



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:29 am GMT

PDB ID : 2JA8  
Title : CPD lesion containing RNA Polymerase II elongation complex D  
Authors : Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.  
Deposited on : 2006-11-23  
Resolution : 3.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

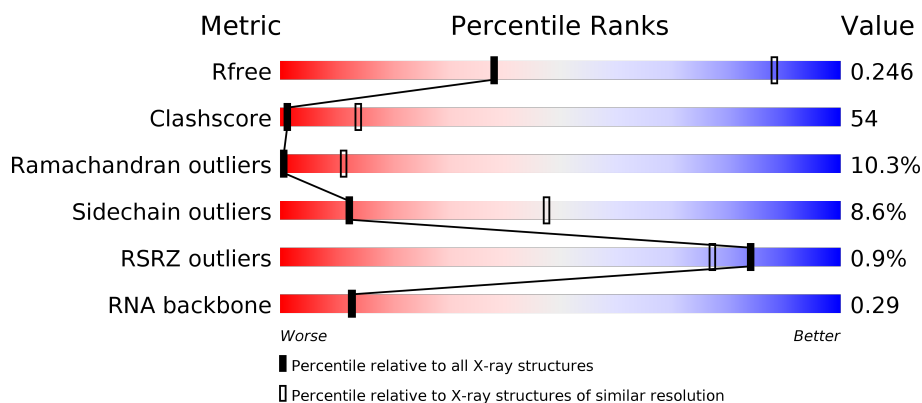
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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))
$R_{free}$	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)
RNA backbone	2435	1016 (4.70-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	1733	
2	B	1224	
3	C	318	
4	D	221	

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	11	
15	T	25	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	TT	T	19	-	-	X	-

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32000 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 DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8866	5614	1553	1644	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

## KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is a DNA chain called 5'-D(\*TP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	8	Total	C	N	O	P	0	0	0
			161	79	29	46	7			

- Molecule 14 is a RNA chain called 5'-R(\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*AP\*GP\*AP\*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	10	Total	C	N	O	P	0	0	0
			209	95	38	67	9			

- Molecule 15 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*TP\*TP\*TTP\*CP\*BRUP\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	19	Total	Br	C	N	O	P	0	0
			401	1	197	61	124	18		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

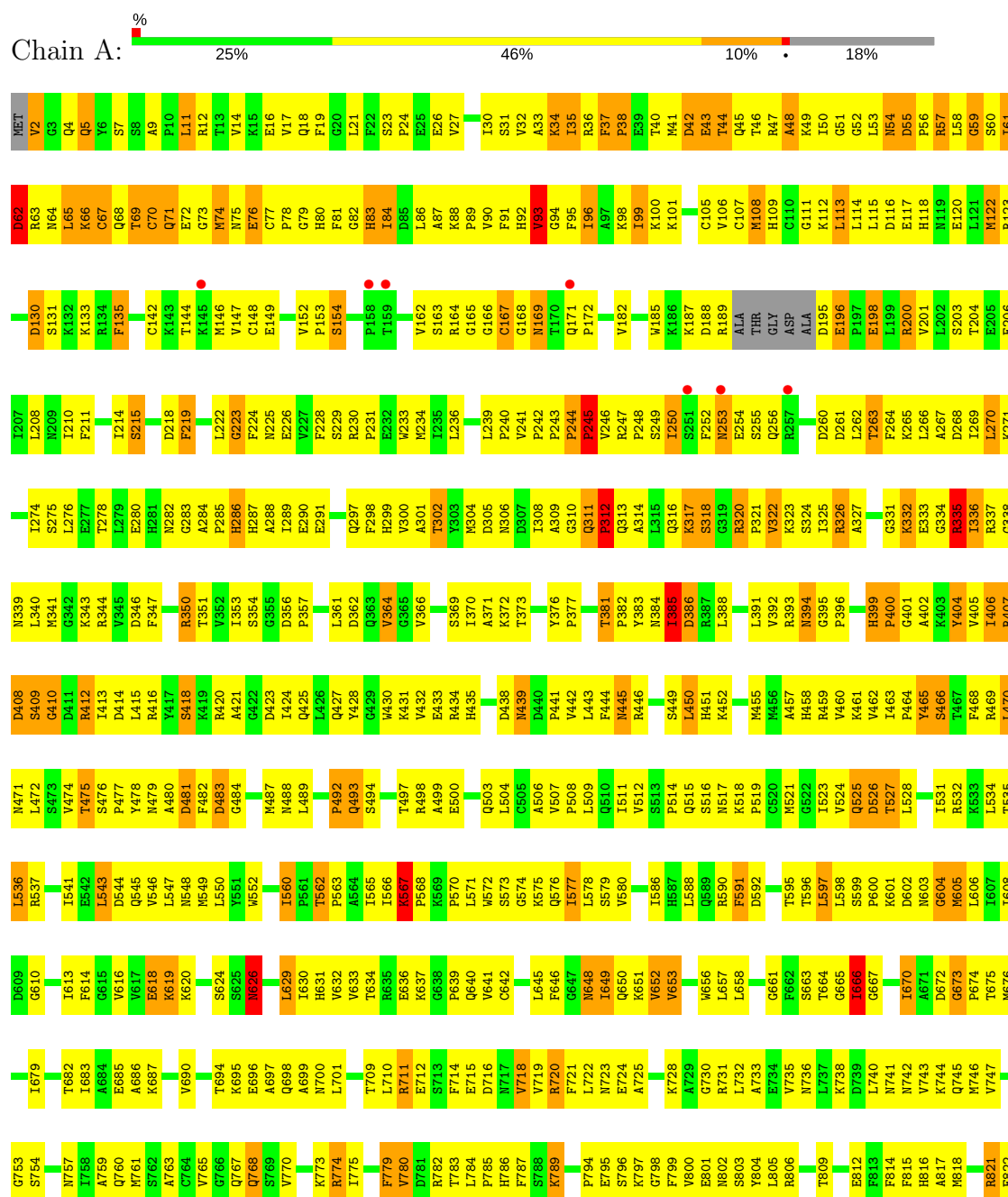
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	8	Total	Zn	0	0
			8	8		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT



● Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE

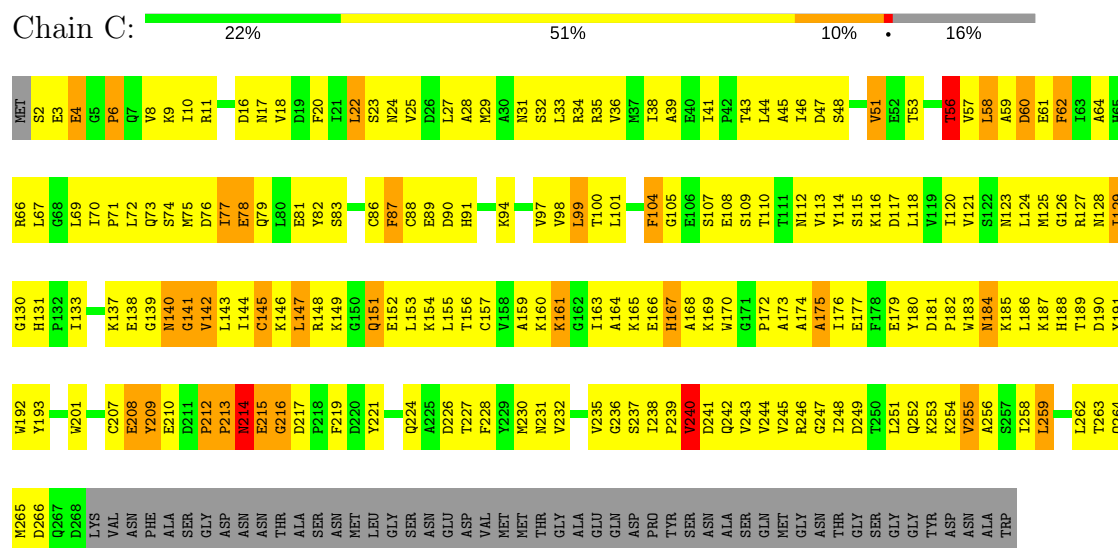




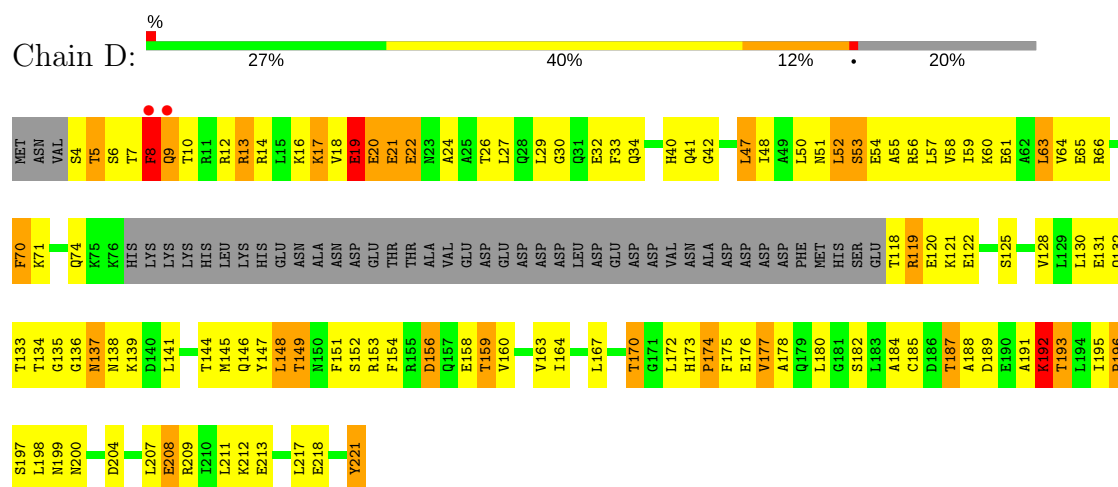
K987	G988	T989	T990	G991	G992	T993	T994	R995	R996	E997	D998	M999	P1000	F1001	T1002	A1003	E1004	T1009	G1005	I1006	V1007	S1008	S1009	T1010	L1011	I1012	M1013	I1017	P1018	L1019	S1019	A1020	M1021	T1022	V1023	A1024	H1025	L1026	I1027	E1028	G1029	L1030	K965	L1031	S1032	K1033	A1034	T1034	A1035	A1036	L1037	S1038	G1039	M1040	E1041	G1042	T1043	T915	T916	T917	F851	T918	S919	P1046	F1047																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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F856	R857	Y858	Y859	M860	D861	Q862	E863	K864	T865	G866	G867	T806	R807	A808	M809	E810	Y811	L812	L813	L814	R815	E816	L817	P818	Q821	M822	N823	A824	V825	A826	L827	Y830	S831	G832	Y833	M834	Q835	E836	D837	S838	M839	I840	M841	N842	Q843	S844	I845	I846	D847	R848	G849	L850	T851	R852	S853	L854	F855																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
F856	R857	Y858	Y859	M860	D861	Q862	E863	K864	T865	G866	G867	T806	R807	A808	M809	E810	Y811	L812	L813	L814	R815	E816	L817	P818	Q821	M822	N823	A824	V825	A826	L827	Y830	S831	G832	Y833	M834	Q835	E836	D837	S838	M839	I840	M841	N842	Q843	S844	I845	I846	D847	R848	G849	L850	T851	R852	S853	L854	F855																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
Q878	R879	T880	N881	T882	L883	R884	Q890	D891	K892	L893	D894	D895	Q896	G897	L898	L899	A900	P901	G902	V903	R904	V905	S906	G907	E908	D909	V910	T911	T912	G913	K914	T915	T916	T917	F918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T996	T997	T998	T999	T1000	T1001	T1002	T1003	T1004	T1005	T1006	T1007	T1008	T1009	T1010	T1011	T1012	T1013	T1014	T1015	T1016	T1017	T1018	T1019	T1020	T1021	T1022	T1023	T1024	T1025	T1026	T1027	T1028	T1029	T1030	T1031	T1032	T1033	T1034	T1035	T1036	T1037	T1038	T1039	T1040	T1041	T1042	T1043	T1044	T1045	T1046	T1047	T1048	T1049	T1050	T1051	T1052	T1053	T1054	T1055	T1056	T1057	T1058	T1059	T1060	T1061	T1062	T1063	T1064	T1065	T1066	T1067	T1068	T1069	T1070	T1071	T1072	T1073	T1074	T1075	T1076	T1077	T1078	T1079	T1080	T1081	T1082	T1083	T1084	T1085	T1086	T1087	T1088	T1089	T1090	T1091	T1092	T1093	T1094	T1095	T1096	T1097	T1098	T1099	T1100	T1101	T1102	T1103	T1104	T1105	T1106	T1107	T1108	T1109	T1110	T1111	T1112	T1113	T1114	T1115	T1116	T1117	T1118	T1119	T1120	T1121	T1122	T1123	T1124	T1125	T1126	T1127	T1128	T1129	T1130	T1131	T1132	T1133	T1134	T1135	T1136	T1137	T1138	T1139	T1140	T1141	T1142	T1143	T1144	T1145	T1146	T1147	T1148	T1149	T1150	T1151	T1152	T1153	T1154	T1155	T1156	T1157	T1158	T1159	T1160	T1161	T1162	T1163	T1164	T1165	T1166	T1167	T1168	T1169	T1170	T1171	T1172	T1173	T1174	T1175	T1176	T1177	T1178	T1179	T1180	T1181	T1182	T1183	T1184	T1185	T1186	T1187	T1188	T1189	T1190	T1191	T1192	T1193	T1194	T1195	T1196	T1197	T1198	T1199	T1200	T1201	T1202	T1203	T1204	T1205	T1206	T1207	T1208	T1209	T1210	T1211	T1212	T1213	T1214	T1215	T1216	T1217	T1218	T1219	T1220	T1221	T1222	T1223	T1224	T1225	T1226	T1227	T1228	T1229	T1230	T1231	T1232	T1233	T1234	T1235	T1236	T1237	T1238	T1239	T1240	T1241	T1242	T1243	T1244	T1245	T1246	T1247	T1248	T1249	T1250	T1251	T1252	T1253	T1254	T1255	T1256	T1257	T1258	T1259	T1260	T1261	T1262	T1263	T1264	T1265	T1266	T1267	T1268	T1269	T1270	T1271	T1272	T1273	T1274	T1275	T1276	T1277	T1278	T1279	T1280	T1281	T1282	T1283	T1284	T1285	T1286	T1287	T1288	T1289	T1290	T1291	T1292	T1293	T1294	T1295	T1296	T1297	T1298	T1299	T1300	T1301	T1302	T1303	T1304	T1305	T1306	T1307	T1308	T1309	T1310	T1311	T1312	T1313	T1314	T1315	T1316	T1317	T1318	T1319	T1320	T1321	T1322	T1323	T1324	T1325	T1326	T1327	T1328	T1329	T1330	T1331	T1332	T1333	T1334	T1335	T1336	T1337	T1338	T1339	T1340	T1341	T1342	T1343	T1344	T1345	T1346	T1347	T1348	T1349	T1350	T1351	T1352	T1353	T1354	T1355	T1356	T1357	T1358	T1359	T1360	T1361	T1362	T1363	T1364	T1365	T1366	T1367	T1368	T1369	T1370	T1371	T1372	T1373	T1374	T1375	T1376	T1377	T1378	T1379	T1380	T1381	T1382	T1383	T1384	T1385	T1386	T1387	T1388	T1389	T1390	T1391	T1392	T1393	T1394	T1395	T1396	T1397	T1398	T1399	T1400	T1401	T1402	T1403	T1404	T1405	T1406	T1407	T1408	T1409	T1410	T1411	T1412	T1413	T1414	T1415	T1416	T1417	T1418	T1419	T1420	T1421	T1422	T1423	T1424	T1425	T1426	T1427	T1428	T1429	T1430	T1431	T1432	T1433	T1434	T1435	T1436	T1437	T1438	T1439	T1440	T1441	T1442	T1443	T1444	T1445	T1446	T1447	T1448	T1449	T1450	T1451	T1452	T1453	T1454	T1455	T1456	T1457	T1458	T1459	T1460	T1461	T1462	T1463	T1464	T1465	T1466	T1467	T1468	T1469	T1470	T1471	T1472	T1473	T1474	T1475	T1476	T1477	T1478	T1479	T1480	T1481	T1482	T1483	T1484	T1485	T1486	T1487	T1488	T1489	T1490	T1491	T1492	T1493	T1494	T1495	T1496	T1497	T1498	T1499	T1500	T1501	T1502	T1503	T1504	T1505	T1506	T1507	T1508	T1509	T1510	T1511	T1512	T1513	T1514	T1515	T1516	T1517	T1518	T1519	T1520	T1521	T1522	T1523	T1524	T1525	T1526	T1527	T1528	T1529	T1530	T1531	T1532	T1533	T1534	T1535	T1536	T1537	T1538	T1539	T1540	T1541	T1542	T1543	T1544	T1545	T1546	T1547	T1548	T1549	T1550	T1551	T1552	T1553	T1554	T1555	T1556	T1557	T1558	T1559	T1560	T1561	T1562	T1563	T1564	T1565	T1566	T1567	T1568	T1569	T1570	T1571	T1572	T1573	T1574	T1575	T1576	T1577	T1578	T1579	T1580	T1581	T1582	T1583	T1584	T1585	T1586	T1587	T1588	T1589	T1590	T1591	T1592	T1593	T1594	T1595	T1596	T1597	T1598	T1599	T1600	T1601	T1602	T1603	T1604	T1605	T1606	T1607	T1608	T1609	T1610	T1611	T1612	T1613	T1614	T1615	T1616	T1617	T1618	T1619	T1620	T1621	T1622	T1623	T1624	T1625	T1626	T1627	T1628	T1629	T1630	T1631	T1632	T1633	T1634	T1635	T1636	T1637	T1638	T1639	T1640	T1641	T1642	T1643	T1644	T1645	T1646	T1647	T1648	T1649	T1650	T1651	T1652	T1653	T1654	T1655	T1656	T1657	T1658	T1659	T1660	T1661	T1662	T1663	T1664	T1665	T1666	T1667	T1668	T1669	T1670	T1671	T1672	T1673	T1674	T1675	T1676	T1677	T1678	T1679	T1680	T1681	T1682	T1683	T1684	T1685	T1686	T1687	T1688	T1689	T1690	T1691	T1692	T1693	T1694	T1695	T1696	T1697	T1698	T1699	T1700	T1701	T1702	T1703	T1704	T1705	T1706	T1707	T1708	T1709	T1710	T1711	T1712	T1713	T1714	T1715	T1716	T1717	T1718	T1719	T1720	T1721	T1722	T1723	T1724	T1725	T1726	T1727	T1728	T1729	T1730	T1731	T1732	T1733	T1734	T1735	T1736	T1737	T1738	T1739	T1740	T1741	T1742	T1743	T1744	T1745	T1746	T1747	T1748	T1749	T1750	T1751	T1752	T1753	T1754	T1755	T1756	T1757	T1758	T1759	T1760	T1761	T1762	T1763	T1764	T1765	T1766	T1767	T1768	T1769	T1770	T1771	T1772	T1773	T1774	T1775	T1776	T1777	T1778	T1779	T1780	T1781	T1782	T1783	T1784	T1785	T1786	T1787	T1788	T1789	T1790	T1791	T1792	T1793	T1794	T1795	T1796	T1797	T1798	T1799	T1800	T1801	T1802	T1803	T1804	T1805	T1806	T1807	T1808	T1809	T1810	T1811	T1812	T1813	T1814	T1815	T1816	T1817	T1818	T1819	T1820	T1821	T1822	T1823	T1824	T1825	T1826	T1827	T1828	T1829	T1830	T1831	T1832	T1833	T1834	T1835	T1836	T1837	T1838	T1839	T1840	T1841	T1842	T1843	T1844	T1845	T1846	T1847	T1848	T1849	T1850	T1851	T1852	T1853	T1854	T1855	T1856	T1857	T1858	T1859	T1860	T1861	T1862	T1863	T1864	T1865	T1866	T1867	T1868	T1869	T1870	T1871	T1872	T1873	T1874	T1875	T1876	T1877	T1878	T1879	T1880	T1881	T1882	T1883	T1884	T1885	T1886	T1887	T1888	T1889	T1890	T1891	T1892	T1893	T1894	T1895	T1896	T1897	T1898	T1899	T1900	T1901	T1902	T1903	T1904	T1905	T1906	T1907	T1908	T1909	T1910	T1911	T1912	T1913	T1914	T1915	T1916	T1917	T1918	T1919	T1920	T1921	T1922	T1923	T1924	T1925	T1926	T1927	T1928	T1929	T1930	T1931	T1932	T1933	T1934	T1935	T1936	T1937	T1938	T1939	T1940	T1941	T1942	T1943	T1944	T1945	T1946	T1947	T1948	T1949	T1950	T1951	T1952	T1953	T1954	T1955	T1956	T1957	T1958	T1959	T1960	T1961	T1962	T1963	T1964	T1965	T1966	T1967	T1968	T1969	T1970	T1971	T1972	T1973	T1974	T1975	T1976	T1977	T1978	T1979	T1980</



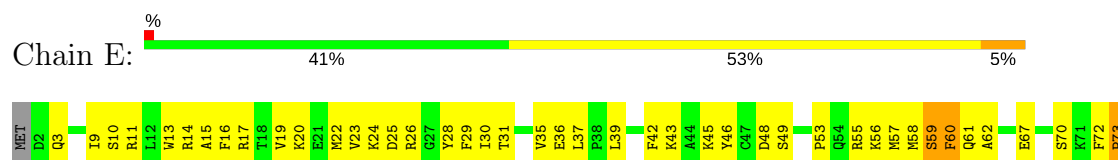
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE

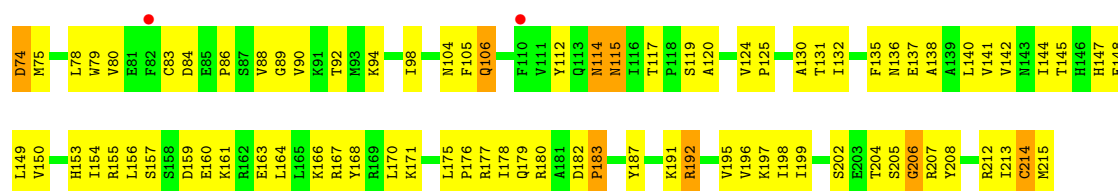


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE

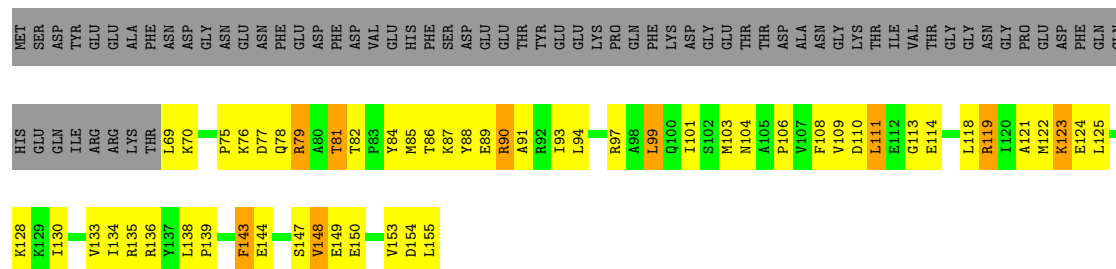


• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE

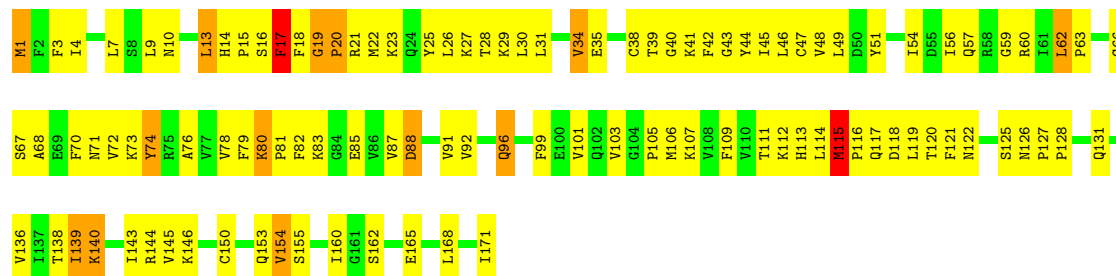




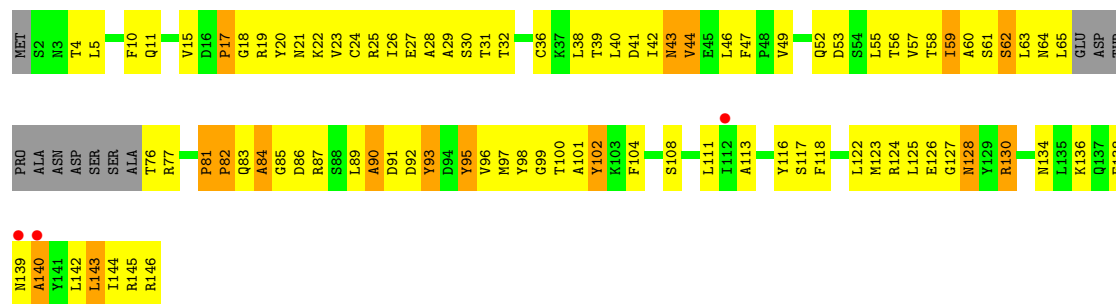
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE



- Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE

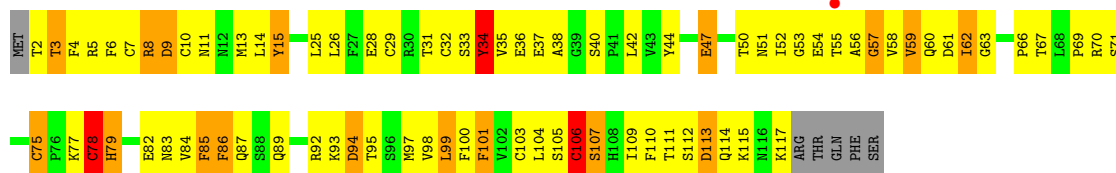


- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

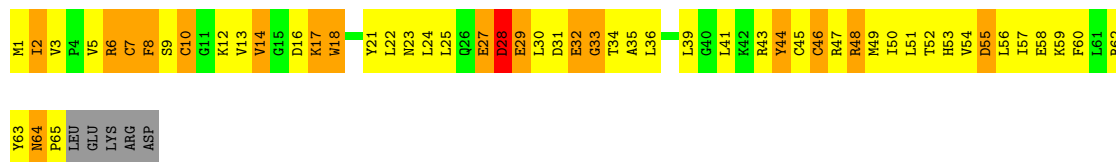
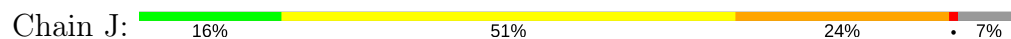


- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9

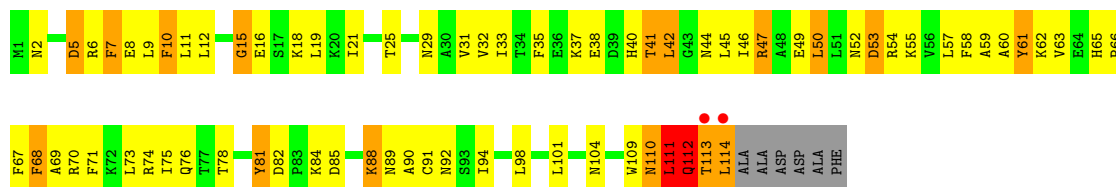




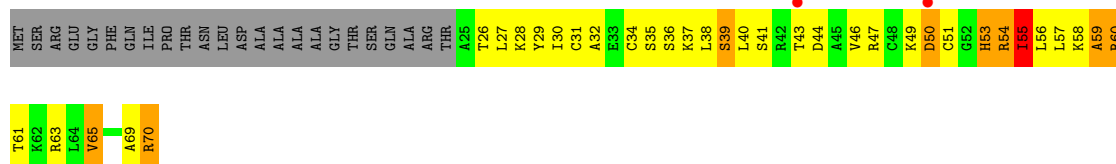
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10



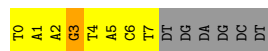
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE



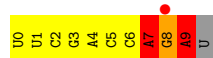
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE



• Molecule 13: 5'-D(\*TP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP \*AP\*GP\*CP\*T)-3'



• Molecule 14: 5'-R(\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*AP\*GP\*AP\*UP)-3'



● Molecule 15: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP \*CP\*TP\*TP\*TP\*TP\*TTP\*CP  
\*BRUP\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'



DA	DG	DC	DT	DC	DA	A10	G11	T12	A13	C14	T15	T16	T17	T18	N19	C21	U22	G23	G24	T25	C26	A27	T28	T29
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.64Å 392.85Å 282.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 48.85 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.80) 99.9 (48.85-3.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.269 , 0.288 0.222 , 0.246	Depositor DCC
$R_{free}$ test set	2410 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	110.0	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 70.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	32000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, BRU, TT

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	0.46	0/11385	0.73	1/15393 (0.0%)
2	B	0.45	0/9037	0.71	2/12181 (0.0%)
3	C	0.48	0/2138	0.71	0/2896
4	D	0.42	0/1437	0.67	0/1925
5	E	0.43	1/1788 (0.1%)	0.62	0/2406
6	F	0.53	0/716	0.77	0/964
7	G	0.49	0/1368	0.73	0/1844
8	H	0.38	0/1102	0.65	0/1492
9	I	0.39	0/962	0.68	0/1295
10	J	0.48	0/541	0.80	0/727
11	K	0.67	3/937 (0.3%)	0.86	4/1265 (0.3%)
12	L	0.41	0/366	0.68	0/485
13	N	1.21	1/180 (0.6%)	1.08	0/276
14	P	0.85	0/233	1.41	2/361 (0.6%)
15	T	1.12	2/380 (0.5%)	1.39	3/580 (0.5%)
All	All	0.49	7/32570 (0.0%)	0.74	12/44090 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
15	T	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	113	THR	N-CA	5.90	1.58	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	113	THR	CA-C	5.73	1.67	1.52
15	T	12	DT	N1-C2	5.38	1.42	1.38
5	E	214	CYS	CB-SG	-5.28	1.73	1.81
11	K	114	LEU	N-CA	5.10	1.56	1.46
15	T	14	DC	N1-C2	5.10	1.45	1.40
13	N	3	DG	N9-C4	5.03	1.42	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	113	THR	N-CA-C	9.56	136.81	111.00
15	T	24	DG	O4'-C1'-N9	7.22	113.06	108.00
15	T	21	DC	O5'-P-OP1	7.09	119.21	110.70
14	P	9	A	C2'-C3'-O3'	7.01	124.92	109.50
14	P	7	A	N9-C1'-C2'	-6.77	104.56	112.00
11	K	111	LEU	N-CA-C	6.32	128.07	111.00
11	K	114	LEU	N-CA-C	5.93	127.00	111.00
2	B	111	ALA	N-CA-C	-5.85	95.21	111.00
11	K	113	THR	C-N-CA	5.83	136.26	121.70
15	T	10	DA	OP2-P-O3'	5.60	117.52	105.20
2	B	1185	CYS	N-CA-C	-5.06	97.34	111.00
1	A	567	LYS	C-N-CD	5.02	138.93	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	486	TYR	Sidechain
15	T	13	DA	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	11186	0	11266	1310	0
2	B	8866	0	8898	1015	0
3	C	2101	0	2055	265	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1427	0	1451	139	0
5	E	1752	0	1776	134	0
6	F	705	0	730	89	0
7	G	1340	0	1357	173	0
8	H	1084	0	1057	127	0
9	I	944	0	900	110	0
10	J	532	0	542	99	0
11	K	919	0	929	107	0
12	L	364	0	386	47	0
13	N	161	0	93	17	0
14	P	209	0	109	28	0
15	T	401	0	231	64	0
16	A	1	0	0	0	0
17	A	8	0	0	0	0
All	All	32000	0	31780	3425	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 54.

All (3425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD23	1:A:54:ASN:N	1.61	1.13
1:A:855:THR:HG21	1:A:857:ARG:HE	1.10	1.11
7:G:14:HIS:CD2	7:G:16:SER:HB2	1.87	1.10
15:T:19:TT:C1'	15:T:19:TT:H5R1	1.83	1.09
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.16	1.09
15:T:17:DT:H2''	15:T:18:DT:H5'	1.32	1.08
2:B:343:ILE:HG23	2:B:347:LYS:HB2	1.16	1.08
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.36	1.08
15:T:19:TT:H5R1	15:T:19:TT:H1'	1.23	1.07
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.15	1.07
2:B:336:ARG:HG2	2:B:348:ARG:HD3	1.31	1.07
7:G:138:THR:HG22	7:G:139:ILE:H	1.20	1.07
15:T:17:DT:C2'	15:T:18:DT:H5'	1.83	1.06
1:A:34:LYS:HD3	1:A:57:ARG:HH22	0.92	1.04
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.16	1.04
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.17	1.03
2:B:882:THR:HG22	2:B:884:ARG:H	1.20	1.03
1:A:40:THR:HG22	1:A:41:MET:HG3	1.39	1.03
1:A:913:LEU:HD12	1:A:914:GLU:H	1.24	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD12	1:A:59:GLY:H	1.23	1.01
1:A:53:LEU:HD23	1:A:54:ASN:H	0.84	1.01
2:B:589:VAL:HG12	2:B:590:HIS:H	1.24	1.01
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	1.94	1.01
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.42	1.01
11:K:111:LEU:C	11:K:112:GLN:HG2	1.76	1.01
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.96	1.00
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.27	1.00
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.38	1.00
1:A:34:LYS:HD3	1:A:57:ARG:NH2	1.77	1.00
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.25	0.99
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.91	0.98
1:A:53:LEU:CD2	1:A:54:ASN:H	1.74	0.98
2:B:65:GLU:HG3	2:B:66:ASP:H	1.27	0.98
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.43	0.98
3:C:43:THR:HG22	3:C:44:LEU:H	1.29	0.97
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.45	0.97
2:B:214:ALA:HB3	2:B:498:THR:HA	1.46	0.97
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.94	0.96
10:J:1:MET:N	10:J:57:ILE:H	1.63	0.96
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.65	0.96
2:B:806:THR:HG22	2:B:808:ALA:H	1.29	0.96
1:A:709:THR:HG23	9:I:94:ASP:HA	1.46	0.96
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.31	0.96
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.80	0.96
15:T:19:TT:H1'	15:T:19:TT:C5R	1.96	0.96
1:A:225:ASN:HD22	1:A:228:PHE:H	1.03	0.95
15:T:18:DT:C2'	15:T:19:TT:H5'1	1.94	0.95
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.06	0.95
2:B:516:ASN:N	2:B:516:ASN:HD22	1.64	0.94
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.48	0.94
4:D:144:THR:O	4:D:148:LEU:HB2	1.67	0.94
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.28	0.94
2:B:502:ILE:HD12	2:B:502:ILE:H	1.31	0.94
1:A:567:LYS:HB3	8:H:96:VAL:H	1.33	0.94
15:T:17:DT:H2''	15:T:18:DT:C5'	1.97	0.94
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.30	0.94
1:A:34:LYS:HE3	1:A:57:ARG:HH12	1.30	0.94
2:B:168:GLY:H	2:B:450:ALA:HB1	1.32	0.94
11:K:110:ASN:O	11:K:111:LEU:HD23	1.68	0.94
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.65	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:486:TYR:OH	2:B:1096:ARG:HB3	1.66	0.93
15:T:19:TT:H5M1	15:T:21:DC:C5	2.03	0.93
1:A:58:LEU:HD21	1:A:243:PRO:HA	1.47	0.93
10:J:1:MET:H1	10:J:57:ILE:N	1.66	0.93
11:K:65:HIS:HD2	11:K:67:PHE:H	1.10	0.93
1:A:58:LEU:CD1	1:A:59:GLY:H	1.82	0.93
1:A:34:LYS:CD	1:A:57:ARG:HH22	1.82	0.93
1:A:754:SER:H	1:A:757:ASN:HD22	1.11	0.93
2:B:336:ARG:HH22	2:B:345:LYS:HE2	1.33	0.92
10:J:48:ARG:HE	10:J:49:MET:HE2	1.31	0.92
15:T:17:DT:C1'	15:T:18:DT:H5'	1.99	0.92
2:B:232:SER:HB3	2:B:261:ARG:HH21	1.32	0.92
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.82	0.92
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.50	0.92
1:A:524:VAL:HG12	1:A:525:GLN:H	1.32	0.92
3:C:6:PRO:HB3	3:C:25:VAL:CG1	1.99	0.92
1:A:254:GLU:HB2	2:B:935:ARG:HH12	1.34	0.92
2:B:515:HIS:H	2:B:518:HIS:HD2	1.16	0.92
6:F:111:LEU:HD12	6:F:111:LEU:H	1.35	0.91
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.05	0.91
14:P:5:C:H2'	14:P:6:C:O4'	1.70	0.91
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.04	0.91
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.51	0.91
8:H:4:THR:HA	8:H:60:ALA:HB2	1.53	0.91
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.53	0.91
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.53	0.91
9:I:85:PHE:H	9:I:85:PHE:HD2	1.18	0.91
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.36	0.91
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.84	0.90
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.53	0.90
8:H:100:THR:HG23	8:H:138:GLU:HA	1.49	0.90
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.34	0.90
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.52	0.90
15:T:22:BRU:H2'	15:T:23:DG:C8	2.07	0.90
1:A:1094:VAL:HG12	1:A:1095:THR:H	1.34	0.90
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.53	0.90
1:A:855:THR:HG21	1:A:857:ARG:NE	1.86	0.90
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.02	0.89
2:B:549:THR:HG22	2:B:550:ASP:H	1.36	0.89
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.08	0.89
15:T:17:DT:H1'	15:T:18:DT:H5'	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:19:TT:H2'1	15:T:19:TT:H2R2	1.55	0.89
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.38	0.89
15:T:19:TT:C2'	15:T:19:TT:H5R1	2.02	0.88
15:T:15:DT:H1'	15:T:16:DT:H5'	1.53	0.88
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.03	0.88
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.56	0.88
1:A:901:LEU:H	1:A:926:GLN:NE2	1.71	0.88
2:B:842:ASN:ND2	2:B:845:SER:H	1.72	0.88
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.08	0.88
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.35	0.88
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.56	0.88
1:A:534:LEU:O	1:A:574:GLY:HA3	1.74	0.87
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.54	0.87
1:A:58:LEU:HD11	1:A:243:PRO:HB3	1.56	0.87
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.55	0.87
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.55	0.86
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.57	0.86
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.56	0.86
1:A:323:LYS:HZ3	14:P:1:U:H4'	1.39	0.86
2:B:942:ARG:HH22	15:T:25:DT:P	1.98	0.86
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.56	0.86
2:B:510:LYS:HG2	2:B:511:PRO:HD3	1.58	0.86
3:C:43:THR:HG22	3:C:44:LEU:N	1.89	0.86
1:A:70:CYS:O	1:A:72:GLU:HG2	1.75	0.85
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.06	0.85
1:A:646:PHE:O	1:A:650:GLN:HG3	1.76	0.85
2:B:343:ILE:HG21	2:B:348:ARG:HG3	1.58	0.85
5:E:19:VAL:O	5:E:23:VAL:HG23	1.76	0.85
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.11	0.85
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.76	0.85
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.77	0.85
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.59	0.85
9:I:115:LYS:HD3	9:I:117:LYS:HE3	1.57	0.85
2:B:343:ILE:CG2	2:B:348:ARG:HG3	2.05	0.85
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.58	0.85
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.57	0.85
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.59	0.85
1:A:320:ARG:HH22	14:P:1:U:H1'	1.40	0.85
1:A:321:PRO:O	1:A:322:VAL:HB	1.76	0.84
2:B:46:GLN:HG3	2:B:47:GLN:H	1.41	0.84
11:K:65:HIS:CD2	11:K:67:PHE:H	1.94	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.59	0.84
1:A:225:ASN:ND2	1:A:228:PHE:H	1.76	0.84
1:A:855:THR:CG2	1:A:857:ARG:HE	1.90	0.84
2:B:847:ASP:HB3	3:C:167:HIS:NE2	1.92	0.84
1:A:535:THR:HG21	1:A:616:VAL:HA	1.60	0.84
2:B:343:ILE:HG21	2:B:348:ARG:N	1.92	0.84
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.59	0.84
14:P:6:C:H2'	14:P:7:A:C8	2.12	0.84
2:B:98:THR:O	2:B:126:SER:HB2	1.78	0.84
6:F:69:LEU:HA	6:F:70:LYS:N	1.91	0.84
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.60	0.83
3:C:32:SER:O	3:C:36:VAL:HG23	1.78	0.83
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.77	0.83
1:A:853:ASP:OD1	1:A:855:THR:HB	1.77	0.83
1:A:1094:VAL:HG12	1:A:1095:THR:N	1.93	0.83
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.59	0.83
1:A:58:LEU:HD12	1:A:59:GLY:N	1.94	0.83
1:A:913:LEU:HD12	1:A:914:GLU:N	1.94	0.83
1:A:1325:THR:O	5:E:148:GLU:HB2	1.79	0.83
1:A:741:ASN:HD22	1:A:744:LYS:H	1.27	0.82
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.14	0.82
1:A:709:THR:HG22	1:A:711:ARG:H	1.44	0.82
2:B:642:ASP:HA	2:B:649:LYS:HA	1.59	0.82
2:B:363:HIS:O	2:B:364:ILE:HB	1.76	0.82
1:A:903:ASN:HD22	1:A:904:THR:N	1.77	0.82
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.60	0.82
1:A:590:ARG:HG3	1:A:590:ARG:NH1	1.94	0.82
8:H:59:ILE:HG22	8:H:60:ALA:N	1.93	0.82
9:I:34:TYR:CD2	9:I:35:VAL:N	2.48	0.82
1:A:472:LEU:O	1:A:475:THR:HB	1.79	0.82
2:B:955:THR:HG22	2:B:956:THR:H	1.44	0.82
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.44	0.81
9:I:105:SER:O	9:I:106:CYS:HB3	1.77	0.81
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.15	0.81
2:B:365:THR:HG23	2:B:367:LEU:H	1.45	0.81
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.14	0.81
11:K:47:ARG:NH1	11:K:47:ARG:HB3	1.96	0.81
2:B:336:ARG:HD3	2:B:348:ARG:HH11	1.46	0.81
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.62	0.81
7:G:80:LYS:HD3	7:G:80:LYS:H	1.45	0.81
7:G:80:LYS:HD3	7:G:80:LYS:N	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:18:DT:C3'	15:T:19:TT:H4'	2.11	0.81
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.96	0.81
7:G:128:PRO:O	7:G:138:THR:HG23	1.81	0.81
1:A:356:ASP:HB2	1:A:469:ARG:NH1	1.96	0.81
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.62	0.81
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.63	0.81
2:B:879:ARG:HH11	2:B:883:LEU:HD22	1.44	0.81
15:T:18:DT:H2''	15:T:19:TT:C5'	2.11	0.81
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.16	0.80
10:J:7:CYS:HB2	10:J:46:CYS:HB3	1.63	0.80
15:T:18:DT:H2'	15:T:19:TT:H5'1	1.62	0.80
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.16	0.80
1:A:743:VAL:O	1:A:747:VAL:HG23	1.82	0.80
5:E:192:ARG:HG3	5:E:192:ARG:HH11	1.45	0.80
3:C:244:VAL:O	3:C:248:ILE:HG13	1.82	0.80
2:B:189:LEU:O	2:B:192:LEU:N	2.14	0.80
2:B:467:GLY:H	2:B:475:SER:HB3	1.46	0.80
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.97	0.80
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.64	0.80
4:D:22:GLU:H	4:D:22:GLU:CD	1.85	0.80
9:I:34:TYR:HD2	9:I:35:VAL:N	1.80	0.80
1:A:767:GLN:NE2	1:A:774:ARG:HB3	1.96	0.79
5:E:22:MET:HE3	5:E:26:ARG:NH2	1.96	0.79
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.12	0.79
15:T:18:DT:H2''	15:T:19:TT:O5'	1.82	0.79
10:J:8:PHE:H	10:J:49:MET:HE1	1.46	0.79
1:A:107:CYS:SG	1:A:171:GLN:HG2	2.21	0.79
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.45	0.79
1:A:886:ILE:HG22	1:A:887:GLY:N	1.96	0.79
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.63	0.79
15:T:18:DT:C2'	15:T:19:TT:C5'	2.60	0.79
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.62	0.79
2:B:467:GLY:N	2:B:475:SER:HB3	1.98	0.79
1:A:567:LYS:HE3	8:H:46:LEU:HB2	1.64	0.79
1:A:768:GLN:CG	1:A:816:HIS:HA	2.12	0.79
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.65	0.79
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.47	0.79
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.82	0.79
2:B:244:LEU:HD21	2:B:366:GLN:NE2	1.97	0.79
2:B:112:LEU:HD12	2:B:113:TYR:H	1.48	0.79
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.48	0.79
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.83	0.78
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.63	0.78
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.83	0.78
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.64	0.78
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.47	0.78
1:A:63:ARG:HA	1:A:74:MET:SD	2.24	0.78
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.66	0.78
2:B:613:VAL:HG13	2:B:627:PHE:O	1.83	0.78
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.65	0.78
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.66	0.78
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.18	0.78
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.65	0.78
1:A:34:LYS:CE	1:A:57:ARG:HH12	1.95	0.78
4:D:153:ARG:NH2	4:D:184:ALA:HA	1.99	0.78
8:H:59:ILE:HG22	8:H:60:ALA:H	1.48	0.78
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.66	0.78
5:E:213:ILE:HG12	5:E:214:CYS:H	1.48	0.78
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.49	0.78
2:B:882:THR:HG22	2:B:884:ARG:N	1.99	0.78
3:C:35:ARG:NH1	11:K:41:THR:H	1.80	0.78
7:G:111:THR:HG22	7:G:113:HIS:H	1.49	0.78
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.66	0.78
1:A:1028:THR:O	1:A:1032:LEU:HD12	1.84	0.78
2:B:654:ARG:H	2:B:657:HIS:HD2	1.28	0.78
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.84	0.77
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.64	0.77
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.24	0.77
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.66	0.77
1:A:528:LEU:O	1:A:531:ILE:HG22	1.84	0.77
1:A:14:VAL:HG21	2:B:1216:LEU:HD13	1.66	0.77
1:A:596:THR:O	1:A:598:LEU:N	2.18	0.77
1:A:308:ILE:HG22	1:A:309:ALA:H	1.48	0.77
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.49	0.77
2:B:65:GLU:HG3	2:B:66:ASP:N	1.97	0.77
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.49	0.77
6:F:82:THR:HG22	6:F:84:TYR:H	1.49	0.77
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.00	0.77
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.85	0.77
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.49	0.77
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:SER:O	2:B:941:LEU:HD23	1.85	0.77
1:A:866:PHE:C	1:A:867:ILE:HD12	2.05	0.77
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.67	0.77
1:A:836:TYR:CD1	15:T:18:DT:H5''	2.19	0.77
1:A:903:ASN:ND2	1:A:905:ASP:H	1.83	0.77
7:G:138:THR:HG22	7:G:139:ILE:N	1.99	0.77
13:N:5:DA:H1'	13:N:6:DC:O5'	1.85	0.77
1:A:269:ILE:HD13	1:A:300:VAL:HG22	1.67	0.76
1:A:323:LYS:NZ	14:P:1:U:H4'	1.99	0.76
2:B:340:ALA:HB2	2:B:343:ILE:HD12	1.67	0.76
2:B:737:THR:HG21	9:I:66:PRO:HA	1.67	0.76
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.21	0.76
14:P:9:A:N1	15:T:19:TT:O4T	2.17	0.76
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.48	0.76
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.16	0.76
2:B:821:GLN:HE22	2:B:851:PHE:HA	1.50	0.76
4:D:47:LEU:HD13	4:D:48:ILE:H	1.49	0.76
8:H:61:SER:O	8:H:62:SER:HB3	1.85	0.76
1:A:466:SER:O	2:B:1103:ILE:HD11	1.85	0.76
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.85	0.76
1:A:106:VAL:HG13	1:A:112:LYS:O	1.85	0.76
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.68	0.76
2:B:114:PRO:HG2	2:B:115:GLN:H	1.51	0.76
13:N:3:DG:H1'	13:N:4:DT:H5'	1.68	0.76
1:A:1171:GLN:HA	1:A:1174:PHE:CE1	2.21	0.76
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.84	0.76
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.01	0.76
2:B:44:VAL:HG11	2:B:199:MET:HG2	1.66	0.76
3:C:213:PRO:O	3:C:214:ASN:HB2	1.84	0.76
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.32	0.76
3:C:73:GLN:HE21	3:C:75:MET:N	1.84	0.76
8:H:36:CYS:HA	8:H:126:GLU:O	1.84	0.76
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.66	0.75
1:A:982:THR:HB	1:A:985:ASP:H	1.49	0.75
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.48	0.75
2:B:708:GLU:O	2:B:710:LEU:N	2.20	0.75
6:F:90:ARG:HD3	6:F:155:LEU:HD11	1.67	0.75
1:A:986:ILE:HG22	1:A:987:VAL:N	2.00	0.75
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.68	0.75
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.67	0.75
1:A:1329:THR:HG22	1:A:1331:SER:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LEU:HD12	1:A:657:LEU:O	1.86	0.75
1:A:885:THR:O	1:A:940:ARG:HD2	1.87	0.75
1:A:666:ILE:HD12	1:A:667:GLY:H	1.51	0.75
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.16	0.75
1:A:230:ARG:H	1:A:233:TRP:HE3	1.35	0.75
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.69	0.75
1:A:385:ILE:HG22	1:A:386:ASP:N	2.01	0.75
1:A:512:VAL:HA	1:A:519:PRO:HA	1.68	0.75
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.22	0.75
3:C:73:GLN:HE21	3:C:75:MET:H	1.31	0.75
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.21	0.75
2:B:516:ASN:ND2	2:B:516:ASN:N	2.35	0.75
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.69	0.75
11:K:12:LEU:HD12	11:K:12:LEU:H	1.50	0.75
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.68	0.75
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.50	0.75
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.17	0.74
1:A:92:HIS:O	1:A:94:GLY:N	2.20	0.74
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.67	0.74
7:G:81:PRO:HG3	7:G:106:MET:SD	2.26	0.74
11:K:47:ARG:HH11	11:K:47:ARG:CB	1.98	0.74
1:A:1387:HIS:CE1	13:N:4:DT:H4'	2.21	0.74
7:G:39:THR:HG22	7:G:41:LYS:H	1.52	0.74
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.28	0.74
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.00	0.74
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.68	0.74
1:A:754:SER:H	1:A:757:ASN:ND2	1.86	0.74
2:B:830:TYR:O	2:B:832:GLY:N	2.20	0.74
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.69	0.74
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.23	0.74
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.68	0.74
2:B:434:ARG:O	2:B:437:GLU:HB2	1.86	0.74
2:B:515:HIS:HD2	2:B:517:THR:H	1.35	0.74
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.52	0.74
12:L:30:ILE:O	12:L:56:LEU:HA	1.87	0.74
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.23	0.74
2:B:549:THR:H	2:B:628:THR:HG23	1.52	0.74
3:C:43:THR:CG2	3:C:44:LEU:H	2.01	0.74
5:E:157:SER:OG	5:E:160:GLU:HG3	1.87	0.74
1:A:858:ASN:HD22	1:A:858:ASN:C	1.91	0.74
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.70	0.74
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.22	0.73
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.03	0.73
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.87	0.73
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.69	0.73
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.68	0.73
12:L:38:LEU:O	12:L:39:SER:HB3	1.88	0.73
2:B:332:ASP:O	2:B:336:ARG:HG3	1.86	0.73
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.23	0.73
7:G:39:THR:HG22	7:G:40:GLY:H	1.54	0.73
1:A:35:ILE:O	1:A:35:ILE:HG22	1.89	0.73
1:A:63:ARG:HA	1:A:74:MET:CE	2.19	0.73
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.49	0.73
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.18	0.73
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.89	0.73
1:A:53:LEU:HD22	1:A:54:ASN:HD22	1.54	0.73
2:B:1072:MET:HE1	2:B:1085:ILE:HB	1.68	0.73
4:D:66:ARG:HD2	4:D:133:THR:HB	1.71	0.73
1:A:254:GLU:HB2	2:B:935:ARG:NH1	2.03	0.73
2:B:232:SER:HB3	2:B:261:ARG:NH2	2.04	0.73
1:A:249:SER:O	1:A:250:ILE:HG13	1.87	0.73
1:A:567:LYS:HB3	8:H:96:VAL:N	2.03	0.73
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.24	0.72
3:C:47:ASP:HA	12:L:69:ALA:CB	2.19	0.72
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.71	0.72
2:B:589:VAL:HG12	2:B:590:HIS:N	2.03	0.72
4:D:130:LEU:O	4:D:132:GLN:N	2.21	0.72
3:C:167:HIS:HD2	3:C:168:ALA:N	1.85	0.72
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.71	0.72
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	1.89	0.72
1:A:67:CYS:O	1:A:70:CYS:HB3	1.89	0.72
2:B:778:MET:HE3	2:B:1094:ARG:HD3	1.71	0.72
3:C:174:ALA:HB2	3:C:235:VAL:CG2	2.19	0.72
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.70	0.72
2:B:336:ARG:NH2	2:B:345:LYS:HG2	2.05	0.72
2:B:879:ARG:NH1	2:B:883:LEU:HD22	2.03	0.72
6:F:103:MET:HE2	7:G:66:GLY:H	1.54	0.72
9:I:111:THR:HG22	9:I:112:SER:N	2.04	0.72
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.71	0.72
1:A:115:LEU:O	1:A:122:MET:HE2	1.90	0.72
1:A:62:ASP:HB3	1:A:64:ASN:ND2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1138:MET:HA	2:B:1138:MET:HE3	1.72	0.72
2:B:343:ILE:CG2	2:B:347:LYS:HB2	2.07	0.72
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.24	0.72
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.19	0.72
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.25	0.72
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.55	0.72
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.71	0.72
1:A:58:LEU:HD13	1:A:80:HIS:O	1.90	0.72
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.72	0.72
2:B:336:ARG:CG	2:B:348:ARG:HD3	2.15	0.72
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.71	0.72
15:T:24:DG:H2''	15:T:25:DT:O5'	1.89	0.72
2:B:1087:PHE:HD2	2:B:1088:GLY:N	1.86	0.72
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.71	0.71
10:J:1:MET:H1	10:J:57:ILE:H	0.80	0.71
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.24	0.71
4:D:134:THR:HG22	4:D:136:GLY:H	1.55	0.71
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.54	0.71
1:A:858:ASN:ND2	1:A:860:LEU:H	1.88	0.71
1:A:325:ILE:HG21	2:B:1210:MET:HG3	1.72	0.71
2:B:516:ASN:H	2:B:516:ASN:HD22	1.37	0.71
14:P:5:C:O2'	14:P:6:C:H5'	1.91	0.71
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.31	0.71
1:A:1171:GLN:HA	1:A:1174:PHE:CD1	2.26	0.71
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.91	0.71
4:D:176:GLU:C	4:D:178:ALA:H	1.94	0.71
13:N:6:DC:H2''	13:N:7:DT:OP2	1.89	0.71
15:T:19:TT:C2'	15:T:19:TT:H2R2	2.19	0.71
2:B:336:ARG:HH22	2:B:345:LYS:CE	2.03	0.71
2:B:310:MET:HE3	2:B:387:LEU:HD12	1.70	0.71
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.72	0.71
2:B:336:ARG:HD3	2:B:348:ARG:NH1	2.05	0.71
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.73	0.71
2:B:515:HIS:H	2:B:518:HIS:CD2	2.04	0.71
2:B:35:SER:HA	2:B:811:TYR:HE2	1.56	0.71
3:C:208:GLU:O	3:C:210:GLU:N	2.24	0.71
8:H:56:THR:HB	8:H:145:ARG:HG2	1.72	0.71
1:A:960:ILE:O	1:A:963:ILE:HG22	1.89	0.71
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.72	0.71
1:A:254:GLU:CB	2:B:935:ARG:HH12	2.04	0.71
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.89	0.71
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.54	0.71
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.05	0.71
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.23	0.71
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.30	0.71
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.55	0.71
2:B:955:THR:HG22	2:B:956:THR:N	2.05	0.71
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.20	0.71
3:C:186:LEU:HD21	3:C:224:GLN:O	1.90	0.71
3:C:35:ARG:NH1	11:K:41:THR:N	2.38	0.71
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.21	0.70
1:A:1437:GLY:O	1:A:1439:GLY:N	2.23	0.70
1:A:326:ARG:HH22	1:A:1407:GLU:HG3	1.53	0.70
1:A:69:THR:O	1:A:71:GLN:N	2.23	0.70
4:D:134:THR:HG22	4:D:135:GLY:N	2.06	0.70
1:A:541:ILE:HD13	1:A:549:MET:CE	2.21	0.70
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.71	0.70
2:B:359:GLU:O	2:B:362:PRO:HD3	1.92	0.70
1:A:546:VAL:O	1:A:550:LEU:HG	1.92	0.70
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.55	0.70
4:D:130:LEU:C	4:D:132:GLN:H	1.94	0.70
5:E:117:THR:HG22	5:E:119:SER:H	1.56	0.70
9:I:111:THR:HG22	9:I:112:SER:H	1.56	0.70
1:A:567:LYS:CB	8:H:95:TYR:HA	2.21	0.70
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.55	0.70
3:C:226:ASP:O	3:C:227:THR:HB	1.90	0.70
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.22	0.70
15:T:18:DT:O3'	15:T:19:TT:H4'	1.90	0.70
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.57	0.70
2:B:1172:ILE:O	2:B:1172:ILE:HG22	1.90	0.70
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.73	0.70
7:G:39:THR:HG22	7:G:40:GLY:N	2.06	0.70
1:A:58:LEU:HD11	1:A:243:PRO:CB	2.21	0.70
1:A:55:ASP:N	1:A:56:PRO:HD3	2.04	0.70
2:B:615:MET:C	2:B:616:ILE:HD12	2.12	0.70
10:J:7:CYS:CB	10:J:46:CYS:HB3	2.21	0.70
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.21	0.70
1:A:438:ASP:O	1:A:439:ASN:HB2	1.90	0.70
4:D:7:THR:HG21	4:D:32:GLU:CD	2.11	0.70
4:D:8:PHE:CE2	4:D:40:HIS:HA	2.25	0.70
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:THR:HG22	1:A:1331:SER:N	2.06	0.70
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.73	0.70
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.55	0.70
2:B:336:ARG:HG2	2:B:348:ARG:CD	2.17	0.70
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.60	0.70
1:A:265:LYS:HD2	1:A:265:LYS:N	2.06	0.70
1:A:34:LYS:H	1:A:57:ARG:NH2	1.90	0.70
8:H:123:MET:HG2	8:H:124:ARG:N	2.07	0.70
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.73	0.69
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.09	0.69
1:A:1035:TYR:O	1:A:1037:LEU:N	2.25	0.69
1:A:996:ASN:O	1:A:998:LEU:HD12	1.91	0.69
2:B:1069:PHE:HD1	2:B:1069:PHE:H	1.39	0.69
2:B:336:ARG:CD	2:B:348:ARG:HH11	2.04	0.69
2:B:824:ILE:CG2	2:B:1087:PHE:HE2	2.05	0.69
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.54	0.69
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.74	0.69
4:D:34:GLN:O	4:D:47:LEU:HD23	1.92	0.69
6:F:111:LEU:N	6:F:111:LEU:HD12	2.06	0.69
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.22	0.69
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.22	0.69
1:A:347:PHE:H	2:B:1107:ALA:HA	1.57	0.69
1:A:471:ASN:OD1	1:A:472:LEU:N	2.25	0.69
15:T:26:DC:H2''	15:T:27:DA:H5'	1.74	0.69
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.74	0.69
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.74	0.69
8:H:100:THR:OG1	8:H:138:GLU:HG3	1.92	0.69
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.75	0.69
2:B:847:ASP:HB3	3:C:167:HIS:HE2	1.54	0.69
1:A:114:LEU:HD13	1:A:171:GLN:HE22	1.56	0.69
2:B:745:PRO:O	2:B:748:ILE:HG12	1.93	0.69
2:B:842:ASN:HD22	2:B:845:SER:CB	2.06	0.69
2:B:857:ARG:HD2	2:B:945:GLU:OE1	1.93	0.69
4:D:213:GLU:O	4:D:217:LEU:HG	1.93	0.69
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.74	0.69
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.73	0.69
2:B:411:PRO:O	2:B:414:ALA:HB3	1.93	0.69
2:B:642:ASP:O	2:B:644:GLU:N	2.26	0.69
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.75	0.69
1:A:836:TYR:HD1	15:T:18:DT:H5''	1.57	0.69
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.92	0.69
2:B:975:GLN:HG2	2:B:976:ILE:H	1.58	0.69
1:A:701:LEU:HA	9:I:115:LYS:HE3	1.75	0.69
10:J:14:VAL:HG12	10:J:14:VAL:O	1.92	0.69
1:A:19:PHE:O	1:A:1416:ALA:HA	1.93	0.69
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.08	0.69
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.57	0.69
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.23	0.69
8:H:4:THR:HA	8:H:60:ALA:CB	2.22	0.69
1:A:1332:PHE:HD2	1:A:1332:PHE:N	1.90	0.69
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.28	0.69
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.74	0.69
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.28	0.69
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.23	0.69
15:T:18:DT:H3'	15:T:19:TT:H4'	1.73	0.69
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.08	0.68
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.75	0.68
11:K:6:ARG:O	11:K:9:LEU:HG	1.93	0.68
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.58	0.68
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.28	0.68
2:B:180:TYR:HD1	2:B:180:TYR:H	1.41	0.68
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.28	0.68
1:A:549:MET:SD	1:A:577:ILE:HD11	2.33	0.68
1:A:856:THR:HB	1:A:865:GLN:HB2	1.75	0.68
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.19	0.68
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.75	0.68
11:K:53:ASP:OD1	11:K:55:LYS:HB2	1.93	0.68
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.92	0.68
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.29	0.68
6:F:76:LYS:O	6:F:79:ARG:HD3	1.94	0.68
1:A:1445:ILE:HG12	7:G:18:PHE:CE2	2.28	0.68
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.94	0.68
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.59	0.68
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.74	0.68
4:D:118:THR:HB	4:D:121:LYS:HB2	1.76	0.68
4:D:189:ASP:O	4:D:193:THR:HB	1.92	0.68
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.76	0.68
2:B:121:ASN:HA	2:B:207:GLY:CA	2.23	0.68
2:B:863:GLU:OE2	2:B:873:THR:HA	1.94	0.68
2:B:882:THR:HB	2:B:934:LYS:O	1.94	0.68
6:F:103:MET:O	6:F:104:ASN:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.29	0.68
11:K:31:VAL:HG12	11:K:32:VAL:N	2.09	0.68
15:T:19:TT:C2R	15:T:19:TT:H2'1	2.23	0.68
1:A:1436:ILE:O	1:A:1437:GLY:C	2.33	0.68
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.74	0.68
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.22	0.68
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.60	0.68
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.24	0.68
2:B:232:SER:CB	2:B:261:ARG:HH21	2.06	0.68
5:E:157:SER:C	5:E:159:ASP:H	1.97	0.68
1:A:58:LEU:HD21	1:A:243:PRO:CA	2.23	0.67
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.56	0.67
8:H:130:ARG:H	8:H:130:ARG:HD2	1.59	0.67
1:A:42:ASP:HB3	1:A:45:GLN:H	1.59	0.67
1:A:903:ASN:HD22	1:A:903:ASN:C	1.96	0.67
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.75	0.67
2:B:351:TYR:O	2:B:355:ILE:HG13	1.95	0.67
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.59	0.67
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.77	0.67
3:C:35:ARG:HH12	11:K:41:THR:H	1.40	0.67
6:F:130:ILE:O	6:F:148:VAL:HG21	1.93	0.67
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.19	0.67
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.75	0.67
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.29	0.67
1:A:1120:LEU:N	1:A:1120:LEU:HD12	2.09	0.67
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.25	0.67
1:A:901:LEU:H	1:A:926:GLN:HE21	1.40	0.67
2:B:953:LEU:O	2:B:953:LEU:HD23	1.94	0.67
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.24	0.67
1:A:34:LYS:HE3	1:A:57:ARG:NH1	2.08	0.67
10:J:1:MET:H3	10:J:56:LEU:N	1.91	0.67
1:A:68:GLN:C	1:A:70:CYS:H	1.97	0.67
1:A:69:THR:C	1:A:71:GLN:H	1.96	0.67
2:B:1174:LYS:O	2:B:1176:ASN:N	2.28	0.67
2:B:871:THR:HG22	2:B:872:GLU:O	1.94	0.67
3:C:56:THR:HG22	3:C:57:VAL:H	1.60	0.67
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.23	0.67
8:H:143:LEU:N	8:H:143:LEU:HD12	2.08	0.67
15:T:19:TT:H5M1	15:T:21:DC:C4	2.29	0.67
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.75	0.67
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:O	1:A:385:ILE:C	2.33	0.67
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.76	0.67
1:A:253:ASN:HB3	2:B:935:ARG:CZ	2.25	0.67
9:I:8:ARG:CG	9:I:34:TYR:HE1	2.06	0.67
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.29	0.67
1:A:450:LEU:HD12	1:A:450:LEU:H	1.60	0.67
1:A:527:THR:CG2	1:A:650:GLN:HA	2.25	0.67
5:E:192:ARG:NH1	5:E:192:ARG:HG3	2.09	0.67
8:H:58:THR:HG22	8:H:59:ILE:H	1.60	0.67
1:A:252:PHE:O	1:A:253:ASN:HB2	1.95	0.66
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.75	0.66
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.25	0.66
8:H:44:VAL:O	8:H:44:VAL:HG12	1.96	0.66
2:B:516:ASN:ND2	2:B:516:ASN:H	1.92	0.66
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.78	0.66
1:A:1450:LEU:HG	1:A:1450:LEU:O	1.96	0.66
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.31	0.66
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.10	0.66
8:H:41:ASP:O	8:H:42:ILE:HG13	1.95	0.66
1:A:881:GLN:NE2	1:A:958:VAL:O	2.28	0.66
2:B:1106:ARG:NH1	2:B:1110:PRO:HG2	2.11	0.66
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.77	0.66
3:C:167:HIS:CD2	3:C:168:ALA:N	2.64	0.66
3:C:43:THR:CG2	3:C:44:LEU:N	2.58	0.66
6:F:109:VAL:HG11	6:F:123:LYS:HD3	1.78	0.66
9:I:75:CYS:SG	9:I:79:HIS:N	2.68	0.66
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.24	0.66
15:T:18:DT:H2"	15:T:19:TT:H5'1	1.72	0.66
1:A:1279:ILE:O	1:A:1279:ILE:HG22	1.96	0.66
2:B:378:LEU:O	2:B:382:ILE:HG13	1.95	0.66
2:B:464:GLY:HA2	2:B:479:VAL:O	1.96	0.66
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.78	0.66
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.64	0.66
2:B:18:PHE:N	2:B:19:GLU:N	2.44	0.66
2:B:825:VAL:CG1	2:B:826:ALA:N	2.58	0.66
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.11	0.66
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	1.93	0.66
2:B:217:ARG:C	2:B:217:ARG:HD2	2.15	0.66
2:B:563:MET:HE3	2:B:580:VAL:HB	1.78	0.66
2:B:794:ASN:O	2:B:795:ILE:HD12	1.95	0.66
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:176:GLU:O	4:D:178:ALA:N	2.29	0.66
11:K:46:ILE:O	11:K:46:ILE:HG22	1.96	0.66
2:B:224:GLN:O	2:B:238:ALA:HA	1.95	0.66
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.77	0.66
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.60	0.66
1:A:84:ILE:HG23	1:A:84:ILE:O	1.96	0.66
2:B:842:ASN:ND2	2:B:845:SER:OG	2.29	0.66
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.11	0.66
14:P:1:U:O2'	14:P:2:C:H5'	1.96	0.66
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.26	0.65
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.25	0.65
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.11	0.65
1:A:728:LYS:O	1:A:732:LEU:HG	1.97	0.65
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.78	0.65
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.26	0.65
1:A:982:THR:H	1:A:985:ASP:HB2	1.61	0.65
1:A:984:LYS:O	1:A:988:LEU:HB2	1.97	0.65
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.44	0.65
2:B:1069:PHE:HA	2:B:1085:ILE:O	1.96	0.65
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.11	0.65
3:C:66:ARG:NH2	10:J:3:VAL:O	2.29	0.65
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.08	0.65
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.12	0.65
1:A:164:ARG:HG3	1:A:165:GLY:N	2.11	0.65
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.11	0.65
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.78	0.65
2:B:557:PHE:C	2:B:557:PHE:CD2	2.70	0.65
11:K:61:TYR:CD2	11:K:61:TYR:C	2.69	0.65
1:A:320:ARG:NH2	14:P:1:U:O2'	2.29	0.65
1:A:50:ILE:C	1:A:52:GLY:H	2.00	0.65
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.27	0.65
2:B:35:SER:O	2:B:39:ARG:HG3	1.97	0.65
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.79	0.65
3:C:167:HIS:HD2	3:C:168:ALA:H	1.43	0.65
8:H:11:GLN:HA	8:H:53:ASP:O	1.96	0.65
1:A:1005:GLU:O	1:A:1009:ASN:HB2	1.97	0.65
1:A:714:PHE:O	1:A:718:VAL:HG23	1.97	0.65
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.11	0.65
2:B:850:LEU:HD12	2:B:851:PHE:N	2.11	0.65
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.78	0.65
5:E:22:MET:CE	5:E:26:ARG:HH21	2.02	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.26	0.65
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.77	0.65
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.79	0.65
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.78	0.65
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.97	0.65
1:A:69:THR:C	1:A:71:GLN:N	2.49	0.65
5:E:114:ASN:O	5:E:115:ASN:HB3	1.97	0.65
1:A:547:LEU:HD22	11:K:58:PHE:HD1	1.60	0.65
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.11	0.64
2:B:770:GLN:HG2	2:B:983:ARG:O	1.97	0.64
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.62	0.64
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.78	0.64
4:D:192:LYS:HE3	4:D:204:ASP:OD1	1.97	0.64
4:D:47:LEU:HD13	4:D:48:ILE:N	2.11	0.64
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.33	0.64
1:A:1445:ILE:HD12	1:A:1445:ILE:N	1.98	0.64
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.79	0.64
1:A:450:LEU:N	1:A:450:LEU:HD12	2.13	0.64
2:B:589:VAL:CG1	2:B:590:HIS:H	2.07	0.64
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.77	0.64
15:T:13:DA:H1'	15:T:14:DC:H5'	1.78	0.64
1:A:105:CYS:O	1:A:114:LEU:HG	1.97	0.64
1:A:591:PHE:HA	1:A:595:THR:HG21	1.80	0.64
1:A:979:SER:OG	1:A:980:ASP:N	2.29	0.64
2:B:185:THR:H	2:B:188:ASP:HB2	1.62	0.64
2:B:467:GLY:H	2:B:475:SER:CB	2.10	0.64
2:B:744:HIS:HD2	2:B:746:SER:OG	1.80	0.64
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.45	0.64
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.27	0.64
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.97	0.64
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.27	0.64
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.11	0.64
2:B:247:GLY:C	2:B:249:ARG:H	1.99	0.64
3:C:183:TRP:O	3:C:185:LYS:N	2.30	0.64
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.32	0.64
2:B:776:GLN:HE22	14:P:8:G:H5'	1.62	0.64
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	1.78	0.64
1:A:35:ILE:HA	1:A:52:GLY:O	1.97	0.64
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.33	0.64
2:B:918:ILE:HB	2:B:935:ARG:HD2	1.80	0.64
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.79	0.64
1:A:1094:VAL:CG1	1:A:1095:THR:H	2.06	0.64
1:A:1134:ILE:O	1:A:1138:ILE:HG13	1.98	0.64
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.62	0.64
2:B:745:PRO:O	2:B:747:MET:N	2.31	0.64
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.80	0.64
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.61	0.64
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.98	0.64
1:A:853:ASP:OD1	1:A:855:THR:CB	2.45	0.64
3:C:133:ILE:HD11	3:C:237:SER:HA	1.80	0.64
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.28	0.64
1:A:254:GLU:O	1:A:256:GLN:N	2.30	0.64
1:A:388:LEU:O	1:A:392:VAL:HG23	1.98	0.64
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.28	0.64
2:B:842:ASN:O	2:B:846:ILE:HG13	1.98	0.64
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.79	0.64
6:F:99:LEU:O	6:F:103:MET:HG2	1.97	0.64
6:F:93:ILE:HD11	6:F:134:ILE:CD1	2.26	0.64
1:A:1444:MET:CG	7:G:60:ARG:HA	2.28	0.64
8:H:81:PRO:CB	8:H:82:PRO:CD	2.75	0.64
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.44	0.64
1:A:34:LYS:CE	1:A:57:ARG:NH1	2.61	0.64
2:B:860:MET:HG2	2:B:861:ASP:H	1.63	0.64
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.33	0.64
11:K:111:LEU:C	11:K:112:GLN:CG	2.59	0.64
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.33	0.63
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.01	0.63
2:B:806:THR:HG22	2:B:808:ALA:N	2.07	0.63
15:T:22:BRU:C2'	15:T:23:DG:O4'	2.46	0.63
1:A:144:THR:O	1:A:146:MET:HG3	1.98	0.63
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.28	0.63
2:B:339:THR:HG22	2:B:339:THR:O	1.98	0.63
2:B:601:ARG:O	2:B:605:ARG:HG3	1.98	0.63
2:B:637:LEU:O	2:B:690:VAL:HG13	1.99	0.63
3:C:133:ILE:CD1	3:C:237:SER:HA	2.28	0.63
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.79	0.63
1:A:477:PRO:CG	1:A:521:MET:HG2	2.29	0.63
1:A:675:THR:O	1:A:679:ILE:HG13	1.98	0.63
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.46	0.63
2:B:211:VAL:O	2:B:480:SER:HA	1.99	0.63
2:B:336:ARG:HH21	2:B:345:LYS:HG2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:23:ASN:C	10:J:25:LEU:H	1.99	0.63
10:J:28:ASP:O	10:J:30:LEU:HG	1.99	0.63
1:A:326:ARG:NH2	1:A:1407:GLU:HG3	2.13	0.63
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.81	0.63
2:B:799:PRO:HB3	2:B:818:PRO:HG2	1.80	0.63
1:A:265:LYS:HD2	1:A:265:LYS:H	1.64	0.63
1:A:518:LYS:HE2	1:A:624:SER:O	1.97	0.63
2:B:125:SER:HA	2:B:171:PRO:HA	1.80	0.63
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.78	0.63
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.80	0.63
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.28	0.63
2:B:957:ASN:O	2:B:959:ASP:N	2.31	0.63
3:C:263:THR:C	3:C:265:MET:H	2.02	0.63
4:D:52:LEU:O	4:D:54:GLU:N	2.32	0.63
7:G:79:PHE:CZ	7:G:106:MET:HE1	2.33	0.63
6:F:69:LEU:CA	6:F:70:LYS:N	2.60	0.63
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.14	0.63
1:A:588:LEU:O	1:A:606:LEU:HA	1.99	0.63
1:A:61:ILE:HG22	1:A:62:ASP:H	1.64	0.63
2:B:365:THR:HG23	2:B:367:LEU:HG	1.79	0.63
2:B:975:GLN:O	2:B:990:ILE:HD12	1.99	0.63
3:C:189:THR:HG22	3:C:190:ASP:N	2.14	0.63
7:G:17:PHE:N	7:G:17:PHE:CD2	2.66	0.63
8:H:93:TYR:HB3	8:H:144:ILE:O	1.99	0.63
1:A:321:PRO:O	1:A:322:VAL:CB	2.46	0.63
2:B:315:LYS:N	2:B:316:PRO:HD2	2.13	0.63
2:B:916:THR:O	2:B:935:ARG:HG3	1.99	0.63
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.80	0.63
4:D:7:THR:HB	7:G:42:PHE:CE2	2.34	0.63
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.14	0.62
2:B:705:MET:H	2:B:710:LEU:HD12	1.63	0.62
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.64	0.62
1:A:57:ARG:O	1:A:68:GLN:HG3	1.99	0.62
1:A:87:ALA:HB1	1:A:276:LEU:HD23	1.80	0.62
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.34	0.62
1:A:730:GLY:O	1:A:732:LEU:N	2.32	0.62
1:A:979:SER:OG	1:A:981:LEU:HG	1.99	0.62
2:B:731:VAL:HG12	2:B:732:SER:H	1.64	0.62
4:D:159:THR:O	4:D:163:VAL:HG23	1.99	0.62
7:G:145:VAL:HG12	7:G:146:LYS:N	2.14	0.62
10:J:12:LYS:O	10:J:14:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:15:DT:C1'	15:T:16:DT:H5'	2.29	0.62
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.63	0.62
2:B:1034:VAL:O	2:B:1037:LEU:N	2.30	0.62
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.80	0.62
2:B:563:MET:CE	2:B:580:VAL:HB	2.29	0.62
2:B:999:MET:HE2	2:B:1000:PRO:HD2	1.80	0.62
3:C:100:THR:OG1	3:C:121:VAL:HG21	1.99	0.62
3:C:104:PHE:HD2	3:C:105:GLY:H	1.47	0.62
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.28	0.62
9:I:61:ASP:C	9:I:63:GLY:H	2.03	0.62
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.81	0.62
1:A:567:LYS:CB	1:A:568:PRO:CD	2.77	0.62
2:B:616:ILE:HD12	2:B:616:ILE:N	2.14	0.62
3:C:35:ARG:HH11	11:K:41:THR:CA	2.12	0.62
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.79	0.62
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.99	0.62
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.29	0.62
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.39	0.62
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	1.98	0.62
1:A:741:ASN:ND2	1:A:744:LYS:H	1.98	0.62
1:A:763:ALA:O	1:A:803:SER:HB3	2.00	0.62
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.98	0.62
2:B:842:ASN:HB3	2:B:845:SER:OG	1.99	0.62
11:K:10:PHE:CD2	11:K:10:PHE:N	2.68	0.62
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.81	0.62
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.80	0.62
1:A:524:VAL:HG12	1:A:525:GLN:N	2.12	0.62
1:A:58:LEU:CG	1:A:59:GLY:H	2.11	0.62
1:A:844:ALA:C	1:A:845:LEU:HD23	2.20	0.62
2:B:465:ASN:HD22	2:B:465:ASN:N	1.98	0.62
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.30	0.62
5:E:39:LEU:O	5:E:42:PHE:HB3	2.00	0.62
5:E:48:ASP:CG	5:E:49:SER:H	2.03	0.62
6:F:97:ARG:O	6:F:101:ILE:HG13	1.99	0.62
11:K:67:PHE:C	11:K:68:PHE:HD2	2.03	0.62
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.29	0.62
2:B:525:ALA:O	2:B:768:THR:HA	2.00	0.62
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.34	0.62
3:C:253:LYS:O	3:C:256:ALA:HB3	2.00	0.62
4:D:8:PHE:CZ	4:D:40:HIS:HA	2.35	0.62
5:E:202:SER:OG	5:E:204:THR:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:90:ARG:HG3	6:F:91:ALA:N	2.14	0.62
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.34	0.62
1:A:53:LEU:CD2	1:A:54:ASN:HD22	2.13	0.62
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.57	0.62
2:B:446:LEU:O	2:B:447:ALA:HB3	1.99	0.62
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.65	0.62
2:B:822:ASN:O	10:J:48:ARG:NH1	2.33	0.62
13:N:5:DA:C2	15:T:13:DA:C2	2.88	0.62
1:A:1244:ARG:HB3	1:A:1245:PRO:HD2	1.80	0.62
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.34	0.62
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.80	0.62
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.29	0.62
1:A:107:CYS:N	1:A:114:LEU:HD21	2.15	0.61
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.30	0.61
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.81	0.61
2:B:433:GLN:O	2:B:437:GLU:HG3	1.99	0.61
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.81	0.61
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.82	0.61
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.82	0.61
1:A:901:LEU:N	1:A:926:GLN:NE2	2.47	0.61
2:B:464:GLY:O	2:B:477:ALA:HA	2.00	0.61
10:J:64:ASN:CB	10:J:65:PRO:HD3	2.30	0.61
2:B:336:ARG:NH2	2:B:345:LYS:HE2	2.10	0.61
2:B:498:THR:HB	2:B:537:LYS:O	2.00	0.61
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.82	0.61
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.29	0.61
10:J:44:TYR:HA	10:J:47:ARG:CB	2.30	0.61
10:J:8:PHE:H	10:J:49:MET:CE	2.12	0.61
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.01	0.61
2:B:168:GLY:N	2:B:450:ALA:HB1	2.12	0.61
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.31	0.61
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.30	0.61
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.66	0.61
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.34	0.61
1:A:907:THR:CG2	1:A:908:LEU:N	2.63	0.61
7:G:143:ILE:HG22	7:G:144:ARG:N	2.15	0.61
3:C:164:ALA:HA	3:C:167:HIS:O	2.00	0.61
1:A:450:LEU:HB3	1:A:838:GLN:NE2	2.15	0.61
2:B:278:GLN:HE22	2:B:337:ARG:HH21	1.47	0.61
2:B:520:GLY:H	2:B:748:ILE:HG22	1.64	0.61
3:C:104:PHE:HD2	3:C:105:GLY:N	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:VAL:H	10:J:16:ASP:HB3	1.66	0.61
3:C:69:LEU:HD12	3:C:69:LEU:N	2.16	0.61
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.82	0.61
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.64	0.61
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.65	0.61
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.81	0.61
3:C:34:ARG:O	3:C:38:ILE:HG13	2.01	0.61
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.65	0.61
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.16	0.61
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.81	0.61
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.66	0.61
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.83	0.61
5:E:29:PHE:O	5:E:30:ILE:HG13	2.00	0.61
8:H:25:ARG:HA	8:H:41:ASP:HA	1.83	0.61
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.19	0.61
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.34	0.60
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.10	0.60
2:B:1084:GLN:NE2	2:B:1084:GLN:H	1.99	0.60
2:B:811:TYR:N	2:B:811:TYR:CD1	2.68	0.60
6:F:103:MET:CE	7:G:66:GLY:H	2.13	0.60
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.24	0.60
10:J:48:ARG:HE	10:J:49:MET:CE	2.10	0.60
13:N:1:DA:H2''	13:N:2:DA:OP2	2.00	0.60
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.66	0.60
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.31	0.60
4:D:5:THR:O	4:D:5:THR:HG23	2.01	0.60
11:K:114:LEU:C	11:K:114:LEU:HD13	2.20	0.60
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.36	0.60
1:A:320:ARG:NH2	14:P:1:U:H1'	2.15	0.60
1:A:1095:THR:O	1:A:1096:SER:HB2	1.99	0.60
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.31	0.60
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.83	0.60
13:N:0:DT:H2''	13:N:1:DA:O5'	2.01	0.60
1:A:886:ILE:CG2	1:A:887:GLY:N	2.64	0.60
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.49	0.60
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.66	0.60
2:B:770:GLN:CD	2:B:983:ARG:HA	2.21	0.60
3:C:147:LEU:N	3:C:147:LEU:HD23	2.16	0.60
10:J:1:MET:N	10:J:56:LEU:N	2.48	0.60
2:B:112:LEU:HD12	2:B:113:TYR:N	2.15	0.60
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:65:HIS:HD2	11:K:67:PHE:N	1.92	0.60
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.36	0.60
1:A:663:SER:OG	1:A:664:THR:N	2.33	0.60
1:A:694:THR:O	1:A:698:GLN:HG3	2.00	0.60
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.36	0.60
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.82	0.60
6:F:130:ILE:O	6:F:148:VAL:CG2	2.49	0.60
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.02	0.60
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.83	0.60
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.36	0.60
11:K:42:LEU:O	11:K:46:ILE:HG13	2.02	0.60
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.83	0.60
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.02	0.60
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.82	0.60
3:C:165:LYS:O	11:K:6:ARG:NH1	2.35	0.60
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.02	0.60
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.12	0.60
1:A:783:THR:HG22	1:A:784:LEU:HG	1.84	0.60
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.83	0.60
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.32	0.60
2:B:515:HIS:CD2	2:B:517:THR:H	2.17	0.60
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.37	0.60
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.17	0.60
1:A:901:LEU:HA	1:A:907:THR:OG1	2.02	0.60
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.70	0.60
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.20	0.60
3:C:100:THR:HG22	3:C:101:LEU:N	2.16	0.60
4:D:138:ASN:OD1	4:D:141:LEU:HB2	2.02	0.60
7:G:1:MET:SD	7:G:79:PHE:CD1	2.95	0.60
11:K:68:PHE:N	11:K:68:PHE:CD2	2.67	0.60
15:T:22:BRU:H2'	15:T:23:DG:O4'	2.01	0.60
3:C:179:GLU:HG2	3:C:180:TYR:N	2.17	0.60
4:D:4:SER:OG	4:D:5:THR:N	2.34	0.60
6:F:77:ASP:C	6:F:79:ARG:H	2.06	0.60
7:G:80:LYS:HG2	7:G:80:LYS:O	2.02	0.60
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.31	0.60
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.84	0.59
2:B:880:THR:O	2:B:881:ASN:HB2	2.01	0.59
3:C:2:SER:N	3:C:3:GLU:N	2.50	0.59
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.15	0.59
1:A:1017:LEU:HB3	5:E:205:SER:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:111:LEU:C	6:F:113:GLY:H	2.05	0.59
7:G:119:LEU:HD12	7:G:131:GLN:O	2.01	0.59
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.01	0.59
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.02	0.59
1:A:384:ASN:O	1:A:386:ASP:N	2.34	0.59
1:A:463:ILE:HD12	1:A:469:ARG:HD2	1.84	0.59
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.32	0.59
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.83	0.59
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.66	0.59
3:C:147:LEU:HD12	3:C:151:GLN:O	2.02	0.59
7:G:49:LEU:HG	7:G:76:ALA:HA	1.82	0.59
8:H:127:GLY:O	8:H:128:ASN:HB2	2.02	0.59
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.31	0.59
15:T:22:BRU:H2'	15:T:23:DG:H8	1.62	0.59
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.02	0.59
1:A:720:ARG:O	1:A:724:GLU:HB2	2.02	0.59
15:T:17:DT:C2'	15:T:18:DT:C5'	2.65	0.59
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.83	0.59
1:A:590:ARG:O	1:A:591:PHE:HB2	2.01	0.59
1:A:809:THR:H	1:A:812:GLU:HB2	1.66	0.59
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.32	0.59
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.83	0.59
2:B:899:ILE:HD13	2:B:905:VAL:HG11	1.82	0.59
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.68	0.59
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.30	0.59
4:D:40:HIS:CB	7:G:73:LYS:HZ3	2.02	0.59
8:H:40:LEU:HD12	8:H:122:LEU:O	2.03	0.59
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.03	0.59
1:A:23:SER:HA	1:A:233:TRP:CD1	2.38	0.59
1:A:289:ILE:C	1:A:291:GLU:H	2.03	0.59
1:A:405:VAL:HG22	1:A:432:VAL:HG13	1.85	0.59
1:A:55:ASP:C	1:A:57:ARG:H	2.04	0.59
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.67	0.59
1:A:738:LYS:HD2	1:A:740:LEU:HD21	1.84	0.59
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.35	0.59
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.66	0.59
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.66	0.59
2:B:603:LEU:HD12	2:B:609:ILE:HG13	1.82	0.59
2:B:942:ARG:NH2	15:T:25:DT:P	2.75	0.59
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.84	0.59
1:A:665:GLY:O	1:A:667:GLY:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:THR:H	2:B:188:ASP:CB	2.14	0.59
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.84	0.59
2:B:731:VAL:HG12	2:B:732:SER:N	2.17	0.59
5:E:177:ARG:C	5:E:212:ARG:HD3	2.22	0.59
10:J:44:TYR:HD2	10:J:44:TYR:H	1.48	0.59
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.18	0.59
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.83	0.59
1:A:596:THR:C	1:A:598:LEU:H	2.05	0.59
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.85	0.59
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.67	0.59
10:J:36:LEU:HD22	10:J:41:LEU:HD12	1.83	0.59
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.02	0.59
1:A:1385:THR:O	1:A:1387:HIS:N	2.36	0.59
3:C:124:LEU:O	3:C:127:ARG:HG2	2.03	0.59
2:B:1005:GLY:HA2	3:C:176:ILE:O	2.02	0.59
15:T:26:DC:H2''	15:T:27:DA:C5'	2.32	0.59
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.02	0.59
1:A:765:VAL:HG23	1:A:802:ASN:O	2.03	0.59
4:D:13:ARG:HB2	4:D:17:LYS:HZ2	1.67	0.59
5:E:15:ALA:O	5:E:19:VAL:HG23	2.03	0.59
8:H:43:ASN:OD1	8:H:46:LEU:HG	2.03	0.59
1:A:75:ASN:O	1:A:76:GLU:CB	2.51	0.59
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.85	0.59
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.33	0.59
2:B:57:TYR:N	2:B:57:TYR:HD1	2.01	0.59
2:B:745:PRO:C	2:B:747:MET:H	2.06	0.59
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.38	0.58
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.18	0.58
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.84	0.58
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.85	0.58
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.38	0.58
1:A:914:GLU:HB2	1:A:979:SER:O	2.03	0.58
4:D:52:LEU:C	4:D:54:GLU:H	2.05	0.58
5:E:157:SER:HG	5:E:160:GLU:HG3	1.68	0.58
7:G:1:MET:SD	7:G:1:MET:O	2.61	0.58
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.84	0.58
10:J:64:ASN:CB	10:J:65:PRO:CD	2.81	0.58
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.03	0.58
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.03	0.58
1:A:33:ALA:HA	1:A:57:ARG:NH2	2.18	0.58
1:A:528:LEU:HD12	1:A:528:LEU:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:CD1	1:A:667:GLY:H	2.17	0.58
1:A:832:ALA:O	1:A:833:GLU:C	2.42	0.58
8:H:38:LEU:HD12	8:H:124:ARG:O	2.03	0.58
15:T:14:DC:H1'	15:T:15:DT:H5'	1.86	0.58
1:A:444:PHE:HB2	1:A:458:HIS:HD2	1.68	0.58
2:B:225:VAL:HA	2:B:237:VAL:O	2.03	0.58
2:B:343:ILE:HG22	2:B:345:LYS:H	1.66	0.58
3:C:174:ALA:O	3:C:175:ALA:HB2	2.04	0.58
4:D:160:VAL:O	4:D:164:ILE:HG13	2.03	0.58
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.33	0.58
1:A:982:THR:O	1:A:985:ASP:HB2	2.04	0.58
2:B:57:TYR:CD1	2:B:57:TYR:N	2.70	0.58
2:B:864:LYS:N	2:B:872:GLU:OE1	2.37	0.58
5:E:178:ILE:HG22	5:E:213:ILE:O	2.04	0.58
6:F:111:LEU:H	6:F:111:LEU:CD1	2.13	0.58
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.04	0.58
1:A:224:PHE:HD2	1:A:229:SER:O	1.86	0.58
1:A:399:HIS:O	1:A:401:GLY:N	2.36	0.58
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.15	0.58
2:B:486:TYR:HH	2:B:1096:ARG:HB3	1.68	0.58
2:B:344:LYS:O	2:B:345:LYS:HB2	2.03	0.58
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.85	0.58
4:D:53:SER:HB3	4:D:153:ARG:H	1.67	0.58
4:D:66:ARG:O	4:D:70:PHE:HB2	2.04	0.58
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.68	0.58
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.33	0.58
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.38	0.58
1:A:34:LYS:HB3	1:A:36:ARG:HE	1.69	0.58
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.01	0.58
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.39	0.58
1:A:964:ILE:O	1:A:967:ALA:N	2.37	0.58
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.50	0.58
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.51	0.58
2:B:990:ILE:HG22	2:B:991:GLY:N	2.19	0.58
5:E:23:VAL:O	5:E:28:TYR:HB2	2.04	0.58
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.34	0.58
1:A:606:LEU:HB3	1:A:614:PHE:CE2	2.39	0.58
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.86	0.58
4:D:192:LYS:HB3	4:D:192:LYS:HZ3	1.69	0.58
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.84	0.58
1:A:1001:ARG:O	1:A:1002:GLY:O	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:THR:CG2	1:A:476:SER:N	2.66	0.58
1:A:492:PRO:O	1:A:493:GLN:NE2	2.36	0.58
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.85	0.58
1:A:648:ASN:O	1:A:649:ILE:C	2.41	0.58
2:B:1159:ARG:NH1	2:B:1159:ARG:HB3	2.18	0.58
2:B:265:SER:O	2:B:266:ALA:HB3	2.04	0.58
2:B:778:MET:CE	2:B:1094:ARG:CD	2.82	0.58
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.34	0.58
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.85	0.58
6:F:99:LEU:C	6:F:99:LEU:HD12	2.24	0.58
11:K:111:LEU:O	11:K:112:GLN:HG2	2.03	0.58
15:T:19:TT:H2'1	15:T:19:TT:H5R1	1.83	0.58
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.19	0.58
4:D:53:SER:HB3	4:D:152:SER:CB	2.33	0.58
6:F:75:PRO:O	6:F:77:ASP:O	2.22	0.58
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.07	0.57
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.19	0.57
1:A:58:LEU:CG	1:A:59:GLY:N	2.66	0.57
1:A:699:ALA:CB	1:A:701:LEU:HG	2.34	0.57
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.03	0.57
4:D:51:ASN:O	4:D:52:LEU:O	2.22	0.57
5:E:207:ARG:CB	5:E:207:ARG:HH11	2.16	0.57
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.03	0.57
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.29	0.57
2:B:229:ALA:CB	2:B:231:PRO:HD2	2.34	0.57
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.69	0.57
4:D:134:THR:CG2	4:D:135:GLY:N	2.66	0.57
4:D:167:LEU:HB3	4:D:177:VAL:HG13	1.85	0.57
7:G:3:PHE:CE1	7:G:80:LYS:HE2	2.38	0.57
12:L:39:SER:O	12:L:40:LEU:HG	2.03	0.57
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.67	0.57
1:A:471:ASN:O	1:A:474:VAL:HG12	2.04	0.57
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.69	0.57
2:B:910:VAL:HG12	2:B:912:ILE:H	1.69	0.57
5:E:213:ILE:HG12	5:E:214:CYS:N	2.19	0.57
1:A:699:ALA:HB1	1:A:701:LEU:HG	1.85	0.57
1:A:754:SER:N	1:A:757:ASN:HD22	1.92	0.57
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.86	0.57
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.34	0.57
1:A:37:PHE:N	1:A:37:PHE:CD1	2.72	0.57
1:A:567:LYS:CG	1:A:568:PRO:CD	2.76	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:486:TYR:CZ	2:B:1096:ARG:HB3	2.39	0.57
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.20	0.57
4:D:18:VAL:O	4:D:18:VAL:HG13	2.05	0.57
7:G:145:VAL:CG1	7:G:146:LYS:N	2.67	0.57
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.45	0.57
14:P:4:A:O2'	14:P:5:C:H5'	2.05	0.57
1:A:42:ASP:HB3	1:A:45:GLN:N	2.19	0.57
1:A:482:PHE:C	1:A:484:GLY:H	2.07	0.57
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.86	0.57
1:A:709:THR:HG21	9:I:93:LYS:O	2.05	0.57
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.36	0.57
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.35	0.57
2:B:1219:ASP:O	2:B:1219:ASP:OD1	2.23	0.57
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.86	0.57
2:B:580:VAL:HG22	2:B:624:LEU:CB	2.35	0.57
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.86	0.57
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.87	0.57
12:L:58:LYS:HG2	12:L:58:LYS:O	2.03	0.57
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.87	0.57
2:B:1023:VAL:O	2:B:1026:LEU:N	2.38	0.57
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.45	0.57
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.39	0.57
1:A:58:LEU:CD1	1:A:243:PRO:HB3	2.33	0.57
1:A:699:ALA:O	1:A:700:ASN:HB3	2.04	0.57
2:B:332:ASP:OD1	2:B:336:ARG:NE	2.38	0.57
2:B:340:ALA:CB	2:B:343:ILE:HD12	2.35	0.57
7:G:154:VAL:HG12	7:G:155:SER:N	2.20	0.57
1:A:1226:VAL:HG13	1:A:1240:CYS:HB3	1.87	0.57
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.18	0.57
2:B:496:ARG:HH11	2:B:496:ARG:HB3	1.69	0.57
2:B:744:HIS:HD2	2:B:746:SER:CB	2.16	0.57
2:B:874:PHE:HA	2:B:913:GLY:O	2.05	0.57
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.87	0.57
4:D:4:SER:O	4:D:5:THR:HB	2.03	0.57
1:A:1095:THR:OG1	1:A:1113:THR:HB	2.05	0.57
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.34	0.57
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.85	0.57
10:J:44:TYR:HA	10:J:47:ARG:HB3	1.87	0.57
1:A:406:ILE:HG13	1:A:431:LYS:HB2	1.87	0.56
1:A:600:PRO:HG2	1:A:601:LYS:H	1.70	0.56
1:A:709:THR:HB	1:A:712:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:SER:O	2:B:182:SER:HB3	2.04	0.56
2:B:386:LEU:O	2:B:388:CYS:N	2.37	0.56
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.39	0.56
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.35	0.56
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.86	0.56
7:G:88:ASP:OD2	7:G:88:ASP:N	2.37	0.56
9:I:15:TYR:CD1	9:I:15:TYR:N	2.73	0.56
11:K:47:ARG:HD2	11:K:47:ARG:O	2.05	0.56
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.05	0.56
1:A:1450:LEU:HD21	7:G:18:PHE:O	2.04	0.56
1:A:853:ASP:OD1	1:A:855:THR:N	2.38	0.56
1:A:982:THR:N	1:A:985:ASP:HB2	2.20	0.56
2:B:1176:ASN:C	2:B:1178:ASN:H	2.08	0.56
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.87	0.56
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.87	0.56
3:C:20:PHE:CE1	3:C:22:LEU:HD12	2.40	0.56
3:C:241:ASP:O	3:C:245:VAL:HG23	2.05	0.56
6:F:81:THR:HG23	6:F:144:GLU:OE2	2.06	0.56
7:G:51:TYR:C	7:G:51:TYR:CD2	2.79	0.56
9:I:62:ILE:HG12	9:I:62:ILE:O	2.05	0.56
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.45	0.56
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.36	0.56
1:A:709:THR:HG22	1:A:710:LEU:N	2.20	0.56
1:A:866:PHE:O	1:A:867:ILE:HD12	2.06	0.56
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.19	0.56
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.54	0.56
2:B:1155:SER:OG	2:B:1156:ASP:N	2.37	0.56
3:C:98:VAL:C	3:C:99:LEU:HD23	2.26	0.56
5:E:168:TYR:HB2	5:E:170:LEU:HG	1.86	0.56
9:I:82:GLU:O	9:I:104:LEU:HG	2.05	0.56
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.05	0.56
1:A:1162:VAL:HG12	1:A:1162:VAL:O	2.06	0.56
1:A:1279:ILE:CD1	1:A:1316:VAL:HG21	2.35	0.56
1:A:222:LEU:O	1:A:224:PHE:N	2.38	0.56
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.86	0.56
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.44	0.56
1:A:525:GLN:HG3	2:B:835:GLN:HG2	1.86	0.56
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.39	0.56
1:A:31:SER:OG	1:A:82:GLY:HA2	2.04	0.56
1:A:858:ASN:ND2	1:A:858:ASN:C	2.59	0.56
1:A:869:GLY:O	5:E:204:THR:HG21	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:GLY:H	2:B:298:LEU:HD23	1.69	0.56
6:F:89:GLU:OE2	6:F:134:ILE:HG21	2.05	0.56
7:G:114:LEU:HG	7:G:162:SER:HB3	1.87	0.56
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	1.87	0.56
1:A:968:GLN:O	1:A:970:THR:N	2.38	0.56
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.41	0.56
2:B:310:MET:HE3	2:B:387:LEU:CD1	2.34	0.56
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.04	0.56
3:C:77:ILE:O	3:C:79:GLN:N	2.39	0.56
8:H:61:SER:O	8:H:62:SER:CB	2.54	0.56
8:H:91:ASP:C	8:H:93:TYR:H	2.08	0.56
10:J:44:TYR:N	10:J:44:TYR:CD2	2.73	0.56
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.87	0.56
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.88	0.56
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.87	0.56
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.88	0.56
1:A:626:ASN:O	1:A:631:HIS:CD2	2.59	0.56
2:B:344:LYS:O	2:B:345:LYS:CB	2.53	0.56
2:B:831:SER:HB3	2:B:994:TYR:OH	2.05	0.56
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.88	0.56
9:I:55:THR:CG2	9:I:58:VAL:HG21	2.36	0.56
9:I:92:ARG:HB3	9:I:95:THR:OG1	2.05	0.56
12:L:58:LYS:O	12:L:59:ALA:O	2.24	0.56
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.25	0.56
1:A:730:GLY:C	1:A:732:LEU:H	2.09	0.56
1:A:867:ILE:HG22	1:A:872:GLY:N	2.21	0.56
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.88	0.56
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.87	0.56
2:B:776:GLN:O	2:B:1095:LEU:HA	2.06	0.56
6:F:99:LEU:HD12	6:F:99:LEU:O	2.05	0.56
7:G:111:THR:HG22	7:G:113:HIS:N	2.17	0.56
8:H:100:THR:HG22	8:H:101:ALA:N	2.20	0.56
8:H:39:THR:O	8:H:123:MET:HA	2.06	0.56
10:J:44:TYR:HD2	10:J:44:TYR:N	2.03	0.56
14:P:3:G:H2'	14:P:4:A:C8	2.41	0.56
1:A:528:LEU:O	1:A:528:LEU:HD12	2.05	0.56
1:A:806:ARG:HH12	2:B:729:ILE:CD1	2.18	0.56
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.87	0.56
2:B:521:LEU:HD13	2:B:633:VAL:HB	1.86	0.56
2:B:557:PHE:C	2:B:557:PHE:HD2	2.09	0.56
3:C:176:ILE:HG22	3:C:177:GLU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.86	0.56
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	1.88	0.56
2:B:343:ILE:HG21	2:B:348:ARG:H	1.70	0.56
2:B:357:GLN:O	2:B:366:GLN:HA	2.04	0.56
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.37	0.56
2:B:658:ILE:HG22	2:B:659:ALA:N	2.21	0.56
8:H:128:ASN:CG	8:H:128:ASN:O	2.44	0.56
10:J:36:LEU:O	10:J:39:LEU:N	2.37	0.56
14:P:7:A:H2'	14:P:8:G:C1'	2.36	0.56
1:A:1387:HIS:NE2	13:N:4:DT:H5''	2.21	0.56
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.87	0.56
1:A:590:ARG:HB3	1:A:605:MET:N	2.20	0.56
1:A:596:THR:C	1:A:598:LEU:N	2.58	0.56
1:A:95:PHE:O	1:A:96:ILE:C	2.44	0.56
1:A:1410:PHE:HA	2:B:1212:ILE:CD1	2.35	0.56
2:B:466:TRP:HA	2:B:466:TRP:CE3	2.41	0.56
2:B:705:MET:H	2:B:710:LEU:CD1	2.19	0.56
2:B:843:GLN:O	2:B:846:ILE:HB	2.06	0.56
2:B:882:THR:HG21	2:B:935:ARG:HA	1.87	0.56
5:E:105:PHE:O	5:E:106:GLN:HB2	2.06	0.56
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.88	0.56
8:H:61:SER:HB2	8:H:139:ASN:HB3	1.87	0.56
11:K:18:LYS:HZ3	11:K:38:GLU:HG2	1.70	0.56
1:A:364:VAL:O	1:A:364:VAL:HG13	2.06	0.56
1:A:920:LEU:HD23	1:A:921:GLY:N	2.20	0.56
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.88	0.56
1:A:942:PHE:HD2	1:A:943:LEU:HD23	1.70	0.56
1:A:98:LYS:O	1:A:99:ILE:C	2.44	0.56
4:D:17:LYS:CA	4:D:17:LYS:HE3	2.35	0.56
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.87	0.56
1:A:108:MET:N	1:A:108:MET:SD	2.79	0.55
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.05	0.55
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.87	0.55
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.86	0.55
1:A:446:ARG:HB2	1:A:487:MET:SD	2.47	0.55
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.63	0.55
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.35	0.55
3:C:243:VAL:HG12	3:C:243:VAL:O	2.05	0.55
5:E:78:LEU:HD23	5:E:78:LEU:C	2.26	0.55
4:D:47:LEU:HD11	7:G:3:PHE:CE2	2.40	0.55
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1377:THR:O	1:A:1379:GLY:N	2.39	0.55
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.33	0.55
1:A:302:THR:HA	1:A:305:ASP:O	2.05	0.55
1:A:449:SER:O	2:B:1133:MET:HB3	2.06	0.55
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.35	0.55
2:B:114:PRO:O	2:B:116:GLU:N	2.39	0.55
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.36	0.55
2:B:51:PHE:O	2:B:54:PHE:HB3	2.06	0.55
3:C:18:VAL:O	3:C:20:PHE:HD2	1.90	0.55
6:F:118:LEU:O	6:F:122:MET:HG3	2.06	0.55
9:I:106:CYS:O	9:I:107:SER:HB2	2.07	0.55
11:K:110:ASN:O	11:K:111:LEU:CD2	2.50	0.55
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.88	0.55
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.71	0.55
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.41	0.55
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.41	0.55
4:D:137:ASN:HD22	4:D:137:ASN:C	2.10	0.55
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.71	0.55
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.35	0.55
7:G:83:LYS:HE2	7:G:150:CYS:H	1.72	0.55
8:H:4:THR:CA	8:H:60:ALA:HB2	2.32	0.55
8:H:64:ASN:O	8:H:65:LEU:HB2	2.05	0.55
8:H:83:GLN:C	8:H:85:GLY:H	2.09	0.55
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.36	0.55
15:T:10:DA:H2''	15:T:11:DG:OP2	2.06	0.55
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.36	0.55
1:A:595:THR:O	1:A:596:THR:HG23	2.05	0.55
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.89	0.55
4:D:128:VAL:O	4:D:132:GLN:HG3	2.06	0.55
5:E:55:ARG:C	5:E:57:MET:H	2.08	0.55
7:G:47:CYS:O	7:G:76:ALA:HB1	2.06	0.55
8:H:40:LEU:HD22	8:H:123:MET:HE2	1.87	0.55
8:H:82:PRO:C	8:H:84:ALA:H	2.09	0.55
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.71	0.55
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.40	0.55
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.54	0.55
1:A:1114:PRO:O	1:A:1115:SER:O	2.24	0.55
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.88	0.55
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.42	0.55
1:A:42:ASP:HB3	1:A:45:GLN:CA	2.36	0.55
1:A:61:ILE:O	1:A:63:ARG:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:ASN:O	1:A:745:GLN:HB2	2.05	0.55
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.86	0.55
2:B:254:LEU:HD23	2:B:381:MET:CE	2.37	0.55
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.89	0.55
4:D:7:THR:O	4:D:9:GLN:N	2.40	0.55
5:E:157:SER:C	5:E:159:ASP:N	2.57	0.55
6:F:125:LEU:O	6:F:125:LEU:HG	2.07	0.55
6:F:69:LEU:N	6:F:70:LYS:CA	2.69	0.55
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.36	0.55
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.42	0.55
2:B:1002:THR:HG21	2:B:1006:ILE:CD1	2.30	0.55
2:B:217:ARG:O	2:B:217:ARG:HD2	2.07	0.55
2:B:466:TRP:O	2:B:468:GLU:N	2.39	0.55
3:C:167:HIS:CD2	3:C:168:ALA:H	2.23	0.55
9:I:52:ILE:HG13	9:I:52:ILE:O	2.06	0.55
11:K:69:ALA:O	11:K:70:ARG:HB3	2.06	0.55
1:A:311:GLN:O	1:A:312:PRO:C	2.45	0.55
2:B:1087:PHE:HD2	2:B:1088:GLY:H	1.50	0.55
1:A:17:VAL:HA	2:B:1215:ARG:O	2.06	0.55
2:B:729:ILE:HG22	2:B:729:ILE:O	2.04	0.55
2:B:792:MET:HA	2:B:856:PHE:O	2.06	0.55
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.06	0.55
7:G:10:ASN:OD1	7:G:71:ASN:HA	2.07	0.55
7:G:20:PRO:HG2	7:G:21:ARG:H	1.70	0.55
15:T:17:DT:H1'	15:T:18:DT:C5'	2.33	0.55
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.07	0.55
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.89	0.55
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.88	0.55
1:A:687:LYS:O	1:A:690:VAL:HB	2.06	0.55
1:A:68:GLN:O	1:A:70:CYS:N	2.39	0.55
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.27	0.55
1:A:14:VAL:CG2	2:B:1216:LEU:HD13	2.34	0.55
2:B:130:VAL:HB	2:B:167:ILE:CD1	2.36	0.55
3:C:90:ASP:O	3:C:91:HIS:HB3	2.05	0.55
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.41	0.55
1:A:1151:GLU:HA	9:I:44:TYR:O	2.07	0.55
10:J:48:ARG:HD2	10:J:49:MET:N	2.21	0.55
14:P:6:C:H2'	14:P:7:A:H8	1.68	0.55
1:A:115:LEU:HB2	1:A:122:MET:HE2	1.89	0.55
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.37	0.55
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:13:TRP:O	5:E:16:PHE:HB3	2.07	0.55
2:B:1077:THR:HG22	11:K:44:ASN:HD21	1.71	0.55
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.42	0.55
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.05	0.55
1:A:47:ARG:HH12	1:A:254:GLU:HG2	1.72	0.55
2:B:129:PHE:HA	2:B:165:VAL:O	2.07	0.55
2:B:343:ILE:CG2	2:B:348:ARG:N	2.66	0.55
2:B:654:ARG:H	2:B:657:HIS:CD2	2.17	0.55
2:B:745:PRO:C	2:B:747:MET:N	2.60	0.55
4:D:176:GLU:C	4:D:178:ALA:N	2.60	0.55
4:D:7:THR:HB	7:G:42:PHE:HE2	1.72	0.55
1:A:1120:LEU:CD1	1:A:1120:LEU:N	2.69	0.54
1:A:265:LYS:HZ3	1:A:322:VAL:HG13	1.71	0.54
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.89	0.54
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.72	0.54
2:B:911:ILE:O	2:B:912:ILE:HG13	2.07	0.54
3:C:189:THR:HG22	3:C:190:ASP:H	1.71	0.54
7:G:18:PHE:HA	7:G:22:MET:CE	2.36	0.54
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.22	0.54
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.07	0.54
1:A:1424:VAL:CG1	1:A:1436:ILE:HD11	2.34	0.54
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.89	0.54
1:A:265:LYS:HE2	1:A:322:VAL:HG11	1.89	0.54
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.37	0.54
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.89	0.54
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.07	0.54
9:I:50:THR:HG22	9:I:52:ILE:H	1.72	0.54
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.22	0.54
2:B:1165:ILE:HG12	4:D:17:LYS:HD2	1.89	0.54
2:B:38:PHE:CD1	2:B:811:TYR:CD2	2.94	0.54
2:B:834:ASN:HA	2:B:838:SER:O	2.06	0.54
4:D:185:CYS:HB2	4:D:211:LEU:HD22	1.88	0.54
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.88	0.54
5:E:35:VAL:C	5:E:37:LEU:H	2.10	0.54
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.90	0.54
1:A:873:MET:C	1:A:1058:VAL:HG23	2.27	0.54
1:A:44:THR:O	1:A:45:GLN:HB2	2.07	0.54
1:A:527:THR:HG23	1:A:650:GLN:HA	1.89	0.54
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.49	0.54
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.56	0.54
2:B:479:VAL:O	2:B:480:SER:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.22	0.54
2:B:542:MET:HG2	2:B:747:MET:HB3	1.89	0.54
2:B:841:MET:O	2:B:993:THR:HA	2.08	0.54
2:B:879:ARG:HH11	2:B:883:LEU:CD2	2.17	0.54
7:G:143:ILE:CG2	7:G:144:ARG:N	2.71	0.54
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.19	0.54
9:I:101:PHE:N	9:I:101:PHE:CD1	2.76	0.54
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.90	0.54
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.38	0.54
2:B:287:ARG:NH1	2:B:324:ILE:O	2.41	0.54
2:B:305:VAL:HG12	2:B:305:VAL:O	2.07	0.54
2:B:865:LYS:NZ	2:B:869:SER:HA	2.23	0.54
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.28	0.54
5:E:55:ARG:C	5:E:57:MET:N	2.61	0.54
10:J:32:GLU:CD	10:J:32:GLU:H	2.10	0.54
1:A:340:LEU:HD21	2:B:1200:ALA:N	2.23	0.54
1:A:695:LYS:C	1:A:697:ALA:H	2.10	0.54
1:A:814:PHE:O	1:A:817:ALA:HB3	2.08	0.54
2:B:372:SER:O	2:B:376:PHE:HD1	1.90	0.54
3:C:100:THR:HG22	3:C:101:LEU:H	1.71	0.54
14:P:7:A:H2'	14:P:8:G:O4'	2.08	0.54
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.43	0.54
2:B:25:ILE:HD11	2:B:653:VAL:O	2.08	0.54
3:C:70:ILE:HD11	3:C:144:ILE:CG1	2.38	0.54
6:F:69:LEU:N	6:F:70:LYS:N	2.56	0.54
7:G:111:THR:HB	7:G:114:LEU:HB2	1.90	0.54
8:H:58:THR:HG22	8:H:59:ILE:N	2.22	0.54
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.29	0.54
1:A:4:GLN:O	1:A:5:GLN:HB2	2.07	0.54
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.90	0.54
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.08	0.54
2:B:687:GLU:O	2:B:689:LEU:HG	2.08	0.54
2:B:705:MET:N	2:B:710:LEU:HD12	2.23	0.54
2:B:850:LEU:HD12	2:B:851:PHE:H	1.72	0.54
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.38	0.54
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.90	0.54
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.37	0.54
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.23	0.54
1:A:71:GLN:O	1:A:73:GLY:N	2.37	0.54
2:B:63:ILE:O	2:B:67:SER:HB3	2.08	0.54
2:B:942:ARG:NH2	15:T:25:DT:OP2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.08	0.54
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.33	0.54
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.41	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.71	0.54
1:A:1171:GLN:HA	1:A:1174:PHE:HE1	1.71	0.54
1:A:164:ARG:HG3	1:A:165:GLY:H	1.72	0.54
1:A:535:THR:CG2	1:A:616:VAL:HA	2.35	0.54
1:A:787:PHE:CE1	1:A:796:SER:HA	2.43	0.54
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.18	0.54
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.42	0.54
2:B:502:ILE:CD1	2:B:502:ILE:H	2.07	0.54
2:B:860:MET:HG2	2:B:861:ASP:N	2.23	0.54
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.23	0.54
11:K:47:ARG:HD3	11:K:59:ALA:O	2.07	0.54
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.73	0.54
1:A:1369:ALA:O	1:A:1372:VAL:HG12	2.08	0.53
1:A:187:LYS:HE3	1:A:198:GLU:OE2	2.08	0.53
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.43	0.53
1:A:500:GLU:OE2	2:B:1145:SER:HB2	2.08	0.53
2:B:549:THR:HG22	2:B:550:ASP:N	2.15	0.53
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.89	0.53
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.90	0.53
1:A:1313:LEU:O	1:A:1315:GLU:N	2.41	0.53
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.90	0.53
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.22	0.53
2:B:327:ARG:O	2:B:331:LEU:HD13	2.07	0.53
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.90	0.53
3:C:73:GLN:HB3	3:C:131:HIS:H	1.73	0.53
12:L:31:CYS:HB3	12:L:34:CYS:C	2.28	0.53
1:A:886:ILE:HG13	1:A:943:LEU:HD12	1.89	0.53
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.23	0.53
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.23	0.53
7:G:138:THR:CG2	7:G:139:ILE:H	2.00	0.53
11:K:109:TRP:O	11:K:111:LEU:N	2.39	0.53
11:K:63:VAL:O	11:K:63:VAL:HG23	2.09	0.53
12:L:32:ALA:CB	12:L:55:ILE:HD12	2.39	0.53
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.42	0.53
1:A:42:ASP:C	1:A:44:THR:H	2.09	0.53
1:A:761:MET:HA	1:A:804:TYR:HB2	1.89	0.53
1:A:958:VAL:O	1:A:958:VAL:HG12	2.08	0.53
2:B:830:TYR:O	2:B:831:SER:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.73	0.53
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.43	0.53
11:K:55:LYS:CB	11:K:81:TYR:HE1	2.21	0.53
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.21	0.53
4:D:198:LEU:O	4:D:200:ASN:N	2.42	0.53
5:E:207:ARG:HB2	5:E:207:ARG:NH1	2.23	0.53
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.08	0.53
1:A:53:LEU:CD2	1:A:54:ASN:N	2.51	0.53
1:A:666:ILE:HD12	1:A:666:ILE:N	2.23	0.53
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.43	0.53
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.90	0.53
1:A:982:THR:HB	1:A:985:ASP:N	2.23	0.53
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.43	0.53
7:G:91:VAL:HB	7:G:139:ILE:O	2.08	0.53
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.74	0.53
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.39	0.53
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.91	0.53
2:B:408:LEU:HG	2:B:409:ALA:H	1.74	0.53
4:D:56:ARG:HD3	4:D:149:THR:HA	1.91	0.53
5:E:163:GLU:O	5:E:164:LEU:C	2.47	0.53
1:A:288:ALA:HA	1:A:291:GLU:OE2	2.09	0.53
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.44	0.53
1:A:478:TYR:O	1:A:479:ASN:HB3	2.08	0.53
2:B:1166:CYS:O	2:B:1168:LEU:N	2.41	0.53
2:B:1180:PHE:O	2:B:1181:GLU:O	2.27	0.53
2:B:343:ILE:CB	2:B:348:ARG:HG3	2.37	0.53
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.08	0.53
4:D:53:SER:HB3	4:D:152:SER:HB2	1.91	0.53
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.90	0.53
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.74	0.53
2:B:54:PHE:O	2:B:58:THR:HB	2.09	0.53
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.39	0.53
3:C:120:ILE:HD13	3:C:124:LEU:HD21	1.91	0.53
9:I:111:THR:CG2	9:I:112:SER:N	2.72	0.53
9:I:112:SER:O	9:I:114:GLN:N	2.42	0.53
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.73	0.53
14:P:1:U:H2'	14:P:2:C:C6	2.43	0.53
15:T:22:BRU:H2''	15:T:23:DG:O4'	2.09	0.53
1:A:1369:ALA:O	1:A:1370:LEU:C	2.46	0.53
1:A:317:LYS:O	1:A:318:SER:HB3	2.09	0.53
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ILE:C	1:A:610:GLY:N	2.63	0.53
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.91	0.53
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.38	0.53
2:B:683:SER:C	2:B:685:LEU:N	2.62	0.53
2:B:756:ILE:O	2:B:759:PRO:HD3	2.08	0.53
3:C:263:THR:C	3:C:265:MET:N	2.63	0.53
4:D:208:GLU:O	4:D:212:LYS:HG3	2.08	0.53
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.09	0.53
7:G:44:TYR:CD2	7:G:105:PRO:HB2	2.44	0.53
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.91	0.53
1:A:1153:TYR:CE1	9:I:42:LEU:HD13	2.44	0.53
13:N:0:DT:H1'	13:N:1:DA:H5'	1.90	0.53
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.10	0.52
1:A:282:ASN:O	1:A:284:ALA:N	2.42	0.52
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.42	0.52
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.88	0.52
2:B:412:LEU:HB3	2:B:466:TRP:HZ2	1.74	0.52
2:B:654:ARG:C	2:B:656:GLY:H	2.11	0.52
3:C:87:PHE:HD1	3:C:87:PHE:H	1.56	0.52
4:D:19:GLU:O	4:D:21:GLU:N	2.42	0.52
9:I:99:LEU:O	9:I:111:THR:HG23	2.09	0.52
9:I:115:LYS:CD	9:I:117:LYS:HE3	2.35	0.52
11:K:60:ALA:O	11:K:73:LEU:HD12	2.09	0.52
14:P:8:G:H8	14:P:8:G:OP2	1.91	0.52
1:A:1187:GLN:O	1:A:1243:VAL:HG13	2.09	0.52
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	1.90	0.52
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.91	0.52
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.44	0.52
1:A:903:ASN:ND2	1:A:903:ASN:C	2.63	0.52
2:B:1183:LYS:CE	2:B:1183:LYS:N	2.72	0.52
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.09	0.52
3:C:263:THR:O	3:C:265:MET:N	2.43	0.52
5:E:168:TYR:CB	5:E:170:LEU:HG	2.38	0.52
7:G:138:THR:HG22	7:G:139:ILE:HG13	1.90	0.52
7:G:1:MET:O	7:G:3:PHE:CE1	2.63	0.52
2:B:954:VAL:O	12:L:55:ILE:O	2.28	0.52
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.90	0.52
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.39	0.52
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.74	0.52
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.91	0.52
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ILE:HG13	2:B:129:PHE:O	2.08	0.52
2:B:546:SER:OG	2:B:631:GLY:N	2.39	0.52
4:D:29:LEU:HD22	7:G:82:PHE:CD2	2.44	0.52
5:E:78:LEU:HD23	5:E:79:TRP:N	2.24	0.52
6:F:85:MET:HE1	6:F:148:VAL:HG12	1.89	0.52
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.39	0.52
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.44	0.52
2:B:223:VAL:HG21	2:B:380:TYR:HE2	1.75	0.52
2:B:525:ALA:O	2:B:768:THR:HG23	2.09	0.52
2:B:787:VAL:HG12	2:B:787:VAL:O	2.09	0.52
2:B:980:PHE:CD2	2:B:1094:ARG:HA	2.44	0.52
6:F:94:LEU:HD21	6:F:122:MET:HA	1.92	0.52
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.91	0.52
7:G:51:TYR:O	7:G:54:ILE:HG13	2.10	0.52
1:A:1095:THR:O	1:A:1096:SER:CB	2.57	0.52
1:A:475:THR:HG23	1:A:476:SER:N	2.25	0.52
1:A:60:SER:C	1:A:61:ILE:HG13	2.29	0.52
1:A:92:HIS:O	1:A:95:PHE:N	2.36	0.52
2:B:1201:LYS:O	2:B:1204:PHE:HB2	2.09	0.52
2:B:274:PRO:O	2:B:275:TYR:HB2	2.09	0.52
2:B:434:ARG:HA	2:B:437:GLU:CD	2.29	0.52
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.45	0.52
3:C:76:ASP:OD2	3:C:128:ASN:N	2.41	0.52
8:H:102:TYR:N	8:H:102:TYR:CD2	2.77	0.52
13:N:3:DG:C1'	13:N:4:DT:H5'	2.38	0.52
1:A:115:LEU:HB2	1:A:122:MET:CE	2.39	0.52
1:A:244:PRO:O	1:A:246:VAL:N	2.43	0.52
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.92	0.52
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.24	0.52
1:A:838:GLN:O	1:A:842:VAL:HG23	2.09	0.52
1:A:840:ARG:O	1:A:841:LEU:C	2.47	0.52
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.74	0.52
3:C:66:ARG:NH1	3:C:144:ILE:O	2.43	0.52
4:D:130:LEU:C	4:D:132:GLN:N	2.62	0.52
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.91	0.52
1:A:836:TYR:HB2	15:T:18:DT:H4'	1.92	0.52
1:A:1394:THR:CG2	1:A:1398:MET:SD	2.89	0.52
1:A:317:LYS:O	1:A:318:SER:CB	2.57	0.52
1:A:881:GLN:O	1:A:953:ASN:HA	2.10	0.52
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.21	0.52
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ILE:O	2:B:37:PHE:N	2.41	0.52
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.91	0.52
7:G:1:MET:HG3	7:G:85:GLU:OE2	2.10	0.52
8:H:4:THR:O	8:H:5:LEU:HD23	2.09	0.52
10:J:23:ASN:C	10:J:25:LEU:N	2.61	0.52
1:A:40:THR:HG22	1:A:41:MET:CG	2.28	0.52
1:A:774:ARG:O	1:A:775:ILE:C	2.47	0.52
1:A:956:LEU:HD23	1:A:957:PRO:HD2	1.92	0.52
2:B:1022:THR:HG23	2:B:1022:THR:O	2.09	0.52
2:B:1099:VAL:HG12	2:B:1100:ASP:N	2.24	0.52
2:B:1177:HIS:O	2:B:1179:GLN:N	2.42	0.52
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.91	0.52
2:B:496:ARG:HH12	2:B:539:LEU:HB2	1.75	0.52
2:B:654:ARG:N	2:B:657:HIS:HD2	2.04	0.52
2:B:899:ILE:O	2:B:952:VAL:HG21	2.09	0.52
3:C:167:HIS:CD2	3:C:169:LYS:H	2.27	0.52
3:C:256:ALA:O	3:C:259:LEU:N	2.42	0.52
5:E:17:ARG:O	5:E:20:LYS:HB2	2.10	0.52
6:F:125:LEU:N	6:F:130:ILE:HD11	2.23	0.52
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.92	0.52
8:H:84:ALA:HA	8:H:87:ARG:CB	2.34	0.52
9:I:13:MET:HG3	9:I:14:LEU:N	2.23	0.52
1:A:114:LEU:HD13	1:A:171:GLN:NE2	2.25	0.52
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.91	0.52
1:A:30:ILE:HD11	2:B:1168:LEU:HD13	1.92	0.52
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.09	0.52
1:A:886:ILE:HG13	1:A:943:LEU:CD1	2.40	0.52
2:B:936:ASP:OD1	2:B:938:SER:N	2.39	0.52
4:D:53:SER:CB	4:D:153:ARG:H	2.22	0.52
8:H:62:SER:C	8:H:64:ASN:H	2.13	0.52
11:K:55:LYS:HB3	11:K:81:TYR:CE1	2.45	0.52
1:A:58:LEU:CD1	1:A:80:HIS:H	2.23	0.52
1:A:67:CYS:O	1:A:68:GLN:HB2	2.09	0.52
2:B:337:ARG:C	2:B:338:GLY:N	2.64	0.52
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.75	0.52
2:B:640:VAL:O	2:B:641:GLU:C	2.47	0.52
3:C:33:LEU:O	3:C:34:ARG:C	2.48	0.52
5:E:177:ARG:HD3	5:E:215:MET:CG	2.40	0.52
1:A:1441:PHE:HZ	6:F:89:GLU:HA	1.74	0.52
7:G:79:PHE:HZ	7:G:106:MET:HE1	1.71	0.52
7:G:3:PHE:CD1	7:G:80:LYS:NZ	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.92	0.52
9:I:2:THR:O	9:I:3:THR:C	2.47	0.52
9:I:61:ASP:O	9:I:63:GLY:N	2.43	0.52
11:K:55:LYS:CB	11:K:81:TYR:CE1	2.93	0.52
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.92	0.51
1:A:84:ILE:HG22	1:A:239:LEU:HB3	1.91	0.51
1:A:264:PHE:O	1:A:267:ALA:HB3	2.10	0.51
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.09	0.51
1:A:381:THR:CG2	1:A:383:TYR:H	2.23	0.51
1:A:613:ILE:O	1:A:614:PHE:HB3	2.09	0.51
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.43	0.51
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.72	0.51
1:A:965:GLN:O	1:A:968:GLN:HB2	2.10	0.51
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.75	0.51
2:B:184:ALA:HB1	2:B:188:ASP:HB3	1.92	0.51
2:B:278:GLN:HG2	2:B:279:ASP:H	1.74	0.51
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.27	0.51
2:B:825:VAL:HG13	2:B:826:ALA:N	2.25	0.51
7:G:139:ILE:HG22	7:G:140:LYS:N	2.24	0.51
9:I:14:LEU:HA	9:I:28:GLU:O	2.10	0.51
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.40	0.51
1:A:168:GLY:O	1:A:169:ASN:C	2.47	0.51
1:A:974:ASP:C	1:A:976:THR:H	2.13	0.51
2:B:343:ILE:CG2	2:B:348:ARG:H	2.22	0.51
1:A:822:GLU:HG3	2:B:513:GLN:NE2	2.26	0.51
3:C:83:SER:OG	3:C:160:LYS:HD3	2.10	0.51
4:D:167:LEU:O	4:D:170:THR:OG1	2.24	0.51
4:D:17:LYS:HA	4:D:17:LYS:HE3	1.92	0.51
5:E:61:GLN:HG2	5:E:62:ALA:N	2.24	0.51
1:A:107:CYS:H	1:A:114:LEU:HD21	1.74	0.51
1:A:1376:THR:O	1:A:1377:THR:C	2.48	0.51
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.51
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.92	0.51
1:A:826:ASP:HB2	1:A:830:LYS:HD3	1.91	0.51
2:B:281:PRO:O	2:B:283:VAL:N	2.43	0.51
2:B:278:GLN:NE2	2:B:337:ARG:HH21	2.08	0.51
2:B:449:ASN:C	2:B:451:LYS:H	2.13	0.51
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.93	0.51
3:C:226:ASP:O	3:C:227:THR:CB	2.58	0.51
4:D:191:ALA:C	4:D:193:THR:H	2.12	0.51
4:D:29:LEU:HD13	7:G:82:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.92	0.51
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.10	0.51
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.38	0.51
1:A:72:GLU:OE2	2:B:1175:LEU:HB2	2.11	0.51
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.91	0.51
2:B:388:CYS:C	2:B:390:LEU:H	2.13	0.51
2:B:37:PHE:HD2	2:B:542:MET:SD	2.33	0.51
2:B:882:THR:O	2:B:883:LEU:HB2	2.10	0.51
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.93	0.51
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.10	0.51
4:D:50:LEU:HD13	4:D:55:ALA:HA	1.93	0.51
2:B:902:GLY:O	12:L:65:VAL:HG11	2.11	0.51
13:N:0:DT:H71	13:N:1:DA:N6	2.24	0.51
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.10	0.51
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.40	0.51
1:A:982:THR:HG22	1:A:984:LYS:H	1.75	0.51
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.45	0.51
2:B:483:LEU:CD1	2:B:491:THR:HG23	2.39	0.51
3:C:56:THR:HG21	3:C:145:CYS:SG	2.51	0.51
7:G:16:SER:HB3	7:G:17:PHE:CD2	2.46	0.51
2:B:852:ARG:NH2	12:L:70:ARG:OXT	2.37	0.51
1:A:2:VAL:HG21	2:B:1157:ALA:C	2.31	0.51
1:A:55:ASP:CG	1:A:55:ASP:O	2.46	0.51
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.46	0.51
2:B:46:GLN:HG3	2:B:47:GLN:N	2.18	0.51
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.11	0.51
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.92	0.51
1:A:626:ASN:O	1:A:631:HIS:HD2	1.93	0.51
1:A:527:THR:HG21	1:A:650:GLN:HA	1.91	0.51
1:A:834:THR:O	1:A:837:ILE:HB	2.10	0.51
2:B:226:PHE:HA	2:B:395:GLN:CG	2.40	0.51
2:B:769:TYR:C	2:B:771:SER:N	2.62	0.51
8:H:58:THR:HB	8:H:143:LEU:HD13	1.93	0.51
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.41	0.51
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.41	0.51
1:A:332:LYS:HG3	1:A:333:GLU:N	2.26	0.51
1:A:730:GLY:C	1:A:732:LEU:N	2.62	0.51
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.91	0.51
2:B:360:PHE:CD2	2:B:360:PHE:C	2.84	0.51
2:B:434:ARG:HA	2:B:437:GLU:OE2	2.10	0.51
2:B:711:GLU:H	2:B:712:PRO:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:825:VAL:HG13	2:B:826:ALA:H	1.76	0.51
3:C:174:ALA:O	10:J:10:CYS:O	2.29	0.51
10:J:36:LEU:HA	10:J:39:LEU:HD12	1.91	0.51
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.26	0.51
1:A:84:ILE:CG2	1:A:84:ILE:O	2.58	0.51
2:B:27:ALA:O	2:B:29:ASP:N	2.44	0.51
2:B:310:MET:CE	2:B:387:LEU:HD12	2.37	0.51
2:B:616:ILE:HG13	2:B:697:GLU:HG3	1.92	0.51
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.43	0.51
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.11	0.51
3:C:77:ILE:HG22	3:C:78:GLU:N	2.26	0.51
8:H:89:LEU:C	8:H:91:ASP:H	2.13	0.51
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.11	0.51
1:A:1362:TYR:HD1	1:A:1363:VAL:N	2.08	0.51
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.11	0.51
1:A:33:ALA:O	1:A:83:HIS:HD2	1.93	0.51
2:B:955:THR:CG2	2:B:956:THR:H	2.19	0.51
4:D:177:VAL:O	4:D:177:VAL:HG12	2.11	0.51
5:E:9:ILE:CD1	5:E:53:PRO:HD3	2.40	0.51
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.93	0.51
1:A:23:SER:O	1:A:24:PRO:C	2.48	0.50
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.41	0.50
1:A:366:VAL:HG21	1:A:460:VAL:HG22	1.93	0.50
2:B:123:THR:O	2:B:125:SER:N	2.44	0.50
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.45	0.50
2:B:552:MET:HA	2:B:555:ILE:HB	1.93	0.50
7:G:1:MET:O	7:G:3:PHE:CD1	2.65	0.50
7:G:1:MET:SD	7:G:1:MET:C	2.89	0.50
11:K:68:PHE:N	11:K:68:PHE:HD2	2.08	0.50
1:A:284:ALA:O	1:A:286:HIS:N	2.36	0.50
1:A:464:PRO:O	1:A:465:TYR:O	2.29	0.50
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.42	0.50
1:A:64:ASN:O	1:A:65:LEU:C	2.50	0.50
2:B:778:MET:HE2	2:B:1094:ARG:CD	2.41	0.50
2:B:43:LEU:HD13	2:B:812:LEU:HD23	1.93	0.50
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.93	0.50
6:F:77:ASP:O	6:F:78:GLN:HB2	2.11	0.50
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.93	0.50
7:G:13:LEU:O	7:G:67:SER:HA	2.12	0.50
8:H:40:LEU:HD22	8:H:123:MET:CE	2.40	0.50
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:737:THR:CG2	9:I:66:PRO:HA	2.38	0.50
1:A:1135:ARG:HH21	1:A:1284:MET:HG3	1.77	0.50
1:A:316:GLN:O	1:A:317:LYS:C	2.49	0.50
1:A:362:ASP:OD2	1:A:459:ARG:HD3	2.10	0.50
1:A:919:ILE:O	1:A:920:LEU:C	2.50	0.50
2:B:1099:VAL:O	2:B:1101:ASP:N	2.44	0.50
2:B:654:ARG:O	2:B:656:GLY:N	2.45	0.50
2:B:955:THR:CG2	2:B:956:THR:N	2.74	0.50
5:E:35:VAL:O	5:E:37:LEU:N	2.44	0.50
9:I:111:THR:CG2	9:I:112:SER:H	2.22	0.50
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.76	0.50
1:A:244:PRO:O	1:A:247:ARG:N	2.43	0.50
1:A:252:PHE:HB2	1:A:256:GLN:NE2	2.27	0.50
1:A:262:LEU:O	1:A:264:PHE:N	2.45	0.50
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.32	0.50
1:A:710:LEU:HD12	1:A:710:LEU:N	2.27	0.50
1:A:786:HIS:CD2	1:A:786:HIS:N	2.79	0.50
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.93	0.50
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.27	0.50
2:B:515:HIS:N	2:B:518:HIS:HD2	1.98	0.50
3:C:179:GLU:HG2	3:C:180:TYR:H	1.77	0.50
3:C:89:GLU:O	3:C:90:ASP:HB3	2.11	0.50
4:D:51:ASN:O	4:D:54:GLU:HB3	2.10	0.50
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.93	0.50
9:I:61:ASP:C	9:I:63:GLY:N	2.63	0.50
11:K:47:ARG:HD2	11:K:47:ARG:C	2.32	0.50
1:A:23:SER:HA	1:A:233:TRP:NE1	2.27	0.50
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.76	0.50
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.73	0.50
2:B:1102:LYS:O	2:B:1103:ILE:C	2.49	0.50
2:B:298:LEU:HD13	2:B:314:LEU:HD13	1.92	0.50
2:B:44:VAL:O	2:B:45:SER:C	2.49	0.50
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.40	0.50
3:C:112:ASN:N	3:C:112:ASN:HD22	2.07	0.50
3:C:140:ASN:O	3:C:141:GLY:O	2.29	0.50
4:D:27:LEU:HD22	4:D:173:HIS:CD2	2.46	0.50
6:F:114:GLU:OE2	6:F:119:ARG:HG2	2.12	0.50
6:F:82:THR:HG22	6:F:84:TYR:N	2.23	0.50
1:A:310:GLY:O	1:A:312:PRO:HD2	2.12	0.50
1:A:432:VAL:O	1:A:433:GLU:C	2.49	0.50
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ARG:NH2	1:A:797:LYS:HG3	2.27	0.50
1:A:58:LEU:HD11	1:A:80:HIS:H	1.76	0.50
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.11	0.50
1:A:960:ILE:O	1:A:961:ARG:C	2.50	0.50
2:B:192:LEU:O	2:B:193:LYS:HB2	2.12	0.50
2:B:510:LYS:HG3	2:B:511:PRO:CD	2.38	0.50
3:C:69:LEU:HD12	3:C:69:LEU:H	1.76	0.50
4:D:24:ALA:C	4:D:26:THR:H	2.15	0.50
5:E:131:THR:HG21	5:E:191:LYS:NZ	2.26	0.50
7:G:96:GLN:HB3	7:G:121:PHE:CE2	2.47	0.50
7:G:88:ASP:HA	7:G:144:ARG:HA	1.92	0.50
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.24	0.50
1:A:269:ILE:CD1	1:A:300:VAL:HA	2.41	0.50
1:A:350:ARG:HA	1:A:468:PHE:HE1	1.77	0.50
1:A:55:ASP:HA	1:A:58:LEU:HB3	1.94	0.50
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.42	0.50
2:B:329:THR:O	2:B:332:ASP:HB3	2.12	0.50
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.59	0.50
6:F:69:LEU:N	6:F:70:LYS:HA	2.26	0.50
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.11	0.50
1:A:130:ASP:O	1:A:131:SER:C	2.50	0.50
1:A:95:PHE:CZ	1:A:1414:ALA:HB2	2.47	0.50
1:A:195:ASP:O	1:A:196:GLU:HB3	2.12	0.50
1:A:265:LYS:HZ3	1:A:322:VAL:HG22	1.75	0.50
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.39	0.50
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.93	0.50
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.94	0.50
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.92	0.50
3:C:22:LEU:HD13	3:C:230:MET:CE	2.42	0.50
4:D:64:VAL:C	4:D:66:ARG:H	2.14	0.50
7:G:18:PHE:HA	7:G:22:MET:HE2	1.93	0.50
12:L:55:ILE:O	12:L:56:LEU:HB2	2.11	0.50
1:A:250:ILE:CD1	14:P:0:U:H1'	2.41	0.50
1:A:58:LEU:HG	1:A:59:GLY:N	2.26	0.50
1:A:853:ASP:C	1:A:853:ASP:OD1	2.50	0.50
2:B:1033:LYS:NZ	2:B:1068:GLY:O	2.45	0.50
2:B:847:ASP:C	2:B:849:GLY:H	2.14	0.50
15:T:19:TT:H2'1	15:T:19:TT:C5R	2.42	0.50
1:A:116:ASP:C	1:A:118:HIS:N	2.66	0.49
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.12	0.49
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.94	0.49
2:B:122:LEU:O	2:B:206:ASN:HA	2.12	0.49
2:B:220:GLY:O	2:B:222:ILE:HG13	2.12	0.49
2:B:365:THR:HG23	2:B:367:LEU:N	2.21	0.49
2:B:549:THR:N	2:B:628:THR:HG23	2.25	0.49
2:B:899:ILE:CG2	2:B:903:VAL:HB	2.42	0.49
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.93	0.49
7:G:59:GLY:CA	7:G:70:PHE:CD2	2.94	0.49
1:A:1329:THR:CG2	1:A:1331:SER:H	2.22	0.49
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.93	0.49
1:A:541:ILE:HG21	1:A:549:MET:CE	2.39	0.49
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.94	0.49
1:A:867:ILE:CG2	1:A:872:GLY:N	2.75	0.49
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.93	0.49
2:B:549:THR:H	2:B:628:THR:CG2	2.22	0.49
3:C:74:SER:HB2	3:C:77:ILE:HG12	1.93	0.49
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.47	0.49
8:H:116:TYR:HE2	8:H:140:ALA:HB1	1.76	0.49
9:I:58:VAL:HG12	9:I:58:VAL:O	2.11	0.49
14:P:5:C:C2'	14:P:6:C:H5'	2.41	0.49
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.42	0.49
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.93	0.49
1:A:947:PHE:CD2	1:A:954:TRP:CE2	3.00	0.49
2:B:199:MET:CE	2:B:492:LEU:HD23	2.43	0.49
2:B:792:MET:HG3	2:B:855:PHE:CE1	2.47	0.49
4:D:14:ARG:N	4:D:17:LYS:HZ3	2.10	0.49
4:D:40:HIS:CG	4:D:41:GLN:N	2.80	0.49
4:D:57:LEU:O	4:D:61:GLU:HB2	2.12	0.49
6:F:143:PHE:C	6:F:143:PHE:CD1	2.85	0.49
7:G:9:LEU:HD12	7:G:10:ASN:H	1.77	0.49
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.42	0.49
15:T:19:TT:H2'1	15:T:19:TT:C3R	2.42	0.49
1:A:1115:SER:OG	1:A:1116:LEU:N	2.45	0.49
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.78	0.49
1:A:767:GLN:HA	1:A:799:PHE:HA	1.94	0.49
2:B:1159:ARG:HD2	2:B:1159:ARG:C	2.33	0.49
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.24	0.49
2:B:980:PHE:HE2	2:B:1094:ARG:HB2	1.78	0.49
3:C:123:ASN:HD21	3:C:125:MET:HA	1.78	0.49
3:C:254:LYS:O	3:C:256:ALA:N	2.45	0.49
5:E:55:ARG:O	5:E:57:MET:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:26:LEU:O	7:G:27:LYS:C	2.50	0.49
7:G:4:ILE:O	7:G:4:ILE:HG22	2.12	0.49
10:J:7:CYS:SG	10:J:8:PHE:N	2.85	0.49
11:K:12:LEU:HD12	11:K:12:LEU:N	2.22	0.49
12:L:34:CYS:O	12:L:36:SER:N	2.46	0.49
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.11	0.49
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.27	0.49
1:A:335:ARG:HH11	2:B:1202:LEU:HD13	1.76	0.49
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.47	0.49
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.95	0.49
3:C:241:ASP:OD1	3:C:242:GLN:N	2.39	0.49
3:C:73:GLN:NE2	3:C:75:MET:N	2.57	0.49
4:D:176:GLU:HB3	4:D:198:LEU:HD21	1.94	0.49
4:D:59:ILE:O	4:D:60:LYS:C	2.50	0.49
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.26	0.49
7:G:15:PRO:O	7:G:16:SER:C	2.50	0.49
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.42	0.49
8:H:18:GLY:O	8:H:19:ARG:HB2	2.12	0.49
9:I:84:VAL:HG13	9:I:84:VAL:O	2.13	0.49
12:L:38:LEU:O	12:L:39:SER:CB	2.60	0.49
1:A:1139:GLU:O	1:A:1275:GLY:HA3	2.12	0.49
1:A:224:PHE:CZ	1:A:234:MET:HE2	2.47	0.49
1:A:93:VAL:HG21	1:A:301:ALA:O	2.13	0.49
1:A:534:LEU:HG	1:A:534:LEU:O	2.11	0.49
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.94	0.49
2:B:294:ASP:O	2:B:296:GLU:N	2.43	0.49
4:D:156:ASP:C	4:D:158:GLU:H	2.15	0.49
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.42	0.49
1:A:1017:LEU:CB	5:E:205:SER:HA	2.42	0.49
2:B:309:GLN:HG3	9:I:52:ILE:HD11	1.94	0.49
3:C:66:ARG:HH12	10:J:2:ILE:HG21	1.75	0.49
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.95	0.49
15:T:17:DT:H2''	15:T:18:DT:O5'	2.12	0.49
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.12	0.49
1:A:1364:ASN:O	1:A:1365:TYR:C	2.51	0.49
1:A:147:VAL:O	1:A:149:GLU:N	2.46	0.49
1:A:381:THR:HG23	1:A:383:TYR:H	1.78	0.49
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.43	0.49
1:A:837:ILE:HA	1:A:840:ARG:HD3	1.95	0.49
2:B:1068:GLY:O	2:B:1069:PHE:O	2.31	0.49
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:TYR:HD1	2:B:259:TYR:H	1.60	0.49
1:A:658:LEU:HD13	2:B:831:SER:N	2.27	0.49
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.27	0.49
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.28	0.49
4:D:53:SER:HB3	4:D:152:SER:CA	2.42	0.49
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.24	0.49
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.45	0.49
1:A:166:GLY:O	1:A:167:CYS:CB	2.60	0.49
1:A:966:ASN:O	1:A:967:ALA:C	2.51	0.49
2:B:1010:LEU:HD23	2:B:1092:TYR:CD1	2.47	0.49
2:B:1084:GLN:HE21	2:B:1084:GLN:N	2.10	0.49
2:B:472:ALA:C	2:B:474:SER:H	2.14	0.49
2:B:46:GLN:CG	2:B:47:GLN:H	2.20	0.49
2:B:758:PHE:N	2:B:759:PRO:CD	2.76	0.49
2:B:769:TYR:C	2:B:771:SER:H	2.16	0.49
3:C:129:ILE:HG23	3:C:130:GLY:N	2.26	0.49
3:C:161:LYS:O	3:C:170:TRP:NE1	2.46	0.49
3:C:254:LYS:C	3:C:256:ALA:H	2.16	0.49
1:A:1334:ASP:O	1:A:1336:MET:N	2.46	0.49
1:A:1389:PHE:CD1	1:A:1390:ASN:N	2.81	0.49
1:A:401:GLY:C	1:A:435:HIS:CD2	2.86	0.49
1:A:50:ILE:C	1:A:52:GLY:N	2.65	0.49
1:A:50:ILE:O	1:A:52:GLY:N	2.45	0.49
1:A:699:ALA:O	1:A:700:ASN:CB	2.60	0.49
1:A:894:GLU:HG3	1:A:933:TYR:OH	2.12	0.49
2:B:180:TYR:N	2:B:180:TYR:CD1	2.81	0.49
2:B:23:ALA:H	2:B:654:ARG:HB3	1.78	0.49
2:B:801:LYS:O	10:J:52:THR:HG23	2.13	0.49
2:B:843:GLN:O	2:B:844:SER:C	2.50	0.49
2:B:843:GLN:O	2:B:846:ILE:N	2.45	0.49
2:B:910:VAL:HG12	2:B:911:ILE:N	2.28	0.49
3:C:191:TYR:CD2	3:C:201:TRP:CD1	3.01	0.49
3:C:208:GLU:C	3:C:210:GLU:H	2.15	0.49
4:D:135:GLY:C	4:D:137:ASN:H	2.15	0.49
1:A:1446:ASP:HB2	6:F:133:VAL:CG2	2.43	0.49
10:J:27:GLU:O	10:J:29:GLU:N	2.40	0.49
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.78	0.49
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.94	0.49
1:A:577:ILE:HG13	1:A:578:LEU:N	2.27	0.49
1:A:901:LEU:HD22	1:A:919:ILE:HG21	1.95	0.49
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1214:PRO:O	2:B:1214:PRO:HG2	2.13	0.49
2:B:222:ILE:O	2:B:240:ILE:HA	2.13	0.49
2:B:386:LEU:O	2:B:387:LEU:C	2.50	0.49
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.61	0.49
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.28	0.49
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.41	0.49
11:K:52:ASN:O	11:K:53:ASP:C	2.51	0.49
1:A:862:ASN:O	1:A:864:ILE:HG13	2.12	0.48
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	1.95	0.48
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.42	0.48
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.95	0.48
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.94	0.48
2:B:863:GLU:O	2:B:961:LEU:HD22	2.12	0.48
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.94	0.48
5:E:136:ASN:OD1	5:E:137:GLU:N	2.46	0.48
9:I:60:GLN:NE2	9:I:107:SER:OG	2.46	0.48
3:C:35:ARG:HH11	11:K:41:THR:N	2.10	0.48
12:L:31:CYS:SG	12:L:34:CYS:N	2.84	0.48
1:A:1115:SER:HB3	1:A:1330:ASN:HD21	1.78	0.48
1:A:1219:THR:HG21	1:A:1271:ILE:CD1	2.43	0.48
1:A:1349:TYR:CA	1:A:1372:VAL:HG21	2.43	0.48
1:A:388:LEU:CD2	1:A:432:VAL:HB	2.43	0.48
1:A:710:LEU:HD12	1:A:710:LEU:H	1.78	0.48
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.78	0.48
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.95	0.48
2:B:1070:GLU:OE1	10:J:44:TYR:OH	2.30	0.48
2:B:1095:LEU:CD1	2:B:1095:LEU:H	2.16	0.48
2:B:1182:CYS:O	2:B:1183:LYS:C	2.51	0.48
2:B:203:PHE:N	2:B:203:PHE:CD1	2.81	0.48
2:B:33:VAL:O	2:B:36:ALA:HB3	2.13	0.48
2:B:344:LYS:O	2:B:345:LYS:HG3	2.13	0.48
2:B:799:PRO:CB	2:B:818:PRO:HG2	2.43	0.48
2:B:978:ASP:O	2:B:989:THR:HB	2.12	0.48
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.94	0.48
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.95	0.48
5:E:10:SER:O	5:E:14:ARG:HG3	2.11	0.48
9:I:69:PRO:HB2	9:I:85:PHE:CE2	2.48	0.48
1:A:1059:HIS:O	1:A:1060:PRO:C	2.52	0.48
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.42	0.48
1:A:300:VAL:O	1:A:300:VAL:HG12	2.11	0.48
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:PHE:CD2	1:A:954:TRP:CZ2	3.02	0.48
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.95	0.48
2:B:254:LEU:HD23	2:B:381:MET:HE3	1.94	0.48
2:B:343:ILE:HB	2:B:348:ARG:HG3	1.95	0.48
8:H:11:GLN:O	8:H:28:ALA:HB1	2.13	0.48
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.95	0.48
12:L:47:ARG:HH21	12:L:54:ARG:NH2	2.11	0.48
13:N:5:DA:H2''	13:N:6:DC:OP2	2.12	0.48
1:A:108:MET:SD	1:A:210:ILE:HD13	2.53	0.48
1:A:718:VAL:O	1:A:721:PHE:HB2	2.12	0.48
1:A:913:LEU:CD1	1:A:914:GLU:N	2.71	0.48
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.41	0.48
2:B:363:HIS:O	2:B:364:ILE:CB	2.55	0.48
2:B:429:PHE:HA	2:B:432:MET:HE3	1.96	0.48
2:B:604:ARG:O	2:B:606:LYS:N	2.46	0.48
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.93	0.48
2:B:758:PHE:CE2	2:B:1044:ALA:CA	2.92	0.48
7:G:117:GLN:C	7:G:119:LEU:H	2.17	0.48
7:G:80:LYS:CD	7:G:80:LYS:N	2.73	0.48
1:A:701:LEU:HD23	9:I:115:LYS:HG3	1.95	0.48
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.78	0.48
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.76	0.48
1:A:43:GLU:O	1:A:44:THR:CB	2.61	0.48
1:A:936:LEU:O	1:A:939:ASP:HB2	2.13	0.48
2:B:34:ILE:O	2:B:35:SER:C	2.52	0.48
2:B:37:PHE:HE1	2:B:41:LYS:CD	2.26	0.48
2:B:810:GLU:HB3	2:B:811:TYR:CE1	2.48	0.48
2:B:899:ILE:HD13	2:B:905:VAL:CG1	2.43	0.48
3:C:209:TYR:H	3:C:209:TYR:HD1	1.58	0.48
7:G:20:PRO:CG	7:G:21:ARG:H	2.26	0.48
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.49	0.48
1:A:399:HIS:CB	1:A:400:PRO:CD	2.88	0.48
1:A:420:ARG:O	1:A:421:ALA:C	2.50	0.48
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.95	0.48
1:A:535:THR:HG22	1:A:536:LEU:N	2.27	0.48
1:A:603:ASN:O	1:A:604:GLY:C	2.51	0.48
2:B:128:LEU:HB2	2:B:168:GLY:O	2.13	0.48
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.78	0.48
2:B:769:TYR:O	2:B:771:SER:N	2.47	0.48
9:I:71:SER:OG	9:I:83:ASN:HB2	2.13	0.48
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LEU:HD12	1:A:504:LEU:N	2.28	0.48
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.84	0.48
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.49	0.48
2:B:213:ILE:O	2:B:215:GLN:HG2	2.13	0.48
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.29	0.48
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.78	0.48
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.44	0.48
3:C:215:GLU:O	3:C:216:GLY:C	2.51	0.48
3:C:88:CYS:SG	3:C:91:HIS:HA	2.53	0.48
6:F:85:MET:CE	6:F:93:ILE:HD12	2.44	0.48
7:G:20:PRO:HG2	7:G:21:ARG:N	2.28	0.48
8:H:63:LEU:HD22	8:H:90:ALA:HB3	1.96	0.48
9:I:85:PHE:N	9:I:85:PHE:CD2	2.68	0.48
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.95	0.48
1:A:1259:MET:C	1:A:1261:LYS:H	2.16	0.48
1:A:844:ALA:O	1:A:845:LEU:HD23	2.13	0.48
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.96	0.48
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.49	0.48
2:B:683:SER:C	2:B:685:LEU:H	2.15	0.48
1:A:701:LEU:HD23	9:I:115:LYS:CG	2.44	0.48
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.21	0.48
1:A:1373:ASP:O	1:A:1376:THR:HG23	2.14	0.48
1:A:218:ASP:O	1:A:219:PHE:O	2.32	0.48
1:A:353:ILE:HB	1:A:470:LEU:CD2	2.43	0.48
1:A:427:GLN:O	1:A:428:TYR:C	2.52	0.48
1:A:618:GLU:O	1:A:619:LYS:C	2.52	0.48
1:A:666:ILE:HD12	1:A:667:GLY:N	2.25	0.48
1:A:71:GLN:C	1:A:73:GLY:H	2.16	0.48
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.95	0.48
2:B:175:ARG:NH1	2:B:175:ARG:HG2	2.27	0.48
2:B:575:PRO:HG2	2:B:576:ASP:H	1.79	0.48
2:B:970:THR:HG22	2:B:971:THR:N	2.28	0.48
3:C:82:TYR:O	3:C:83:SER:C	2.51	0.48
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.29	0.48
11:K:110:ASN:C	11:K:111:LEU:HG	2.34	0.48
1:A:130:ASP:O	1:A:133:LYS:N	2.38	0.48
1:A:1325:THR:CG2	1:A:1325:THR:O	2.61	0.48
1:A:21:LEU:HG	1:A:1413:GLY:O	2.14	0.48
1:A:1445:ILE:N	1:A:1445:ILE:CD1	2.68	0.48
2:B:259:TYR:N	2:B:259:TYR:CD1	2.82	0.48
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:LEU:O	2:B:447:ALA:CB	2.62	0.48
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.49	0.48
2:B:653:VAL:HG22	2:B:689:LEU:HD13	1.95	0.48
2:B:899:ILE:HD12	2:B:911:ILE:HG23	1.95	0.48
3:C:235:VAL:HG13	10:J:13:VAL:HG23	1.95	0.48
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.95	0.48
5:E:180:ARG:NH2	5:E:192:ARG:HB2	2.25	0.48
1:A:1446:ASP:HB2	6:F:133:VAL:HG23	1.96	0.48
8:H:111:LEU:HD23	8:H:127:GLY:O	2.14	0.48
10:J:23:ASN:O	10:J:25:LEU:N	2.47	0.48
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.96	0.48
1:A:1387:HIS:CE1	13:N:4:DT:H5"	2.48	0.48
1:A:1377:THR:HA	5:E:212:ARG:HH21	1.79	0.47
1:A:1377:THR:O	1:A:1378:GLN:C	2.52	0.47
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.13	0.47
1:A:541:ILE:HD13	1:A:549:MET:HE3	1.93	0.47
2:B:1047:PHE:N	2:B:1047:PHE:CD1	2.76	0.47
2:B:1099:VAL:HG12	2:B:1100:ASP:H	1.79	0.47
2:B:247:GLY:C	2:B:249:ARG:N	2.67	0.47
2:B:310:MET:O	2:B:313:MET:HB2	2.14	0.47
2:B:579:ARG:N	2:B:589:VAL:HG13	2.29	0.47
2:B:30:SER:HB3	2:B:743:ILE:O	2.14	0.47
3:C:31:ASN:O	3:C:34:ARG:HB3	2.14	0.47
7:G:35:GLU:CG	7:G:48:VAL:HG23	2.44	0.47
1:A:789:LYS:HE3	9:I:67:THR:OG1	2.14	0.47
11:K:19:LEU:HD22	11:K:33:ILE:CG2	2.43	0.47
3:C:29:MET:HE1	11:K:98:LEU:HG	1.95	0.47
1:A:224:PHE:CE2	1:A:231:PRO:HA	2.49	0.47
1:A:401:GLY:C	1:A:435:HIS:HD2	2.16	0.47
1:A:600:PRO:C	1:A:602:ASP:H	2.16	0.47
2:B:1050:ILE:HG22	2:B:1051:THR:H	1.79	0.47
1:A:466:SER:HB2	2:B:1099:VAL:HG11	1.96	0.47
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.94	0.47
2:B:185:THR:O	2:B:188:ASP:HB2	2.13	0.47
2:B:205:ILE:N	2:B:205:ILE:HD12	2.28	0.47
2:B:459:TYR:CD2	2:B:459:TYR:C	2.88	0.47
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.49	0.47
3:C:31:ASN:O	3:C:32:SER:C	2.51	0.47
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.95	0.47
1:A:399:HIS:CG	1:A:400:PRO:N	2.81	0.47
1:A:722:LEU:O	1:A:725:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1033:LYS:CE	2:B:1070:GLU:OE1	2.62	0.47
2:B:1031:LEU:HA	2:B:1055:ILE:HD13	1.96	0.47
2:B:1147:LEU:HD23	2:B:1147:LEU:C	2.35	0.47
2:B:100:PRO:HD3	2:B:172:ILE:HD12	1.96	0.47
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.49	0.47
2:B:882:THR:CB	2:B:934:LYS:O	2.62	0.47
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.95	0.47
3:C:242:GLN:C	3:C:244:VAL:H	2.16	0.47
3:C:36:VAL:HG11	3:C:251:LEU:HB2	1.96	0.47
7:G:115:MET:CB	7:G:116:PRO:HD2	2.44	0.47
7:G:154:VAL:HG12	7:G:155:SER:H	1.79	0.47
7:G:25:TYR:O	7:G:28:THR:HB	2.14	0.47
8:H:26:ILE:CG2	8:H:27:GLU:N	2.77	0.47
8:H:31:THR:O	8:H:31:THR:HG22	2.13	0.47
1:A:325:ILE:O	1:A:326:ARG:C	2.52	0.47
1:A:500:GLU:O	1:A:504:LEU:HD13	2.14	0.47
1:A:735:VAL:HG12	1:A:735:VAL:O	2.14	0.47
1:A:770:VAL:HA	1:A:822:GLU:OE1	2.14	0.47
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.27	0.47
2:B:1110:PRO:HB2	2:B:1119:VAL:HG21	1.96	0.47
2:B:1162:ILE:C	2:B:1171:VAL:HG21	2.34	0.47
2:B:298:LEU:N	2:B:298:LEU:CD2	2.77	0.47
2:B:696:GLU:O	2:B:699:GLU:HB2	2.14	0.47
3:C:242:GLN:HB3	3:C:246:ARG:HG3	1.97	0.47
3:C:254:LYS:C	3:C:256:ALA:N	2.67	0.47
7:G:34:VAL:HG12	7:G:45:ILE:CG2	2.39	0.47
11:K:40:HIS:O	11:K:41:THR:C	2.53	0.47
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	2.13	0.47
1:A:326:ARG:HG2	1:A:327:ALA:N	2.30	0.47
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.30	0.47
1:A:921:GLY:O	1:A:922:ASP:C	2.52	0.47
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.29	0.47
2:B:841:MET:SD	2:B:846:ILE:HD11	2.54	0.47
14:P:7:A:C2'	14:P:8:G:O4'	2.62	0.47
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.14	0.47
1:A:1356:ILE:O	1:A:1356:ILE:HG22	2.14	0.47
1:A:88:LYS:HE3	1:A:280:GLU:OE2	2.15	0.47
1:A:331:GLY:O	1:A:332:LYS:HB3	2.15	0.47
1:A:369:SER:HB2	11:K:2:ASN:OD1	2.15	0.47
1:A:867:ILE:HG22	1:A:872:GLY:H	1.79	0.47
2:B:1064:TYR:O	2:B:1065:GLN:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.96	0.47
2:B:386:LEU:O	2:B:389:ALA:N	2.47	0.47
2:B:794:ASN:C	2:B:795:ILE:HD12	2.35	0.47
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.50	0.47
7:G:3:PHE:CG	7:G:80:LYS:NZ	2.73	0.47
8:H:142:LEU:C	8:H:143:LEU:HD12	2.35	0.47
9:I:33:SER:O	9:I:34:TYR:O	2.32	0.47
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.30	0.47
12:L:30:ILE:HG22	12:L:31:CYS:N	2.29	0.47
12:L:61:THR:HG22	12:L:63:ARG:HG2	1.96	0.47
1:A:243:PRO:O	1:A:244:PRO:C	2.53	0.47
1:A:298:PHE:O	1:A:301:ALA:HB3	2.13	0.47
1:A:339:ASN:O	1:A:343:LYS:HG2	2.14	0.47
1:A:350:ARG:HG3	1:A:350:ARG:HH11	1.79	0.47
1:A:41:MET:HB3	1:A:48:ALA:O	2.15	0.47
1:A:888:GLY:O	1:A:940:ARG:NH2	2.48	0.47
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	2.14	0.47
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.30	0.47
4:D:119:ARG:HG2	4:D:120:GLU:N	2.29	0.47
4:D:134:THR:CG2	4:D:135:GLY:H	2.26	0.47
4:D:191:ALA:O	4:D:193:THR:N	2.47	0.47
8:H:93:TYR:N	8:H:93:TYR:CD1	2.82	0.47
1:A:1151:GLU:HB3	1:A:1153:TYR:HE1	1.79	0.47
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.13	0.47
1:A:1313:LEU:HD23	1:A:1338:VAL:CB	2.45	0.47
1:A:402:ALA:CB	1:A:434:ARG:HA	2.45	0.47
1:A:565:ILE:O	1:A:570:PRO:HA	2.14	0.47
1:A:829:VAL:C	1:A:831:THR:N	2.68	0.47
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.97	0.47
1:A:982:THR:H	1:A:985:ASP:CB	2.27	0.47
2:B:839:MET:HB3	2:B:1012:ILE:HG22	1.96	0.47
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.15	0.47
2:B:37:PHE:CD2	2:B:542:MET:SD	3.08	0.47
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.97	0.47
2:B:950:ASP:O	2:B:951:GLN:HB2	2.15	0.47
5:E:31:THR:O	5:E:35:VAL:HG23	2.13	0.47
5:E:84:ASP:O	5:E:86:PRO:HD3	2.15	0.47
6:F:88:TYR:N	6:F:88:TYR:CD1	2.83	0.47
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.95	0.47
8:H:128:ASN:O	8:H:128:ASN:OD1	2.32	0.47
8:H:55:LEU:HD22	8:H:144:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:52:ASN:O	11:K:54:ARG:N	2.48	0.47
11:K:89:ASN:O	11:K:92:ASN:N	2.48	0.47
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.97	0.47
1:A:1323:ASP:C	1:A:1325:THR:H	2.18	0.47
1:A:37:PHE:HD1	1:A:37:PHE:N	2.13	0.47
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.50	0.47
1:A:632:VAL:O	1:A:633:VAL:C	2.53	0.47
1:A:63:ARG:HA	1:A:74:MET:HE2	1.95	0.47
1:A:774:ARG:H	1:A:774:ARG:HG2	1.42	0.47
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.72	0.47
2:B:949:VAL:HG12	2:B:950:ASP:N	2.29	0.47
4:D:20:GLU:HA	4:D:20:GLU:OE2	2.14	0.47
5:E:175:LEU:HD23	5:E:176:PRO:HD2	1.95	0.47
7:G:1:MET:SD	7:G:79:PHE:CE1	3.08	0.47
10:J:7:CYS:SG	10:J:49:MET:HE3	2.54	0.47
11:K:12:LEU:H	11:K:12:LEU:CD1	2.24	0.47
12:L:60:ARG:HG2	12:L:61:THR:H	1.80	0.47
1:A:42:ASP:HA	1:A:46:THR:O	2.15	0.47
1:A:853:ASP:O	1:A:854:ASN:HB2	2.15	0.47
1:A:901:LEU:N	1:A:926:GLN:HE21	2.08	0.47
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.80	0.47
2:B:1107:ALA:O	2:B:1108:ARG:HG2	2.15	0.47
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.50	0.47
2:B:582:VAL:HA	2:B:626:ILE:O	2.15	0.47
2:B:730:ARG:O	2:B:731:VAL:O	2.33	0.47
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.50	0.47
3:C:168:ALA:O	3:C:170:TRP:N	2.48	0.47
7:G:25:TYR:HE2	7:G:29:LYS:HD2	1.80	0.47
11:K:101:LEU:HD23	11:K:101:LEU:O	2.15	0.47
1:A:1280:GLU:O	1:A:1281:ARG:O	2.33	0.47
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.96	0.47
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.30	0.47
1:A:43:GLU:O	1:A:44:THR:HB	2.15	0.47
1:A:588:LEU:O	1:A:606:LEU:HD12	2.14	0.47
1:A:1410:PHE:HD2	2:B:1212:ILE:HD12	1.80	0.47
2:B:388:CYS:C	2:B:390:LEU:N	2.67	0.47
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.51	0.47
2:B:461:LEU:N	2:B:461:LEU:HD12	2.29	0.47
5:E:205:SER:O	5:E:206:GLY:C	2.52	0.47
7:G:23:LYS:HG3	7:G:56:ILE:HD12	1.96	0.47
11:K:111:LEU:O	11:K:112:GLN:CG	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:THR:O	1:A:278:THR:HG22	2.15	0.46
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.80	0.46
2:B:640:VAL:HG12	2:B:640:VAL:O	2.16	0.46
2:B:999:MET:HA	2:B:999:MET:CE	2.45	0.46
3:C:146:LYS:C	3:C:147:LEU:HD23	2.36	0.46
3:C:256:ALA:C	3:C:258:ILE:N	2.68	0.46
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.15	0.46
7:G:39:THR:CG2	7:G:40:GLY:H	2.26	0.46
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.45	0.46
8:H:42:ILE:O	8:H:44:VAL:HG23	2.15	0.46
1:A:698:GLN:HA	9:I:97:MET:O	2.14	0.46
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.15	0.46
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.98	0.46
1:A:224:PHE:HZ	1:A:234:MET:CE	2.27	0.46
1:A:353:ILE:HG21	1:A:487:MET:CG	2.41	0.46
1:A:586:ILE:CD1	1:A:633:VAL:HG22	2.45	0.46
2:B:1109:GLY:O	2:B:1110:PRO:C	2.54	0.46
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.45	0.46
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.97	0.46
2:B:823:ALA:O	2:B:825:VAL:N	2.48	0.46
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.15	0.46
1:A:253:ASN:HB3	2:B:935:ARG:NH1	2.30	0.46
6:F:123:LYS:O	6:F:124:GLU:C	2.54	0.46
8:H:4:THR:HG22	8:H:5:LEU:N	2.29	0.46
10:J:16:ASP:O	10:J:18:TRP:N	2.48	0.46
11:K:42:LEU:HD21	11:K:46:ILE:HD11	1.96	0.46
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.50	0.46
15:T:11:DG:H2"	15:T:12:DT:OP2	2.15	0.46
1:A:1175:SER:O	1:A:1176:LEU:HB2	2.15	0.46
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.30	0.46
1:A:1193:LEU:HD22	1:A:1260:LEU:HD11	1.97	0.46
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.96	0.46
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.50	0.46
1:A:289:ILE:C	1:A:291:GLU:N	2.68	0.46
1:A:438:ASP:OD1	1:A:461:LYS:HA	2.15	0.46
1:A:634:THR:HG1	1:A:642:CYS:HG	1.63	0.46
1:A:967:ALA:O	1:A:968:GLN:O	2.33	0.46
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.40	0.46
2:B:185:THR:N	2:B:188:ASP:HB2	2.27	0.46
2:B:230:ALA:N	2:B:231:PRO:CD	2.78	0.46
2:B:467:GLY:N	2:B:475:SER:CB	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:821:GLN:NE2	2:B:851:PHE:HA	2.23	0.46
2:B:861:ASP:OD1	2:B:862:GLN:N	2.48	0.46
3:C:141:GLY:HA2	10:J:16:ASP:HB3	1.97	0.46
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.30	0.46
4:D:156:ASP:C	4:D:158:GLU:N	2.69	0.46
4:D:54:GLU:O	4:D:58:VAL:HG23	2.14	0.46
7:G:1:MET:CE	7:G:1:MET:O	2.64	0.46
9:I:98:VAL:HG11	9:I:113:ASP:OD1	2.15	0.46
1:A:1219:THR:HG21	1:A:1271:ILE:HG13	1.97	0.46
1:A:261:ASP:O	1:A:264:PHE:HB2	2.15	0.46
1:A:393:ARG:O	1:A:395:GLY:N	2.49	0.46
1:A:42:ASP:C	1:A:44:THR:N	2.68	0.46
1:A:499:ALA:O	1:A:503:GLN:HG2	2.15	0.46
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.15	0.46
2:B:383:ASN:O	2:B:384:ARG:C	2.53	0.46
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.45	0.46
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.14	0.46
2:B:683:SER:O	2:B:685:LEU:N	2.48	0.46
2:B:990:ILE:CG2	2:B:991:GLY:N	2.78	0.46
3:C:123:ASN:ND2	3:C:125:MET:SD	2.89	0.46
4:D:10:THR:O	4:D:10:THR:HG23	2.16	0.46
4:D:151:PHE:N	4:D:151:PHE:CD1	2.83	0.46
5:E:16:PHE:HZ	5:E:20:LYS:HE2	1.77	0.46
5:E:67:GLU:O	5:E:70:SER:HB3	2.15	0.46
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.97	0.46
11:K:10:PHE:CD1	11:K:11:LEU:CD2	2.99	0.46
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.96	0.46
1:A:114:LEU:O	1:A:115:LEU:HG	2.14	0.46
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.64	0.46
1:A:167:CYS:SG	1:A:167:CYS:O	2.73	0.46
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.50	0.46
1:A:34:LYS:HB3	1:A:36:ARG:NE	2.31	0.46
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.98	0.46
1:A:470:LEU:HD22	1:A:487:MET:CE	2.46	0.46
1:A:637:LYS:CB	1:A:641:VAL:HG11	2.45	0.46
2:B:388:CYS:O	2:B:390:LEU:N	2.49	0.46
2:B:604:ARG:C	2:B:606:LYS:H	2.18	0.46
2:B:520:GLY:N	2:B:748:ILE:HG22	2.29	0.46
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.98	0.46
3:C:152:GLU:OE2	3:C:154:LYS:HE3	2.15	0.46
8:H:123:MET:HE3	8:H:142:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:51:ASN:O	9:I:54:GLU:HG3	2.16	0.46
1:A:1053:PHE:O	1:A:1055:ARG:N	2.49	0.46
1:A:560:ILE:HG12	1:A:560:ILE:H	1.46	0.46
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.80	0.46
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.46	0.46
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.97	0.46
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.76	0.46
2:B:763:GLN:C	2:B:765:PRO:HD2	2.36	0.46
2:B:814:PHE:C	2:B:816:GLU:N	2.69	0.46
3:C:115:SER:HB3	3:C:142:VAL:HB	1.98	0.46
3:C:168:ALA:C	3:C:170:TRP:N	2.68	0.46
3:C:87:PHE:CD1	3:C:87:PHE:N	2.84	0.46
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.96	0.46
5:E:207:ARG:CB	5:E:207:ARG:NH1	2.78	0.46
7:G:138:THR:CG2	7:G:139:ILE:N	2.68	0.46
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.79	0.46
3:C:175:ALA:HB3	10:J:43:ARG:HH22	1.81	0.46
11:K:85:ASP:O	11:K:88:LYS:HB2	2.15	0.46
1:A:23:SER:CB	1:A:233:TRP:NE1	2.79	0.46
1:A:34:LYS:NZ	1:A:57:ARG:CZ	2.79	0.46
1:A:566:ILE:O	1:A:567:LYS:O	2.34	0.46
1:A:826:ASP:O	1:A:827:THR:C	2.52	0.46
2:B:244:LEU:C	2:B:246:LYS:N	2.68	0.46
2:B:360:PHE:O	2:B:361:LEU:C	2.54	0.46
2:B:801:LYS:O	10:J:52:THR:CG2	2.64	0.46
2:B:859:TYR:OH	2:B:941:LEU:CD1	2.60	0.46
3:C:114:TYR:HB3	3:C:140:ASN:O	2.16	0.46
9:I:115:LYS:HD3	9:I:117:LYS:CE	2.38	0.46
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.45	0.46
10:J:27:GLU:C	10:J:29:GLU:H	2.17	0.46
1:A:1385:THR:O	1:A:1388:GLY:N	2.46	0.46
1:A:1418:LEU:HD12	1:A:1419:ASP:N	2.30	0.46
1:A:262:LEU:C	1:A:264:PHE:N	2.69	0.46
1:A:49:LYS:NZ	1:A:61:ILE:CG1	2.74	0.46
1:A:652:VAL:O	1:A:653:VAL:C	2.55	0.46
1:A:7:SER:C	1:A:9:ALA:H	2.19	0.46
1:A:835:GLY:HA3	15:T:19:TT:O1P	2.16	0.46
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.43	0.46
4:D:64:VAL:O	4:D:66:ARG:N	2.49	0.46
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.50	0.46
7:G:106:MET:CG	7:G:107:LYS:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:LEU:HB3	7:G:82:PHE:HE2	1.81	0.46
1:A:1152:ILE:HG13	9:I:44:TYR:HD2	1.81	0.46
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.15	0.46
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.51	0.46
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.51	0.46
1:A:494:SER:O	1:A:497:THR:N	2.49	0.46
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.46	0.46
2:B:1110:PRO:HG3	2:B:1125:ASP:HB3	1.98	0.46
1:A:343:LYS:HZ3	2:B:1197:PRO:HB3	1.81	0.46
14:P:8:G:H2'	14:P:9:A:C8	2.51	0.46
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.16	0.46
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.97	0.46
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.15	0.46
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.16	0.46
1:A:241:VAL:HG13	1:A:266:LEU:HD13	1.97	0.46
1:A:474:VAL:C	1:A:477:PRO:HD2	2.36	0.46
1:A:639:PRO:HG2	1:A:640:GLN:H	1.81	0.46
1:A:818:MET:HA	2:B:514:LEU:HB3	1.98	0.46
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.98	0.46
2:B:1045:SER:O	2:B:1046:PRO:O	2.34	0.46
2:B:244:LEU:O	2:B:246:LYS:N	2.49	0.46
2:B:210:LYS:HG3	2:B:461:LEU:O	2.16	0.46
2:B:510:LYS:CG	2:B:511:PRO:CD	2.82	0.46
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.80	0.46
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.51	0.46
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.98	0.46
12:L:49:LYS:O	12:L:50:ASP:CB	2.63	0.46
1:A:332:LYS:NZ	15:T:19:TT:H7C2	2.31	0.46
1:A:244:PRO:HG2	1:A:245:PRO:CD	2.46	0.45
1:A:695:LYS:C	1:A:697:ALA:N	2.69	0.45
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.49	0.45
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.33	0.45
1:A:514:PRO:CB	1:A:875:ALA:HB3	2.47	0.45
1:A:981:LEU:HD21	1:A:1038:THR:C	2.36	0.45
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.30	0.45
2:B:37:PHE:HE2	2:B:542:MET:HA	1.81	0.45
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.46	0.45
3:C:41:ILE:HD11	3:C:247:GLY:CA	2.46	0.45
3:C:73:GLN:NE2	3:C:74:SER:H	2.14	0.45
12:L:40:LEU:HB3	12:L:41:SER:H	1.68	0.45
12:L:55:ILE:H	12:L:55:ILE:HG12	1.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.16	0.45
1:A:1445:ILE:HG12	7:G:18:PHE:HE2	1.78	0.45
1:A:409:SER:O	1:A:410:GLY:C	2.54	0.45
1:A:800:VAL:HA	1:A:812:GLU:OE2	2.16	0.45
1:A:874:ASP:O	1:A:876:ALA:N	2.49	0.45
2:B:102:VAL:HG12	2:B:104:GLU:HG2	1.98	0.45
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.37	0.45
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.97	0.45
3:C:167:HIS:ND1	12:L:70:ARG:HB3	2.31	0.45
2:B:798:TYR:CE2	3:C:62:PHE:CZ	3.04	0.45
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.51	0.45
4:D:52:LEU:C	4:D:54:GLU:N	2.69	0.45
7:G:22:MET:O	7:G:23:LYS:C	2.54	0.45
7:G:39:THR:O	7:G:43:GLY:HA2	2.15	0.45
14:P:2:C:O2'	14:P:3:G:H5'	2.16	0.45
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.98	0.45
1:A:1381:LEU:HA	1:A:1381:LEU:HD23	1.77	0.45
1:A:332:LYS:C	1:A:334:GLY:H	2.20	0.45
1:A:500:GLU:OE2	2:B:1145:SER:N	2.49	0.45
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.48	0.45
1:A:71:GLN:HG3	1:A:72:GLU:N	2.31	0.45
1:A:730:GLY:O	1:A:733:ALA:N	2.49	0.45
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.16	0.45
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.82	0.45
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.16	0.45
1:A:1171:GLN:HA	1:A:1174:PHE:HD1	1.80	0.45
1:A:1394:THR:O	1:A:1395:GLY:O	2.34	0.45
1:A:361:LEU:HA	1:A:471:ASN:ND2	2.31	0.45
1:A:370:ILE:O	1:A:371:ALA:C	2.52	0.45
1:A:915:SER:O	1:A:919:ILE:HG13	2.16	0.45
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.47	0.45
2:B:1184:GLY:C	2:B:1186:ASP:H	2.16	0.45
2:B:96:TYR:HE1	2:B:131:ASP:OD2	1.99	0.45
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.97	0.45
2:B:364:ILE:CG1	2:B:585:VAL:HG13	2.38	0.45
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.80	0.45
3:C:184:ASN:HD21	3:C:187:LYS:HA	1.80	0.45
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.51	0.45
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.51	0.45
9:I:29:CYS:SG	9:I:31:THR:N	2.86	0.45
10:J:45:CYS:O	10:J:48:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:6:DC:H1'	13:N:7:DT:H5'	1.97	0.45
1:A:1111:MET:HE3	1:A:1113:THR:O	2.16	0.45
1:A:396:PRO:HG3	1:A:416:ARG:HB3	1.97	0.45
1:A:885:THR:O	1:A:885:THR:HG22	2.16	0.45
2:B:1182:CYS:O	2:B:1183:LYS:O	2.35	0.45
3:C:113:VAL:CG2	3:C:147:LEU:HD21	2.47	0.45
3:C:22:LEU:HD13	3:C:230:MET:HE1	1.99	0.45
3:C:242:GLN:C	3:C:244:VAL:N	2.70	0.45
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.52	0.45
5:E:156:LEU:HD12	5:E:195:VAL:CB	2.47	0.45
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.99	0.45
11:K:11:LEU:N	11:K:11:LEU:HD22	2.32	0.45
11:K:65:HIS:CG	11:K:66:PRO:HD2	2.51	0.45
2:B:833:TYR:CZ	11:K:66:PRO:HG3	2.51	0.45
12:L:27:LEU:N	12:L:27:LEU:HD23	2.32	0.45
1:A:11:LEU:HB2	2:B:1193:GLN:OE1	2.16	0.45
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.52	0.45
1:A:381:THR:HG23	1:A:382:PRO:CD	2.47	0.45
1:A:32:VAL:HG21	1:A:68:GLN:NE2	2.32	0.45
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.50	0.45
2:B:502:ILE:CD1	2:B:502:ILE:N	2.78	0.45
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.80	0.45
3:C:123:ASN:ND2	3:C:125:MET:CG	2.79	0.45
3:C:176:ILE:CG2	3:C:177:GLU:N	2.79	0.45
3:C:190:ASP:O	3:C:191:TYR:C	2.55	0.45
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.34	0.45
3:C:20:PHE:HE1	3:C:22:LEU:CD1	2.30	0.45
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.84	0.45
8:H:99:GLY:HA3	8:H:117:SER:O	2.17	0.45
10:J:43:ARG:O	10:J:47:ARG:HB2	2.17	0.45
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.16	0.45
1:A:19:PHE:HE1	1:A:1396:ALA:HB3	1.82	0.45
1:A:23:SER:O	1:A:26:GLU:N	2.49	0.45
2:B:1060:ARG:C	2:B:1062:HIS:H	2.19	0.45
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.99	0.45
2:B:58:THR:O	2:B:62:ILE:HG13	2.17	0.45
2:B:999:MET:HE2	2:B:1000:PRO:CD	2.47	0.45
8:H:4:THR:HG22	8:H:5:LEU:H	1.81	0.45
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.52	0.45
11:K:15:GLY:O	11:K:16:GLU:HG3	2.17	0.45
1:A:166:GLY:O	1:A:167:CYS:SG	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.47	0.45
2:B:1006:ILE:HD13	10:J:44:TYR:CZ	2.51	0.45
2:B:1031:LEU:HD11	2:B:1042:GLY:HA3	1.99	0.45
2:B:223:VAL:HG21	2:B:380:TYR:CE2	2.51	0.45
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.52	0.45
2:B:800:GLN:O	2:B:801:LYS:C	2.55	0.45
2:B:839:MET:HE3	2:B:1010:LEU:CD2	2.44	0.45
2:B:860:MET:CG	2:B:861:ASP:N	2.80	0.45
3:C:99:LEU:HD23	3:C:99:LEU:N	2.32	0.45
5:E:124:VAL:HB	5:E:125:PRO:CD	2.47	0.45
12:L:36:SER:O	12:L:37:LYS:C	2.54	0.45
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	1.99	0.45
1:A:120:GLU:HA	1:A:123:ARG:HG3	1.99	0.45
1:A:1211:GLN:O	1:A:1212:VAL:C	2.55	0.45
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.52	0.45
1:A:482:PHE:O	1:A:484:GLY:N	2.49	0.45
1:A:508:PRO:O	1:A:511:ILE:HG13	2.16	0.45
1:A:549:MET:SD	1:A:577:ILE:CD1	3.04	0.45
1:A:666:ILE:CD1	1:A:667:GLY:N	2.80	0.45
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.81	0.45
2:B:360:PHE:CD2	2:B:361:LEU:HB2	2.51	0.45
2:B:582:VAL:HG12	2:B:587:HIS:NE2	2.32	0.45
2:B:802:PRO:HB3	2:B:1091:TYR:CD2	2.51	0.45
2:B:911:ILE:O	2:B:911:ILE:HG22	2.17	0.45
2:B:954:VAL:HA	2:B:964:VAL:HG22	1.98	0.45
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.51	0.45
9:I:34:TYR:O	9:I:35:VAL:HG23	2.17	0.45
9:I:70:ARG:HH11	9:I:84:VAL:HB	1.81	0.45
11:K:82:ASP:O	11:K:85:ASP:HB2	2.17	0.45
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.99	0.45
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.17	0.45
1:A:1333:ILE:HG22	1:A:1334:ASP:N	2.32	0.45
1:A:313:GLN:O	1:A:314:ALA:HB3	2.17	0.45
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.52	0.45
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.38	0.45
1:A:710:LEU:HD13	9:I:94:ASP:O	2.16	0.45
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.16	0.45
2:B:19:GLU:O	2:B:20:ASP:C	2.55	0.45
2:B:405:ARG:HA	2:B:631:GLY:O	2.16	0.45
3:C:215:GLU:O	3:C:217:ASP:N	2.50	0.45
3:C:27:LEU:HD13	3:C:228:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:24:LYS:CG	5:E:25:ASP:N	2.79	0.45
5:E:29:PHE:C	5:E:30:ILE:HG13	2.37	0.45
7:G:20:PRO:CG	7:G:21:ARG:N	2.80	0.45
8:H:10:PHE:CE1	8:H:57:VAL:HB	2.52	0.45
8:H:138:GLU:O	8:H:139:ASN:C	2.54	0.45
11:K:31:VAL:O	11:K:74:ARG:HA	2.17	0.45
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.51	0.44
2:B:1138:MET:HA	2:B:1138:MET:CE	2.38	0.44
2:B:118:ARG:CG	2:B:204:ILE:HD13	2.47	0.44
2:B:295:GLY:O	2:B:299:GLU:HG3	2.18	0.44
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.44	0.44
2:B:364:ILE:HG12	2:B:585:VAL:CG1	2.38	0.44
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.99	0.44
3:C:35:ARG:HH11	11:K:41:THR:HA	1.81	0.44
4:D:33:PHE:CZ	7:G:80:LYS:HE3	2.53	0.44
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.52	0.44
5:E:163:GLU:O	5:E:166:LYS:N	2.50	0.44
6:F:109:VAL:HG12	6:F:110:ASP:N	2.31	0.44
7:G:7:LEU:O	7:G:73:LYS:HD2	2.17	0.44
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.99	0.44
7:G:9:LEU:HD23	7:G:30:LEU:HD12	2.00	0.44
10:J:56:LEU:O	10:J:59:LYS:N	2.44	0.44
11:K:35:PHE:CD1	11:K:71:PHE:CE1	3.05	0.44
15:T:16:DT:H1'	15:T:17:DT:H5'	1.98	0.44
1:A:1213:GLY:O	1:A:1214:GLU:C	2.56	0.44
1:A:1265:ASN:O	1:A:1268:LEU:N	2.47	0.44
1:A:285:PRO:O	1:A:287:HIS:N	2.50	0.44
1:A:34:LYS:CB	1:A:36:ARG:HE	2.28	0.44
1:A:469:ARG:NH2	2:B:991:GLY:O	2.50	0.44
1:A:567:LYS:HE3	8:H:46:LEU:CB	2.42	0.44
1:A:572:TRP:HA	1:A:576:GLN:OE1	2.17	0.44
1:A:67:CYS:O	1:A:68:GLN:CB	2.65	0.44
1:A:75:ASN:O	1:A:76:GLU:HB2	2.17	0.44
2:B:283:VAL:O	2:B:286:PHE:N	2.50	0.44
2:B:25:ILE:HD11	2:B:653:VAL:C	2.37	0.44
5:E:30:ILE:HG22	5:E:31:THR:N	2.31	0.44
6:F:90:ARG:CG	6:F:91:ALA:N	2.81	0.44
8:H:143:LEU:N	8:H:143:LEU:CD1	2.79	0.44
8:H:91:ASP:O	8:H:93:TYR:N	2.50	0.44
11:K:6:ARG:O	11:K:8:GLU:N	2.50	0.44
2:B:776:GLN:NE2	14:P:8:G:H5'	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:HH12	15:T:18:DT:P	2.39	0.44
1:A:1265:ASN:C	1:A:1267:MET:N	2.69	0.44
1:A:524:VAL:HG12	1:A:525:GLN:HE21	1.81	0.44
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.52	0.44
2:B:847:ASP:C	2:B:849:GLY:N	2.71	0.44
2:B:848:ARG:HD2	10:J:7:CYS:O	2.18	0.44
2:B:893:LEU:HD22	2:B:897:GLY:C	2.38	0.44
3:C:45:ALA:HA	3:C:72:LEU:CD1	2.47	0.44
5:E:147:HIS:CD2	5:E:149:LEU:H	2.35	0.44
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.17	0.44
6:F:77:ASP:C	6:F:79:ARG:N	2.70	0.44
7:G:106:MET:HG2	7:G:107:LYS:N	2.31	0.44
7:G:117:GLN:C	7:G:119:LEU:N	2.71	0.44
7:G:1:MET:SD	7:G:79:PHE:HD1	2.40	0.44
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.52	0.44
9:I:78:CYS:HB3	9:I:106:CYS:SG	2.58	0.44
9:I:55:THR:O	9:I:55:THR:HG22	2.18	0.44
10:J:56:LEU:O	10:J:57:ILE:C	2.54	0.44
10:J:57:ILE:HA	10:J:60:PHE:HB2	1.98	0.44
15:T:15:DT:H6	15:T:15:DT:H2'	1.61	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.99	0.44
1:A:1334:ASP:O	1:A:1337:GLU:N	2.50	0.44
1:A:1389:PHE:C	1:A:1389:PHE:CD1	2.90	0.44
1:A:260:ASP:O	1:A:261:ASP:C	2.56	0.44
1:A:42:ASP:O	1:A:44:THR:N	2.38	0.44
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.52	0.44
1:A:825:ILE:O	1:A:826:ASP:C	2.55	0.44
2:B:1223:ASP:HB3	2:B:1224:PHE:H	1.58	0.44
2:B:240:ILE:O	2:B:240:ILE:HG23	2.17	0.44
3:C:239:PRO:O	3:C:240:VAL:C	2.55	0.44
3:C:3:GLU:O	3:C:4:GLU:HG3	2.18	0.44
4:D:7:THR:HG23	4:D:7:THR:O	2.17	0.44
7:G:91:VAL:HG12	7:G:92:VAL:N	2.32	0.44
9:I:50:THR:HG22	9:I:51:ASN:N	2.32	0.44
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.17	0.44
1:A:401:GLY:O	1:A:435:HIS:CD2	2.71	0.44
1:A:404:TYR:CE2	1:A:414:ASP:HA	2.53	0.44
1:A:415:LEU:HA	1:A:415:LEU:HD23	1.69	0.44
1:A:452:LYS:HB3	1:A:452:LYS:HE2	1.71	0.44
1:A:506:ALA:O	1:A:509:LEU:HB2	2.17	0.44
1:A:806:ARG:NH1	2:B:729:ILE:HG13	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:VAL:C	1:A:831:THR:H	2.20	0.44
1:A:979:SER:HG	1:A:981:LEU:HG	1.80	0.44
1:A:929:LEU:CD2	1:A:983:ILE:HG21	2.48	0.44
1:A:996:ASN:C	1:A:998:LEU:HD12	2.36	0.44
2:B:1099:VAL:C	2:B:1101:ASP:H	2.21	0.44
2:B:1152:MET:HE1	2:B:1157:ALA:HA	1.99	0.44
2:B:313:MET:HE2	2:B:386:LEU:HD22	2.00	0.44
2:B:43:LEU:HD11	2:B:811:TYR:O	2.17	0.44
2:B:210:LYS:HA	2:B:481:GLN:O	2.18	0.44
2:B:487:THR:CG2	2:B:488:TYR:N	2.81	0.44
2:B:560:GLU:O	2:B:561:TRP:CD1	2.71	0.44
3:C:18:VAL:O	3:C:20:PHE:CD2	2.70	0.44
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.53	0.44
4:D:146:GLN:O	4:D:149:THR:HG22	2.17	0.44
4:D:27:LEU:HG	4:D:197:SER:HB2	1.98	0.44
5:E:161:LYS:C	5:E:163:GLU:N	2.69	0.44
5:E:23:VAL:HG13	5:E:78:LEU:HD13	2.00	0.44
5:E:48:ASP:CG	5:E:49:SER:N	2.69	0.44
7:G:73:LYS:HE2	7:G:74:TYR:O	2.18	0.44
11:K:82:ASP:OD1	11:K:84:LYS:N	2.46	0.44
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.32	0.44
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.82	0.44
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.33	0.44
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.99	0.44
1:A:56:PRO:O	1:A:57:ARG:HG3	2.18	0.44
1:A:664:THR:CG2	1:A:665:GLY:N	2.80	0.44
1:A:68:GLN:C	1:A:70:CYS:N	2.66	0.44
1:A:816:HIS:CD2	2:B:764:SER:H	2.36	0.44
1:A:986:ILE:HD12	1:A:1032:LEU:HD11	1.98	0.44
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.48	0.44
2:B:314:LEU:O	2:B:317:CYS:HB3	2.17	0.44
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.89	0.44
2:B:782:LEU:CD1	2:B:788:ARG:HH11	2.29	0.44
3:C:44:LEU:HD21	3:C:159:ALA:HB1	1.99	0.44
3:C:77:ILE:C	3:C:79:GLN:H	2.21	0.44
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.99	0.44
11:K:18:LYS:NZ	11:K:37:LYS:O	2.51	0.44
1:A:1062:GLU:OE2	6:F:88:TYR:OH	2.35	0.44
1:A:577:ILE:O	1:A:578:LEU:C	2.52	0.44
1:A:673:GLY:O	1:A:676:MET:HB2	2.17	0.44
1:A:709:THR:CG2	1:A:710:LEU:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLN:C	1:A:73:GLY:N	2.71	0.44
2:B:293:PRO:HG2	2:B:296:GLU:HB3	2.00	0.44
2:B:591:ARG:O	2:B:592:ASN:C	2.55	0.44
2:B:682:SER:O	2:B:685:LEU:HB3	2.17	0.44
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.99	0.44
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.81	0.44
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.33	0.44
3:C:259:LEU:CD1	11:K:91:CYS:HB2	2.47	0.44
5:E:90:VAL:O	5:E:90:VAL:HG22	2.17	0.44
6:F:89:GLU:HB3	6:F:134:ILE:HD13	2.00	0.44
7:G:29:LYS:O	7:G:30:LEU:C	2.54	0.44
9:I:15:TYR:HD1	9:I:15:TYR:N	2.14	0.44
9:I:32:CYS:SG	9:I:33:SER:N	2.90	0.44
9:I:70:ARG:NH1	9:I:84:VAL:HB	2.33	0.44
14:P:4:A:C2'	14:P:5:C:H5'	2.47	0.44
15:T:18:DT:C3'	15:T:19:TT:C5'	2.96	0.44
1:A:1094:VAL:CG1	1:A:1095:THR:N	2.63	0.44
1:A:113:LEU:HG	1:A:218:ASP:OD1	2.17	0.44
1:A:719:VAL:O	1:A:721:PHE:N	2.51	0.44
1:A:760:GLN:HG2	1:A:765:VAL:O	2.17	0.44
2:B:1087:PHE:CD2	2:B:1088:GLY:N	2.76	0.44
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.99	0.44
2:B:259:TYR:HD1	2:B:259:TYR:N	2.16	0.44
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.45	0.44
5:E:197:LYS:HE2	5:E:199:ILE:HD11	2.00	0.44
7:G:125:SER:OG	7:G:128:PRO:HA	2.18	0.44
9:I:110:PHE:H	9:I:110:PHE:HD2	1.66	0.44
1:A:548:ASN:OD1	11:K:60:ALA:HB1	2.18	0.44
13:N:3:DG:H2''	13:N:4:DT:OP2	2.18	0.44
1:A:1385:THR:C	1:A:1387:HIS:N	2.70	0.44
1:A:34:LYS:H	1:A:57:ARG:HH21	1.66	0.44
1:A:388:LEU:HD22	1:A:432:VAL:HG21	2.00	0.44
1:A:523:ILE:HG22	1:A:528:LEU:HB2	2.00	0.44
1:A:34:LYS:HZ1	1:A:57:ARG:NH1	2.15	0.44
1:A:773:LYS:HG3	1:A:773:LYS:H	1.49	0.44
1:A:82:GLY:O	1:A:241:VAL:N	2.37	0.44
2:B:1135:ARG:O	2:B:1136:ASP:C	2.56	0.44
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.17	0.44
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.53	0.44
2:B:343:ILE:HG21	2:B:348:ARG:CA	2.47	0.44
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.48	0.44
3:C:36:VAL:HG21	3:C:251:LEU:HD22	2.00	0.44
3:C:255:VAL:O	3:C:255:VAL:HG12	2.18	0.44
3:C:70:ILE:HG22	3:C:70:ILE:O	2.17	0.44
6:F:128:LYS:HD3	6:F:149:GLU:O	2.18	0.44
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.99	0.44
7:G:31:LEU:CD2	7:G:48:VAL:HG21	2.48	0.44
7:G:39:THR:CG2	7:G:40:GLY:N	2.76	0.44
8:H:40:LEU:HG	8:H:41:ASP:O	2.18	0.44
14:P:5:C:C2'	14:P:6:C:O4'	2.55	0.44
1:A:230:ARG:N	1:A:233:TRP:CE3	2.65	0.43
1:A:242:PRO:HA	1:A:243:PRO:HD2	1.75	0.43
1:A:265:LYS:CE	1:A:322:VAL:HG13	2.47	0.43
1:A:37:PHE:H	1:A:37:PHE:HD1	1.65	0.43
1:A:783:THR:CG2	1:A:815:PHE:CE2	3.00	0.43
1:A:935:GLN:O	1:A:936:LEU:C	2.56	0.43
2:B:1183:LYS:HE3	2:B:1183:LYS:N	2.33	0.43
2:B:377:PHE:CD2	2:B:381:MET:HE2	2.53	0.43
2:B:465:ASN:N	2:B:465:ASN:ND2	2.64	0.43
2:B:640:VAL:HB	2:B:738:PHE:O	2.19	0.43
3:C:107:SER:C	3:C:109:SER:H	2.21	0.43
2:B:798:TYR:CE2	3:C:62:PHE:CE2	3.06	0.43
2:B:798:TYR:HE2	3:C:62:PHE:HZ	1.63	0.43
4:D:18:VAL:O	4:D:19:GLU:HB3	2.18	0.43
5:E:157:SER:O	5:E:159:ASP:N	2.51	0.43
6:F:75:PRO:HG2	6:F:78:GLN:HB2	2.00	0.43
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.83	0.43
7:G:80:LYS:O	7:G:82:PHE:CE1	2.71	0.43
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.47	0.43
1:A:442:VAL:O	1:A:457:ALA:HA	2.17	0.43
1:A:474:VAL:HG22	1:A:474:VAL:O	2.19	0.43
1:A:577:ILE:O	1:A:580:VAL:HG23	2.18	0.43
1:A:907:THR:HG22	1:A:908:LEU:N	2.33	0.43
1:A:935:GLN:O	1:A:938:LYS:N	2.50	0.43
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.48	0.43
2:B:331:LEU:HD12	2:B:331:LEU:N	2.33	0.43
2:B:449:ASN:O	2:B:451:LYS:N	2.51	0.43
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.74	0.43
2:B:642:ASP:HB3	2:B:649:LYS:HG3	2.00	0.43
3:C:249:ASP:O	3:C:252:GLN:HB3	2.18	0.43
4:D:122:GLU:HA	4:D:125:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:LEU:HA	4:D:141:LEU:HD12	1.80	0.43
6:F:111:LEU:C	6:F:113:GLY:N	2.70	0.43
9:I:7:CYS:HB2	9:I:34:TYR:CD1	2.53	0.43
1:A:547:LEU:HB3	11:K:58:PHE:CE1	2.52	0.43
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.32	0.43
15:T:24:DG:C2'	15:T:25:DT:O5'	2.63	0.43
1:A:1243:VAL:HG12	1:A:1244:ARG:N	2.32	0.43
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.19	0.43
1:A:1341:ILE:O	1:A:1344:GLY:N	2.51	0.43
1:A:1450:LEU:HD11	6:F:108:PHE:HZ	1.79	0.43
1:A:248:PRO:O	1:A:260:ASP:HB2	2.18	0.43
1:A:699:ALA:HB2	9:I:114:GLN:NE2	2.32	0.43
1:A:780:VAL:O	1:A:782:ARG:HG2	2.18	0.43
2:B:234:ILE:HD12	2:B:234:ILE:N	2.33	0.43
2:B:616:ILE:CD1	2:B:616:ILE:N	2.81	0.43
2:B:707:PRO:O	2:B:711:GLU:HG3	2.18	0.43
2:B:34:ILE:HD13	2:B:747:MET:HE2	1.99	0.43
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.84	0.43
3:C:8:VAL:HG12	3:C:9:LYS:H	1.83	0.43
4:D:209:ARG:O	4:D:212:LYS:HB2	2.19	0.43
7:G:17:PHE:C	7:G:19:GLY:H	2.20	0.43
7:G:99:PHE:CD1	7:G:99:PHE:C	2.91	0.43
8:H:59:ILE:O	8:H:60:ALA:HB3	2.18	0.43
9:I:85:PHE:CD1	9:I:99:LEU:HD13	2.54	0.43
1:A:1213:GLY:O	1:A:1216:ILE:N	2.52	0.43
1:A:1305:VAL:CG1	1:A:1306:LEU:N	2.81	0.43
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.99	0.43
1:A:388:LEU:HD22	1:A:432:VAL:HB	1.99	0.43
1:A:353:ILE:CG2	1:A:487:MET:HG3	2.45	0.43
1:A:347:PHE:CE2	1:A:493:GLN:OE1	2.72	0.43
1:A:546:VAL:O	1:A:546:VAL:HG12	2.18	0.43
1:A:639:PRO:HG2	1:A:640:GLN:N	2.33	0.43
1:A:699:ALA:HB1	9:I:114:GLN:HB2	2.00	0.43
1:A:802:ASN:ND2	1:A:812:GLU:OE1	2.42	0.43
2:B:114:PRO:HG2	2:B:115:GLN:N	2.28	0.43
2:B:1156:ASP:O	2:B:1157:ALA:O	2.37	0.43
2:B:1181:GLU:O	2:B:1182:CYS:HB2	2.17	0.43
2:B:281:PRO:O	2:B:282:ILE:C	2.56	0.43
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.34	0.43
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.48	0.43
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:661:LEU:C	2:B:663:ALA:N	2.70	0.43
2:B:681:TRP:O	2:B:684:LEU:N	2.51	0.43
2:B:957:ASN:O	2:B:960:GLY:N	2.47	0.43
2:B:997:GLU:H	2:B:997:GLU:CD	2.22	0.43
4:D:55:ALA:HB3	4:D:148:LEU:HD21	1.99	0.43
5:E:88:VAL:HG12	5:E:89:GLY:N	2.33	0.43
7:G:26:LEU:HA	7:G:26:LEU:HD23	1.85	0.43
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.99	0.43
8:H:23:VAL:HG22	8:H:43:ASN:HA	2.00	0.43
15:T:10:DA:HI'	15:T:11:DG:C8	2.54	0.43
2:B:1123:SER:HB3	15:T:24:DG:P	2.58	0.43
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.48	0.43
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	2.00	0.43
1:A:1316:VAL:HG12	1:A:1316:VAL:O	2.19	0.43
1:A:1404:GLU:O	1:A:1407:GLU:HB2	2.18	0.43
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.89	0.43
1:A:608:ILE:HG13	1:A:613:ILE:HD12	2.01	0.43
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.52	0.43
1:A:92:HIS:O	1:A:93:VAL:C	2.56	0.43
1:A:958:VAL:HG12	1:A:960:ILE:HG13	2.01	0.43
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	2.00	0.43
2:B:496:ARG:NH1	2:B:496:ARG:HB3	2.33	0.43
2:B:765:PRO:O	2:B:768:THR:N	2.51	0.43
3:C:213:PRO:O	3:C:214:ASN:CB	2.60	0.43
3:C:86:CYS:O	3:C:88:CYS:N	2.52	0.43
4:D:51:ASN:C	4:D:52:LEU:O	2.56	0.43
5:E:153:HIS:O	5:E:154:ILE:CG1	2.67	0.43
5:E:46:TYR:CE2	5:E:58:MET:HA	2.54	0.43
6:F:118:LEU:HG	6:F:118:LEU:O	2.18	0.43
7:G:9:LEU:HD12	7:G:10:ASN:N	2.34	0.43
10:J:34:THR:O	10:J:35:ALA:C	2.56	0.43
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.34	0.43
13:N:0:DT:O4	15:T:18:DT:O2	2.35	0.43
1:A:335:ARG:N	1:A:339:ASN:HD22	2.17	0.43
1:A:47:ARG:O	1:A:48:ALA:HB2	2.18	0.43
1:A:618:GLU:OE2	1:A:620:LYS:HB2	2.19	0.43
1:A:723:ASN:C	1:A:725:ALA:N	2.72	0.43
1:A:795:GLU:CD	1:A:795:GLU:H	2.22	0.43
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	2.00	0.43
2:B:247:GLY:O	2:B:249:ARG:N	2.51	0.43
2:B:628:THR:CG2	2:B:628:THR:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:825:VAL:HG12	2:B:826:ALA:N	2.33	0.43
2:B:857:ARG:HH21	2:B:942:ARG:NH1	2.16	0.43
3:C:189:THR:CG2	3:C:190:ASP:N	2.81	0.43
4:D:13:ARG:HB2	4:D:17:LYS:NZ	2.34	0.43
4:D:47:LEU:CD1	4:D:48:ILE:N	2.81	0.43
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.46	0.43
5:E:136:ASN:OD1	5:E:138:ALA:N	2.52	0.43
6:F:121:ALA:O	6:F:122:MET:C	2.57	0.43
7:G:99:PHE:CZ	7:G:143:ILE:HD13	2.54	0.43
9:I:33:SER:O	9:I:35:VAL:HG23	2.18	0.43
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.32	0.43
1:A:1313:LEU:HD23	1:A:1338:VAL:HB	2.01	0.43
1:A:1362:TYR:HD1	1:A:1363:VAL:H	1.65	0.43
1:A:1385:THR:O	1:A:1386:ARG:C	2.57	0.43
1:A:265:LYS:HE2	1:A:322:VAL:HG13	1.98	0.43
1:A:696:GLU:HG2	1:A:696:GLU:O	2.18	0.43
1:A:857:ARG:NH2	6:F:139:PRO:HG3	2.33	0.43
1:A:877:HIS:O	1:A:878:ILE:HG12	2.19	0.43
2:B:1184:GLY:C	2:B:1186:ASP:N	2.68	0.43
2:B:189:LEU:O	2:B:190:TYR:C	2.55	0.43
2:B:258:LEU:HG	2:B:258:LEU:O	2.18	0.43
2:B:29:ASP:HB3	2:B:658:ILE:HD11	1.99	0.43
2:B:410:GLY:O	2:B:412:LEU:N	2.52	0.43
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.31	0.43
2:B:895:ASP:C	2:B:897:GLY:H	2.22	0.43
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.84	0.43
3:C:69:LEU:HB3	10:J:6:ARG:HD3	1.99	0.43
4:D:71:LYS:HA	4:D:74:GLN:CB	2.46	0.43
7:G:112:LYS:NZ	7:G:120:THR:HA	2.33	0.43
11:K:44:ASN:N	11:K:61:TYR:CE1	2.87	0.43
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	2.01	0.43
1:A:35:ILE:HB	1:A:83:HIS:O	2.18	0.43
2:B:515:HIS:O	2:B:518:HIS:HB2	2.19	0.43
2:B:583:ASN:OD1	2:B:628:THR:N	2.50	0.43
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.99	0.43
7:G:51:TYR:O	7:G:51:TYR:CD2	2.71	0.43
12:L:43:THR:O	12:L:43:THR:HG22	2.19	0.43
1:A:370:ILE:O	1:A:373:THR:N	2.43	0.43
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.37	0.43
1:A:506:ALA:C	1:A:508:PRO:HD2	2.39	0.43
1:A:570:PRO:O	1:A:571:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:O	1:A:78:PRO:HD3	2.19	0.43
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.63	0.43
2:B:1064:TYR:O	2:B:1065:GLN:O	2.37	0.43
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.33	0.43
2:B:1147:LEU:CD2	2:B:1151:LEU:HD22	2.48	0.43
2:B:47:GLN:O	2:B:173:MET:HE1	2.19	0.43
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.65	0.43
2:B:642:ASP:CA	2:B:649:LYS:HA	2.40	0.43
2:B:797:TYR:HB2	2:B:852:ARG:O	2.19	0.43
3:C:176:ILE:HG22	3:C:177:GLU:O	2.19	0.43
5:E:195:VAL:HG22	5:E:213:ILE:HG13	2.01	0.43
8:H:39:THR:HB	8:H:124:ARG:HB3	2.00	0.43
8:H:30:SER:CB	8:H:36:CYS:HB3	2.48	0.43
10:J:2:ILE:HG22	10:J:3:VAL:O	2.18	0.43
11:K:5:ASP:O	11:K:6:ARG:C	2.57	0.43
11:K:57:LEU:HB2	11:K:76:GLN:HG2	2.01	0.43
1:A:1127:ASP:O	1:A:1128:GLN:C	2.57	0.43
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.19	0.43
1:A:577:ILE:C	1:A:579:SER:N	2.69	0.43
1:A:601:LYS:HB2	1:A:603:ASN:HD21	1.84	0.43
1:A:49:LYS:CE	1:A:61:ILE:HD12	2.42	0.43
1:A:672:ASP:O	1:A:673:GLY:C	2.58	0.43
1:A:877:HIS:C	1:A:878:ILE:CG1	2.87	0.43
1:A:341:MET:HE3	2:B:1135:ARG:NH1	2.33	0.43
1:A:78:PRO:HB2	2:B:1201:LYS:HE3	2.01	0.43
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.39	0.43
2:B:251:ILE:HG22	2:B:251:ILE:O	2.19	0.43
2:B:343:ILE:HB	2:B:348:ARG:HE	1.84	0.43
2:B:361:LEU:N	2:B:362:PRO:CD	2.81	0.43
2:B:785:TYR:C	2:B:785:TYR:CD1	2.91	0.43
2:B:890:TYR:O	2:B:892:LYS:N	2.51	0.43
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.19	0.43
3:C:120:ILE:HD11	3:C:130:GLY:O	2.19	0.43
3:C:38:ILE:HA	3:C:173:ALA:HB2	2.00	0.43
3:C:27:LEU:HD13	3:C:228:PHE:CE2	2.54	0.43
3:C:3:GLU:O	3:C:4:GLU:CG	2.67	0.43
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.52	0.43
4:D:60:LYS:O	4:D:64:VAL:HG23	2.19	0.43
5:E:55:ARG:HD2	5:E:83:CYS:O	2.19	0.43
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.84	0.43
11:K:57:LEU:N	11:K:76:GLN:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.19	0.42
1:A:1025:ARG:O	1:A:1026:LEU:HD23	2.19	0.42
1:A:203:SER:OG	1:A:206:GLU:HB2	2.19	0.42
1:A:350:ARG:HG3	1:A:350:ARG:NH1	2.33	0.42
1:A:40:THR:C	1:A:41:MET:HG3	2.39	0.42
1:A:925:LEU:O	1:A:927:VAL:N	2.52	0.42
2:B:382:ILE:O	2:B:386:LEU:HG	2.19	0.42
2:B:764:SER:HB3	2:B:765:PRO:CD	2.49	0.42
3:C:27:LEU:O	3:C:28:ALA:C	2.57	0.42
3:C:61:GLU:HA	3:C:64:ALA:HB3	2.00	0.42
4:D:145:MET:O	4:D:149:THR:HB	2.19	0.42
6:F:101:ILE:HD11	6:F:124:GLU:OE1	2.18	0.42
7:G:79:PHE:CE2	7:G:105:PRO:HG2	2.54	0.42
8:H:139:ASN:O	8:H:140:ALA:HB2	2.19	0.42
9:I:56:ALA:O	9:I:57:GLY:C	2.57	0.42
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.82	0.42
1:A:1205:LYS:O	1:A:1206:ASP:C	2.57	0.42
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.01	0.42
1:A:92:HIS:HD2	1:A:304:MET:CE	2.32	0.42
1:A:335:ARG:O	1:A:336:ILE:C	2.55	0.42
1:A:674:PRO:C	1:A:676:MET:N	2.72	0.42
1:A:412:ARG:NH2	2:B:1108:ARG:HH12	2.17	0.42
2:B:1197:PRO:O	2:B:1200:ALA:N	2.51	0.42
2:B:654:ARG:C	2:B:656:GLY:N	2.72	0.42
2:B:693:ILE:HG22	2:B:694:ASP:O	2.20	0.42
3:C:41:ILE:HD11	3:C:247:GLY:HA2	2.00	0.42
5:E:160:GLU:O	5:E:163:GLU:HB3	2.19	0.42
6:F:85:MET:HE1	6:F:93:ILE:HD12	2.01	0.42
7:G:66:GLY:O	7:G:67:SER:C	2.55	0.42
8:H:56:THR:HG21	8:H:145:ARG:HE	1.84	0.42
9:I:101:PHE:HB2	9:I:110:PHE:CE2	2.55	0.42
9:I:59:VAL:C	9:I:61:ASP:H	2.22	0.42
1:A:1400:CYS:O	1:A:1405:THR:HG23	2.20	0.42
1:A:1430:LEU:HB2	1:A:1432:GLN:HG3	2.00	0.42
1:A:1437:GLY:O	1:A:1438:THR:C	2.58	0.42
1:A:299:HIS:C	1:A:301:ALA:H	2.23	0.42
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.81	0.42
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.84	0.42
1:A:870:GLU:HG2	5:E:208:TYR:CD1	2.54	0.42
1:A:907:THR:HG23	1:A:908:LEU:N	2.33	0.42
2:B:1162:ILE:O	2:B:1171:VAL:HG21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:PHE:CE2	2:B:542:MET:HA	2.55	0.42
2:B:857:ARG:NH2	2:B:942:ARG:NH1	2.68	0.42
4:D:118:THR:HG22	4:D:118:THR:O	2.19	0.42
5:E:179:GLN:HB2	5:E:182:ASP:HB2	2.01	0.42
5:E:61:GLN:HG2	5:E:62:ALA:H	1.83	0.42
6:F:79:ARG:HH22	6:F:150:GLU:CD	2.22	0.42
7:G:13:LEU:HD21	7:G:17:PHE:CB	2.28	0.42
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.83	0.42
1:A:122:MET:O	1:A:123:ARG:C	2.58	0.42
1:A:1386:ARG:HE	1:A:1386:ARG:HB3	1.68	0.42
1:A:1387:HIS:CE1	13:N:4:DT:C4'	3.00	0.42
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.48	0.42
2:B:221:ASN:OD1	2:B:242:SER:HA	2.18	0.42
2:B:364:ILE:HG22	2:B:365:THR:N	2.33	0.42
2:B:45:SER:O	2:B:46:GLN:C	2.57	0.42
2:B:467:GLY:CA	2:B:475:SER:HB3	2.49	0.42
3:C:45:ALA:O	3:C:159:ALA:HA	2.20	0.42
8:H:95:TYR:CE2	8:H:97:MET:CG	3.02	0.42
9:I:53:GLY:O	9:I:89:GLN:HB2	2.18	0.42
11:K:61:TYR:O	11:K:61:TYR:CD2	2.72	0.42
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	2.01	0.42
1:A:1315:GLU:C	1:A:1317:MET:N	2.72	0.42
1:A:1370:LEU:O	1:A:1373:ASP:HB2	2.20	0.42
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	2.19	0.42
1:A:208:LEU:HD23	1:A:208:LEU:O	2.20	0.42
1:A:817:ALA:O	1:A:818:MET:C	2.56	0.42
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.83	0.42
1:A:907:THR:HG23	1:A:908:LEU:H	1.85	0.42
1:A:964:ILE:O	1:A:965:GLN:C	2.57	0.42
2:B:1222:ARG:HG2	2:B:1222:ARG:O	2.19	0.42
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.37	0.42
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.35	0.42
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.34	0.42
2:B:45:SER:OG	2:B:46:GLN:N	2.49	0.42
2:B:758:PHE:N	2:B:759:PRO:HD2	2.34	0.42
2:B:806:THR:HG22	2:B:808:ALA:CB	2.49	0.42
3:C:239:PRO:O	3:C:241:ASP:N	2.53	0.42
3:C:94:LYS:HB2	3:C:94:LYS:HE3	1.87	0.42
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.54	0.42
6:F:86:THR:HG23	6:F:89:GLU:CD	2.39	0.42
7:G:115:MET:CB	7:G:116:PRO:CD	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:PHE:HA	8:H:29:ALA:O	2.18	0.42
1:A:477:PRO:HG3	1:A:521:MET:HG2	2.02	0.42
1:A:543:LEU:HD12	1:A:547:LEU:HG	2.01	0.42
1:A:53:LEU:O	1:A:54:ASN:C	2.57	0.42
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.54	0.42
1:A:842:VAL:O	1:A:844:ALA:N	2.52	0.42
2:B:1208:MET:O	2:B:1211:ASN:N	2.51	0.42
2:B:597:MET:C	2:B:599:THR:N	2.73	0.42
2:B:641:GLU:HA	2:B:641:GLU:OE1	2.20	0.42
4:D:7:THR:HB	7:G:42:PHE:CZ	2.55	0.42
5:E:180:ARG:NH2	5:E:192:ARG:HD2	2.34	0.42
8:H:95:TYR:HE2	8:H:97:MET:CG	2.32	0.42
9:I:100:PHE:CD1	9:I:100:PHE:N	2.88	0.42
10:J:32:GLU:O	10:J:33:GLY:C	2.57	0.42
12:L:29:TYR:CD2	12:L:29:TYR:N	2.84	0.42
12:L:60:ARG:HG2	12:L:61:THR:N	2.35	0.42
3:C:47:ASP:CA	12:L:69:ALA:CB	2.94	0.42
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.35	0.42
1:A:1226:VAL:HG22	1:A:1240:CYS:CB	2.50	0.42
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.20	0.42
1:A:1315:GLU:C	1:A:1317:MET:H	2.22	0.42
1:A:1389:PHE:C	1:A:1391:ARG:H	2.22	0.42
1:A:507:VAL:N	1:A:508:PRO:CD	2.82	0.42
1:A:746:MET:CE	2:B:1018:PRO:HG2	2.50	0.42
1:A:846:GLU:HB2	1:A:847:ASP:H	1.68	0.42
2:B:559:SER:HA	2:B:563:MET:HB3	2.02	0.42
2:B:519:TRP:HE1	2:B:635:ARG:NH2	2.18	0.42
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.54	0.42
2:B:781:PHE:O	2:B:782:LEU:HD23	2.19	0.42
3:C:98:VAL:C	3:C:99:LEU:CD2	2.88	0.42
6:F:87:LYS:HG3	6:F:88:TYR:CE1	2.54	0.42
12:L:28:LYS:HB2	12:L:39:SER:HA	2.02	0.42
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	2.19	0.42
1:A:274:ILE:O	1:A:275:SER:C	2.57	0.42
1:A:381:THR:O	1:A:384:ASN:N	2.50	0.42
1:A:665:GLY:O	1:A:666:ILE:C	2.58	0.42
1:A:841:LEU:O	1:A:845:LEU:HG	2.20	0.42
2:B:102:VAL:HG23	2:B:112:LEU:HB2	2.02	0.42
2:B:458:LYS:O	2:B:459:TYR:C	2.58	0.42
3:C:124:LEU:HD22	3:C:129:ILE:HG22	2.01	0.42
4:D:170:THR:CG2	4:D:172:LEU:HG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:81:THR:HB	6:F:136:ARG:HH11	1.85	0.42
7:G:56:ILE:O	7:G:57:GLN:HB2	2.20	0.42
10:J:1:MET:H3	10:J:56:LEU:H	1.68	0.42
15:T:12:DT:H2"	15:T:13:DA:OP2	2.18	0.42
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.55	0.42
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.46	0.42
1:A:162:VAL:HG12	1:A:163:SER:N	2.34	0.42
1:A:270:LEU:O	1:A:271:LYS:C	2.57	0.42
1:A:598:LEU:O	1:A:599:SER:C	2.58	0.42
1:A:608:ILE:C	1:A:610:GLY:H	2.22	0.42
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.52	0.42
2:B:1085:ILE:CD1	2:B:1085:ILE:N	2.79	0.42
2:B:235:SER:HA	2:B:261:ARG:NH1	2.34	0.42
2:B:597:MET:O	2:B:599:THR:N	2.53	0.42
2:B:616:ILE:HG12	2:B:697:GLU:HA	2.01	0.42
2:B:914:LYS:HD3	2:B:937:ALA:CB	2.50	0.42
3:C:166:GLU:O	3:C:167:HIS:HB2	2.20	0.42
3:C:208:GLU:C	3:C:210:GLU:N	2.71	0.42
3:C:213:PRO:HG2	3:C:214:ASN:H	1.84	0.42
3:C:23:SER:O	3:C:24:ASN:HB3	2.19	0.42
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.36	0.42
4:D:64:VAL:C	4:D:66:ARG:N	2.73	0.42
5:E:73:PRO:O	5:E:75:MET:N	2.48	0.42
1:A:1441:PHE:CE2	6:F:89:GLU:HG2	2.55	0.42
9:I:4:PHE:HE1	9:I:6:PHE:CE2	2.38	0.42
1:A:975:HIS:HA	1:A:1036:ARG:HG3	2.02	0.42
1:A:1215:ARG:HA	1:A:1215:ARG:HD2	1.72	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:OG1	2.20	0.42
1:A:353:ILE:HD13	1:A:487:MET:CE	2.49	0.42
1:A:382:PRO:CB	1:A:428:TYR:CE2	2.97	0.42
1:A:472:LEU:O	1:A:475:THR:CB	2.60	0.42
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.53	0.42
1:A:856:THR:CB	1:A:865:GLN:HB2	2.47	0.42
1:A:925:LEU:C	1:A:927:VAL:H	2.23	0.42
2:B:1006:ILE:HD13	10:J:44:TYR:HE2	1.81	0.42
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.49	0.42
2:B:28:GLU:HG3	2:B:28:GLU:O	2.20	0.42
2:B:763:GLN:O	2:B:765:PRO:N	2.53	0.42
2:B:882:THR:HG21	2:B:884:ARG:HB2	2.02	0.42
5:E:144:ILE:HD13	5:E:183:PRO:HB3	2.01	0.42
7:G:144:ARG:O	7:G:168:LEU:HD22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:38:CYS:HB3	7:G:155:SER:HA	2.02	0.42
8:H:10:PHE:HE1	8:H:57:VAL:HB	1.85	0.42
8:H:98:TYR:C	8:H:118:PHE:HD2	2.23	0.42
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.50	0.42
14:P:1:U:O2'	14:P:2:C:C5'	2.67	0.42
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.02	0.41
1:A:146:MET:HA	1:A:171:GLN:HB2	2.01	0.41
1:A:61:ILE:HG22	1:A:62:ASP:N	2.32	0.41
1:A:786:HIS:O	1:A:787:PHE:HD2	2.03	0.41
2:B:753:ALA:O	2:B:755:ILE:N	2.53	0.41
2:B:769:TYR:O	2:B:772:ALA:N	2.53	0.41
2:B:957:ASN:O	2:B:958:GLN:C	2.58	0.41
2:B:953:LEU:HD23	2:B:965:LYS:H	1.85	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.83	0.41
7:G:91:VAL:HA	7:G:101:VAL:HA	2.02	0.41
7:G:22:MET:O	7:G:25:TYR:N	2.53	0.41
11:K:42:LEU:HD21	11:K:46:ILE:CD1	2.50	0.41
1:A:108:MET:O	1:A:109:HIS:HB2	2.19	0.41
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.35	0.41
1:A:469:ARG:HB3	1:A:469:ARG:HH11	1.85	0.41
1:A:719:VAL:C	1:A:721:PHE:N	2.73	0.41
1:A:842:VAL:O	1:A:843:LYS:C	2.57	0.41
1:A:98:LYS:O	1:A:101:LYS:N	2.54	0.41
2:B:263:GLY:O	2:B:264:SER:C	2.58	0.41
2:B:523:CYS:SG	2:B:524:PRO:HD2	2.60	0.41
2:B:53:GLN:NE2	2:B:57:TYR:HB2	2.35	0.41
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.68	0.41
2:B:862:GLN:CG	2:B:963:PHE:HD1	2.33	0.41
3:C:51:VAL:HG22	3:C:155:LEU:HD22	2.01	0.41
3:C:53:THR:O	3:C:153:LEU:HA	2.20	0.41
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.88	0.41
5:E:157:SER:OG	5:E:159:ASP:HB2	2.21	0.41
5:E:177:ARG:HD3	5:E:215:MET:HG2	2.02	0.41
5:E:92:THR:HG22	5:E:92:THR:O	2.20	0.41
8:H:20:TYR:O	8:H:22:LYS:N	2.52	0.41
8:H:76:THR:HG22	8:H:76:THR:O	2.19	0.41
9:I:54:GLU:HB3	9:I:100:PHE:CE2	2.55	0.41
1:A:117:GLU:H	1:A:117:GLU:CD	2.23	0.41
1:A:1329:THR:CG2	1:A:1331:SER:HB3	2.51	0.41
1:A:697:ALA:C	1:A:699:ALA:H	2.23	0.41
1:A:722:LEU:HD21	1:A:794:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:O	1:A:846:GLU:C	2.58	0.41
1:A:90:VAL:HG12	1:A:91:PHE:N	2.34	0.41
2:B:169:ARG:N	2:B:454:THR:OG1	2.54	0.41
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.19	0.41
2:B:429:PHE:HA	2:B:432:MET:CE	2.50	0.41
2:B:95:ILE:HB	2:B:130:VAL:HG22	2.01	0.41
3:C:236:GLY:O	3:C:237:SER:C	2.59	0.41
3:C:29:MET:HE1	11:K:98:LEU:CD2	2.50	0.41
6:F:143:PHE:C	6:F:143:PHE:HD1	2.23	0.41
8:H:83:GLN:O	8:H:85:GLY:N	2.53	0.41
10:J:28:ASP:O	10:J:29:GLU:C	2.59	0.41
11:K:91:CYS:O	11:K:94:ILE:HB	2.21	0.41
1:A:1157:ASP:C	1:A:1159:ARG:H	2.24	0.41
1:A:11:LEU:HG	1:A:11:LEU:O	2.16	0.41
1:A:1444:MET:HG2	7:G:59:GLY:O	2.20	0.41
1:A:596:THR:O	1:A:597:LEU:C	2.59	0.41
1:A:825:ILE:O	1:A:828:ALA:N	2.48	0.41
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.82	0.41
2:B:1115:THR:CG2	2:B:1117:GLN:CG	2.98	0.41
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.56	0.41
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.85	0.41
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.01	0.41
2:B:336:ARG:NH2	2:B:345:LYS:CE	2.77	0.41
2:B:48:LEU:O	2:B:51:PHE:N	2.51	0.41
2:B:581:PHE:HA	2:B:585:VAL:O	2.20	0.41
4:D:153:ARG:C	4:D:154:PHE:CD1	2.93	0.41
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.82	0.41
10:J:22:LEU:O	10:J:25:LEU:HB2	2.20	0.41
10:J:2:ILE:HG12	10:J:57:ILE:HD12	2.02	0.41
1:A:1010:ALA:O	1:A:1011:GLN:C	2.59	0.41
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.20	0.41
1:A:1445:ILE:H	1:A:1445:ILE:CD1	1.98	0.41
1:A:265:LYS:NZ	1:A:322:VAL:HG13	2.36	0.41
1:A:305:ASP:CG	1:A:326:ARG:HD2	2.41	0.41
1:A:335:ARG:HB3	1:A:336:ILE:H	1.68	0.41
1:A:353:ILE:HG21	1:A:487:MET:CE	2.49	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.87	0.41
1:A:818:MET:HG2	2:B:514:LEU:HG	2.03	0.41
1:A:886:ILE:HG22	1:A:887:GLY:H	1.78	0.41
2:B:980:PHE:HE2	2:B:1094:ARG:CB	2.33	0.41
2:B:1142:GLY:O	2:B:1144:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:LEU:HD23	2:B:446:LEU:N	2.36	0.41
2:B:705:MET:CE	2:B:745:PRO:HB3	2.51	0.41
2:B:750:GLY:O	2:B:751:VAL:C	2.59	0.41
2:B:806:THR:C	2:B:808:ALA:N	2.71	0.41
2:B:807:ARG:O	2:B:811:TYR:HE1	2.03	0.41
3:C:116:LYS:HD3	3:C:140:ASN:HA	2.02	0.41
3:C:70:ILE:HA	3:C:71:PRO:HD2	1.89	0.41
4:D:40:HIS:C	4:D:42:GLY:N	2.72	0.41
10:J:32:GLU:O	10:J:35:ALA:N	2.53	0.41
10:J:53:HIS:CD2	10:J:54:VAL:N	2.88	0.41
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.50	0.41
1:A:116:ASP:C	1:A:118:HIS:H	2.24	0.41
1:A:860:LEU:HD11	1:A:1393:ASN:HB2	2.02	0.41
1:A:47:ARG:HH12	1:A:254:GLU:CG	2.33	0.41
1:A:62:ASP:HB3	1:A:64:ASN:HD21	1.83	0.41
1:A:920:LEU:HD23	1:A:920:LEU:C	2.40	0.41
2:B:1002:THR:CG2	2:B:1006:ILE:HG13	2.49	0.41
2:B:1074:ASN:O	2:B:1078:GLY:N	2.51	0.41
2:B:1110:PRO:HB2	2:B:1119:VAL:CG2	2.51	0.41
2:B:400:HIS:O	2:B:402:GLY:N	2.53	0.41
2:B:458:LYS:O	2:B:462:ALA:N	2.54	0.41
2:B:651:LEU:HD11	2:B:707:PRO:CB	2.51	0.41
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.20	0.41
3:C:76:ASP:O	3:C:79:GLN:HG2	2.21	0.41
5:E:42:PHE:O	5:E:43:LYS:C	2.59	0.41
6:F:147:SER:OG	6:F:150:GLU:HG3	2.20	0.41
7:G:165:GLU:HB2	7:G:168:LEU:HD12	2.02	0.41
7:G:62:LEU:HD23	7:G:62:LEU:HA	1.89	0.41
10:J:21:TYR:C	10:J:21:TYR:CD2	2.94	0.41
12:L:40:LEU:HD22	12:L:44:ASP:CB	2.51	0.41
14:P:6:C:H2'	14:P:7:A:O4'	2.20	0.41
1:A:252:PHE:HB2	1:A:256:GLN:CD	2.41	0.41
1:A:42:ASP:OD1	1:A:45:GLN:O	2.39	0.41
1:A:526:ASP:O	1:A:527:THR:C	2.59	0.41
1:A:629:LEU:O	1:A:633:VAL:HG23	2.21	0.41
1:A:65:LEU:O	1:A:66:LYS:C	2.59	0.41
1:A:699:ALA:HB2	9:I:114:GLN:CD	2.41	0.41
1:A:89:PRO:HB3	1:A:208:LEU:HD12	2.03	0.41
2:B:1023:VAL:O	2:B:1024:ALA:C	2.59	0.41
2:B:324:ILE:CG2	2:B:325:GLN:N	2.83	0.41
2:B:469:GLN:HB2	2:B:470:LYS:H	1.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.50	0.41
3:C:59:ALA:O	3:C:60:ASP:C	2.58	0.41
5:E:114:ASN:O	5:E:115:ASN:CB	2.63	0.41
6:F:97:ARG:NH2	6:F:106:PRO:O	2.54	0.41
10:J:57:ILE:HG23	10:J:58:GLU:N	2.35	0.41
15:T:16:DT:C4	15:T:17:DT:C4	3.09	0.41
1:A:1076:ALA:HA	1:A:1079:MET:HE3	2.01	0.41
1:A:1170:ILE:HG13	1:A:1170:ILE:H	1.55	0.41
1:A:1214:GLU:OE1	1:A:1214:GLU:HA	2.21	0.41
1:A:135:PHE:HB2	1:A:223:GLY:H	1.85	0.41
1:A:268:ASP:O	1:A:269:ILE:C	2.59	0.41
1:A:322:VAL:HG12	1:A:322:VAL:O	2.19	0.41
1:A:56:PRO:O	1:A:57:ARG:NE	2.47	0.41
1:A:715:GLU:O	1:A:716:ASP:C	2.59	0.41
1:A:77:CYS:C	1:A:78:PRO:O	2.55	0.41
1:A:98:LYS:O	1:A:100:LYS:N	2.53	0.41
2:B:1034:VAL:O	2:B:1036:ALA:N	2.54	0.41
2:B:762:ASN:OD1	2:B:1024:ALA:HB3	2.21	0.41
3:C:143:LEU:HD21	3:C:146:LYS:HE2	2.03	0.41
3:C:256:ALA:O	3:C:258:ILE:N	2.54	0.41
3:C:66:ARG:CZ	10:J:2:ILE:CG2	2.98	0.41
4:D:187:THR:HG22	4:D:188:ALA:H	1.84	0.41
6:F:147:SER:O	6:F:148:VAL:C	2.58	0.41
6:F:89:GLU:O	6:F:93:ILE:HG13	2.20	0.41
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.51	0.41
9:I:101:PHE:CE1	9:I:112:SER:HB2	2.56	0.41
10:J:31:ASP:O	10:J:32:GLU:C	2.59	0.41
12:L:60:ARG:HH21	12:L:65:VAL:HG21	1.86	0.41
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.55	0.41
1:A:269:ILE:HG12	1:A:299:HIS:HB3	2.03	0.41
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.86	0.41
1:A:335:ARG:CA	1:A:339:ASN:HD22	2.28	0.41
1:A:573:SER:OG	1:A:576:GLN:HB2	2.21	0.41
1:A:68:GLN:HE22	1:A:80:HIS:CG	2.39	0.41
1:A:722:LEU:HD22	1:A:799:PHE:CG	2.56	0.41
1:A:976:THR:HG23	8:H:136:LYS:NZ	2.36	0.41
2:B:1010:LEU:HA	2:B:1010:LEU:HD12	1.81	0.41
2:B:1107:ALA:O	2:B:1108:ARG:O	2.39	0.41
2:B:181:LEU:O	2:B:182:SER:C	2.59	0.41
2:B:583:ASN:HD21	2:B:628:THR:HB	1.86	0.41
2:B:603:LEU:HA	2:B:603:LEU:HD22	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:751:VAL:HG13	2:B:812:LEU:CD2	2.47	0.41
2:B:812:LEU:O	2:B:813:LYS:C	2.59	0.41
3:C:236:GLY:C	3:C:238:ILE:N	2.73	0.41
4:D:176:GLU:HG2	4:D:197:SER:OG	2.21	0.41
4:D:56:ARG:NH2	4:D:57:LEU:HD21	2.35	0.41
5:E:153:HIS:O	5:E:154:ILE:HG13	2.20	0.41
5:E:56:LYS:HE3	5:E:84:ASP:HB2	2.02	0.41
5:E:58:MET:O	5:E:59:SER:O	2.38	0.41
7:G:27:LYS:O	7:G:30:LEU:N	2.54	0.41
8:H:83:GLN:C	8:H:85:GLY:N	2.74	0.41
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.56	0.41
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.50	0.41
15:T:18:DT:O3'	15:T:19:TT:C4'	2.63	0.41
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.35	0.41
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.92	0.41
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.56	0.41
1:A:265:LYS:O	1:A:269:ILE:HG13	2.21	0.41
1:A:337:ARG:CZ	1:A:839:ARG:NH1	2.84	0.41
1:A:41:MET:O	1:A:50:ILE:HG13	2.21	0.41
1:A:608:ILE:O	1:A:610:GLY:N	2.54	0.41
2:B:189:LEU:O	2:B:192:LEU:HB2	2.21	0.41
2:B:205:ILE:N	2:B:205:ILE:CD1	2.83	0.41
2:B:24:PRO:O	2:B:655:LYS:HB2	2.21	0.41
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.51	0.41
2:B:597:MET:C	2:B:599:THR:H	2.22	0.41
2:B:909:ASP:N	2:B:909:ASP:OD1	2.51	0.41
1:A:106:VAL:HA	1:A:114:LEU:HD21	2.04	0.41
1:A:1074:GLU:C	1:A:1076:ALA:H	2.25	0.41
1:A:1332:PHE:HE1	1:A:1348:LEU:HD13	1.85	0.41
1:A:188:ASP:OD1	1:A:189:ARG:N	2.53	0.41
1:A:354:SER:HA	1:A:482:PHE:CD2	2.56	0.41
1:A:532:ARG:O	1:A:535:THR:HB	2.21	0.41
1:A:604:GLY:O	1:A:605:MET:HB2	2.21	0.41
2:B:245:GLU:C	2:B:246:LYS:HG3	2.41	0.41
2:B:743:ILE:H	2:B:743:ILE:HG12	1.64	0.41
2:B:895:ASP:C	2:B:897:GLY:N	2.74	0.41
2:B:953:LEU:HD22	2:B:965:LYS:HB2	1.98	0.41
3:C:174:ALA:O	3:C:175:ALA:CB	2.67	0.41
3:C:97:VAL:HG12	3:C:99:LEU:HD21	2.03	0.41
5:E:191:LYS:O	5:E:192:ARG:C	2.58	0.41
7:G:21:ARG:HD3	7:G:21:ARG:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.56	0.41
8:H:145:ARG:O	8:H:146:ARG:HB2	2.21	0.41
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.41	0.41
9:I:77:LYS:O	9:I:79:HIS:N	2.54	0.41
10:J:57:ILE:O	10:J:60:PHE:HB2	2.21	0.41
11:K:42:LEU:O	11:K:42:LEU:HG	2.22	0.41
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.56	0.41
1:A:219:PHE:O	1:A:222:LEU:O	2.38	0.40
1:A:26:GLU:O	1:A:27:VAL:C	2.59	0.40
1:A:31:SER:HA	1:A:81:PHE:O	2.22	0.40
1:A:391:LEU:O	1:A:394:ASN:HB2	2.21	0.40
1:A:606:LEU:CB	1:A:614:PHE:CE2	3.03	0.40
2:B:999:MET:HG2	2:B:1007:VAL:HG22	2.02	0.40
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.51	0.40
2:B:29:ASP:O	2:B:30:SER:C	2.60	0.40
2:B:313:MET:CE	2:B:386:LEU:HD22	2.51	0.40
2:B:337:ARG:C	2:B:338:GLY:CA	2.90	0.40
2:B:638:PHE:HB3	2:B:651:LEU:HD22	2.03	0.40
2:B:710:LEU:O	2:B:711:GLU:OE2	2.38	0.40
2:B:744:HIS:CD2	2:B:746:SER:HB3	2.56	0.40
2:B:834:ASN:CA	2:B:838:SER:O	2.69	0.40
3:C:172:PRO:O	3:C:235:VAL:HG23	2.20	0.40
4:D:192:LYS:HB3	4:D:192:LYS:NZ	2.34	0.40
4:D:195:ILE:N	4:D:196:PRO:CD	2.85	0.40
8:H:39:THR:O	8:H:124:ARG:N	2.52	0.40
8:H:82:PRO:C	8:H:84:ALA:N	2.73	0.40
9:I:34:TYR:O	9:I:35:VAL:CG2	2.69	0.40
10:J:13:VAL:C	10:J:14:VAL:HG23	2.40	0.40
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.56	0.40
1:A:1364:ASN:C	1:A:1364:ASN:HD22	2.24	0.40
1:A:1405:THR:HB	1:A:1406:VAL:H	1.55	0.40
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.21	0.40
1:A:308:ILE:HG22	1:A:309:ALA:N	2.25	0.40
1:A:376:TYR:HA	1:A:377:PRO:HD2	1.93	0.40
1:A:525:GLN:HG3	2:B:836:GLU:HG2	2.02	0.40
1:A:567:LYS:NZ	8:H:47:PHE:HB3	2.36	0.40
1:A:824:LEU:HD23	1:A:824:LEU:HA	1.85	0.40
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.53	0.40
1:A:964:ILE:O	1:A:966:ASN:N	2.54	0.40
2:B:175:ARG:NH1	2:B:175:ARG:CG	2.84	0.40
2:B:298:LEU:N	2:B:298:LEU:HD22	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:448:ILE:O	2:B:450:ALA:N	2.55	0.40
2:B:773:MET:HB3	2:B:1095:LEU:HD23	2.02	0.40
3:C:181:ASP:N	3:C:182:PRO:CD	2.84	0.40
4:D:192:LYS:HG2	4:D:207:LEU:CD2	2.51	0.40
5:E:72:PHE:CE2	5:E:155:ARG:NH2	2.89	0.40
8:H:59:ILE:CG2	8:H:60:ALA:N	2.65	0.40
9:I:103:CYS:CB	9:I:106:CYS:SG	3.09	0.40
11:K:46:ILE:O	11:K:50:LEU:HB2	2.21	0.40
11:K:50:LEU:HD11	11:K:75:ILE:HD13	2.04	0.40
12:L:46:VAL:O	12:L:46:VAL:HG12	2.22	0.40
12:L:49:LYS:O	12:L:50:ASP:HB3	2.22	0.40
1:A:1031:VAL:HG12	1:A:1031:VAL:O	2.22	0.40
1:A:1053:PHE:O	1:A:1056:SER:N	2.51	0.40
1:A:1450:LEU:CD1	6:F:108:PHE:CZ	3.04	0.40
1:A:225:ASN:HD22	1:A:228:PHE:N	1.88	0.40
1:A:230:ARG:N	1:A:233:TRP:HE3	2.11	0.40
1:A:34:LYS:H	1:A:57:ARG:HH22	1.68	0.40
1:A:356:ASP:HB2	1:A:469:ARG:HH12	1.81	0.40
1:A:408:ASP:C	1:A:410:GLY:H	2.24	0.40
1:A:481:ASP:OD1	1:A:483:ASP:CG	2.60	0.40
1:A:482:PHE:C	1:A:484:GLY:N	2.71	0.40
1:A:58:LEU:HG	1:A:59:GLY:H	1.82	0.40
1:A:834:THR:HG22	1:A:835:GLY:N	2.35	0.40
1:A:869:GLY:O	1:A:870:GLU:HB2	2.21	0.40
1:A:925:LEU:C	1:A:927:VAL:N	2.73	0.40
2:B:774:GLY:HA2	2:B:1093:GLN:HE22	1.85	0.40
2:B:315:LYS:N	2:B:316:PRO:CD	2.83	0.40
2:B:658:ILE:O	2:B:661:LEU:N	2.42	0.40
2:B:824:ILE:CG2	2:B:1087:PHE:CE2	2.95	0.40
3:C:16:ASP:O	3:C:17:ASN:CG	2.59	0.40
7:G:109:PHE:O	7:G:160:ILE:HA	2.22	0.40
7:G:17:PHE:N	7:G:17:PHE:HD2	2.17	0.40
7:G:27:LYS:O	7:G:30:LEU:HB3	2.20	0.40
9:I:8:ARG:O	9:I:10:CYS:N	2.54	0.40
2:B:309:GLN:CG	9:I:52:ILE:HD11	2.51	0.40
9:I:56:ALA:O	9:I:57:GLY:O	2.39	0.40
1:A:1134:ILE:O	1:A:1135:ARG:C	2.59	0.40
1:A:263:THR:HG22	1:A:263:THR:O	2.22	0.40
1:A:332:LYS:O	1:A:334:GLY:N	2.55	0.40
1:A:388:LEU:HD22	1:A:432:VAL:CB	2.51	0.40
1:A:466:SER:HB3	2:B:1103:ILE:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:O	1:A:714:PHE:HB3	2.21	0.40
1:A:823:GLY:O	1:A:825:ILE:N	2.55	0.40
2:B:1030:LEU:HA	2:B:1030:LEU:HD12	1.96	0.40
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.49	0.40
2:B:294:ASP:C	2:B:296:GLU:H	2.24	0.40
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.57	0.40
2:B:498:THR:CG2	2:B:499:ASN:N	2.84	0.40
2:B:22:SER:HA	2:B:654:ARG:HG3	2.03	0.40
2:B:732:SER:HB2	2:B:734:HIS:CD2	2.57	0.40
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.21	0.40
3:C:10:ILE:HG22	3:C:11:ARG:O	2.21	0.40
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.56	0.40
3:C:58:LEU:N	3:C:58:LEU:CD2	2.84	0.40
3:C:58:LEU:N	3:C:58:LEU:HD22	2.37	0.40
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.56	0.40
7:G:14:HIS:ND1	7:G:15:PRO:CD	2.78	0.40
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.51	0.40
1:A:1019:CYS:O	1:A:1022:LEU:N	2.54	0.40
1:A:1036:ARG:NH1	1:A:1036:ARG:CG	2.80	0.40
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.21	0.40
1:A:1260:LEU:CG	1:A:1260:LEU:O	2.70	0.40
1:A:299:HIS:C	1:A:301:ALA:N	2.74	0.40
1:A:414:ASP:OD1	1:A:414:ASP:C	2.60	0.40
1:A:545:GLN:C	1:A:547:LEU:N	2.73	0.40
1:A:56:PRO:O	1:A:57:ARG:CG	2.70	0.40
1:A:34:LYS:N	1:A:57:ARG:NH2	2.65	0.40
1:A:682:THR:HG22	1:A:682:THR:O	2.22	0.40
1:A:685:GLU:HG3	1:A:686:ALA:N	2.36	0.40
1:A:939:ASP:O	1:A:940:ARG:C	2.59	0.40
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.51	0.40
2:B:225:VAL:O	2:B:226:PHE:CD2	2.74	0.40
2:B:223:VAL:HG11	2:B:381:MET:HG2	2.03	0.40
2:B:765:PRO:O	2:B:766:ARG:C	2.59	0.40
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.73	0.40
2:B:785:TYR:CD1	2:B:786:ASN:N	2.89	0.40
3:C:137:LYS:HB3	3:C:138:GLU:OE1	2.21	0.40
4:D:207:LEU:O	4:D:211:LEU:HG	2.22	0.40
5:E:114:ASN:HD22	5:E:114:ASN:HA	1.68	0.40
5:E:11:ARG:HH21	5:E:141:VAL:HG21	1.87	0.40
5:E:35:VAL:C	5:E:37:LEU:N	2.75	0.40
6:F:111:LEU:O	6:F:113:GLY:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:110:ASN:C	11:K:111:LEU:CG	2.89	0.40
11:K:62:LYS:O	11:K:71:PHE:HB2	2.21	0.40
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1410/1733 (81%)	962 (68%)	299 (21%)	149 (11%)	0	10
2	B	1096/1224 (90%)	767 (70%)	219 (20%)	110 (10%)	1	12
3	C	264/318 (83%)	171 (65%)	62 (24%)	31 (12%)	0	8
4	D	173/221 (78%)	125 (72%)	29 (17%)	19 (11%)	0	9
5	E	212/215 (99%)	157 (74%)	44 (21%)	11 (5%)	2	29
6	F	84/155 (54%)	67 (80%)	15 (18%)	2 (2%)	7	45
7	G	169/171 (99%)	125 (74%)	34 (20%)	10 (6%)	2	26
8	H	131/146 (90%)	84 (64%)	30 (23%)	17 (13%)	0	6
9	I	114/122 (93%)	80 (70%)	21 (18%)	13 (11%)	0	9
10	J	63/70 (90%)	35 (56%)	13 (21%)	15 (24%)	0	1
11	K	112/120 (93%)	86 (77%)	16 (14%)	10 (9%)	1	15
12	L	44/70 (63%)	17 (39%)	17 (39%)	10 (23%)	0	1
All	All	3872/4565 (85%)	2676 (69%)	799 (21%)	397 (10%)	0	11

All (397) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	THR

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Mol	Chain	Res	Type
1	A	48	ALA
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU
1	A	74	MET
1	A	93	VAL
1	A	167	CYS
1	A	219	PHE
1	A	223	GLY
1	A	255	SER
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	318	SER
1	A	322	VAL
1	A	335	ARG
1	A	385	ILE
1	A	423	ASP
1	A	465	TYR
1	A	536	LEU
1	A	543	LEU
1	A	567	LYS
1	A	597	LEU
1	A	626	ASN
1	A	666	ILE
1	A	753	GLY
1	A	789	LYS
1	A	847	ASP
1	A	875	ALA
1	A	968	GLN
1	A	969	GLN
1	A	986	ILE
1	A	1002	GLY
1	A	1036	ARG
1	A	1096	SER
1	A	1114	PRO
1	A	1115	SER
1	A	1122	PRO
1	A	1212	VAL
1	A	1223	ASP
1	A	1281	ARG
1	A	1314	SER

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Mol	Chain	Res	Type
1	A	1341	ILE
1	A	1365	TYR
1	A	1378	GLN
1	A	1405	THR
1	A	1438	THR
2	B	45	SER
2	B	46	GLN
2	B	108	VAL
2	B	115	GLN
2	B	186	GLU
2	B	258	LEU
2	B	345	LYS
2	B	367	LEU
2	B	467	GLY
2	B	474	SER
2	B	643	ASP
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	764	SER
2	B	831	SER
2	B	943	SER
2	B	958	GLN
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1108	ARG
2	B	1156	ASP
2	B	1157	ALA
2	B	1167	GLY
2	B	1175	LEU
2	B	1178	ASN
2	B	1181	GLU
2	B	1182	CYS
2	B	1188	LYS
3	C	4	GLU
3	C	6	PRO
3	C	78	GLU
3	C	87	PHE
3	C	141	GLY
3	C	149	LYS
3	C	156	THR

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Mol	Chain	Res	Type
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	214	ASN
3	C	215	GLU
4	D	5	THR
4	D	8	PHE
4	D	19	GLU
4	D	20	GLU
4	D	52	LEU
4	D	131	GLU
4	D	177	VAL
4	D	199	ASN
5	E	3	GLN
5	E	36	GLU
5	E	59	SER
5	E	73	PRO
5	E	74	ASP
5	E	106	GLN
5	E	130	ALA
5	E	206	GLY
7	G	63	PRO
7	G	139	ILE
8	H	17	PRO
8	H	62	SER
8	H	81	PRO
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
9	I	3	THR
9	I	9	ASP
9	I	79	HIS
10	J	2	ILE
10	J	6	ARG
10	J	32	GLU
10	J	64	ASN
11	K	110	ASN
12	L	35	SER
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	42	ASP

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Mol	Chain	Res	Type
1	A	54	ASN
1	A	59	GLY
1	A	61	ILE
1	A	66	LYS
1	A	70	CYS
1	A	76	GLU
1	A	84	ILE
1	A	148	CYS
1	A	154	SER
1	A	250	ILE
1	A	253	ASN
1	A	283	GLY
1	A	386	ASP
1	A	394	ASN
1	A	399	HIS
1	A	439	ASN
1	A	517	ASN
1	A	619	LYS
1	A	661	GLY
1	A	731	ARG
1	A	780	VAL
1	A	979	SER
1	A	1054	LEU
1	A	1116	LEU
1	A	1120	LEU
1	A	1124	HIS
1	A	1127	ASP
1	A	1233	ASP
1	A	1280	GLU
1	A	1377	THR
1	A	1386	ARG
1	A	1395	GLY
1	A	1402	PHE
2	B	28	GLU
2	B	48	LEU
2	B	65	GLU
2	B	260	GLY
2	B	264	SER
2	B	266	ALA
2	B	282	ILE
2	B	387	LEU
2	B	401	PHE

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Mol	Chain	Res	Type
2	B	450	ALA
2	B	466	TRP
2	B	605	ARG
2	B	613	VAL
2	B	619	ILE
2	B	641	GLU
2	B	655	LYS
2	B	708	GLU
2	B	746	SER
2	B	751	VAL
2	B	792	MET
2	B	869	SER
2	B	881	ASN
2	B	891	ASP
2	B	907	GLY
2	B	945	GLU
2	B	1065	GLN
2	B	1100	ASP
2	B	1155	SER
2	B	1171	VAL
2	B	1183	LYS
2	B	1186	ASP
3	C	81	GLU
3	C	110	THR
3	C	175	ALA
3	C	213	PRO
3	C	216	GLY
3	C	240	VAL
4	D	12	ARG
4	D	21	GLU
4	D	65	GLU
4	D	192	LYS
5	E	45	LYS
7	G	19	GLY
8	H	21	ASN
8	H	32	THR
8	H	59	ILE
8	H	77	ARG
8	H	84	ALA
8	H	140	ALA
9	I	11	ASN
9	I	34	TYR

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Mol	Chain	Res	Type
9	I	57	GLY
9	I	78	CYS
9	I	106	CYS
10	J	14	VAL
10	J	17	LYS
10	J	27	GLU
10	J	28	ASP
10	J	29	GLU
11	K	7	PHE
11	K	15	GLY
12	L	26	THR
12	L	53	HIS
12	L	55	ILE
1	A	263	THR
1	A	336	ILE
1	A	409	SER
1	A	418	SER
1	A	424	ILE
1	A	525	GLN
1	A	526	ASP
1	A	544	ASP
1	A	592	ASP
1	A	648	ASN
1	A	649	ILE
1	A	673	GLY
1	A	759	ALA
1	A	846	GLU
1	A	871	ASP
1	A	1014	ALA
1	A	1165	GLU
1	A	1221	LYS
1	A	1335	ILE
1	A	1392	SER
2	B	94	LYS
2	B	114	PRO
2	B	124	TYR
2	B	259	TYR
2	B	591	ARG
2	B	629	ASP
2	B	711	GLU
2	B	754	SER
2	B	772	ALA

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Mol	Chain	Res	Type
2	B	818	PRO
2	B	951	GLN
2	B	1041	GLU
3	C	51	VAL
3	C	56	THR
3	C	60	ASP
3	C	148	ARG
3	C	264	GLN
4	D	6	SER
4	D	9	GLN
4	D	30	GLY
4	D	53	SER
5	E	115	ASN
5	E	192	ARG
6	F	81	THR
7	G	140	LYS
8	H	92	ASP
9	I	47	GLU
9	I	62	ILE
10	J	24	LEU
10	J	33	GLY
10	J	55	ASP
11	K	29	ASN
11	K	53	ASP
11	K	88	LYS
11	K	104	ASN
1	A	113	LEU
1	A	169	ASN
1	A	245	PRO
1	A	317	LYS
1	A	332	LYS
1	A	483	ASP
1	A	516	SER
1	A	591	PHE
1	A	605	MET
1	A	636	GLU
1	A	975	HIS
1	A	1277	GLU
1	A	1366	ARG
1	A	1454	MET
2	B	56	ASP
2	B	58	THR

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Mol	Chain	Res	Type
2	B	229	ALA
2	B	257	LYS
2	B	283	VAL
2	B	322	PHE
2	B	389	ALA
2	B	894	ASP
2	B	1003	ALA
2	B	1017	ILE
2	B	1035	ALA
3	C	117	ASP
3	C	167	HIS
6	F	154	ASP
7	G	17	PHE
7	G	20	PRO
7	G	62	LEU
7	G	154	VAL
8	H	52	GLN
8	H	90	ALA
9	I	107	SER
9	I	113	ASP
10	J	8	PHE
10	J	63	TYR
11	K	90	ALA
1	A	69	THR
1	A	86	LEU
1	A	226	GLU
1	A	244	PRO
1	A	290	GLU
1	A	400	PRO
1	A	604	GLY
1	A	720	ARG
1	A	824	LEU
1	A	895	LYS
1	A	926	GLN
1	A	958	VAL
1	A	1389	PHE
2	B	61	ASP
2	B	231	PRO
2	B	245	GLU
2	B	248	SER
2	B	365	THR
2	B	369	GLY

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Mol	Chain	Res	Type
2	B	571	PRO
2	B	728	ARG
2	B	770	GLN
2	B	848	ARG
2	B	880	THR
2	B	1103	ILE
3	C	142	VAL
3	C	208	GLU
4	D	119	ARG
4	D	218	GLU
7	G	115	MET
8	H	43	ASN
8	H	44	VAL
9	I	59	VAL
10	J	18	TRP
11	K	112	GLN
12	L	39	SER
12	L	57	LEU
1	A	43	GLU
1	A	71	GLN
1	A	96	ILE
1	A	111	GLY
1	A	135	PHE
1	A	825	ILE
2	B	100	PRO
2	B	341	LEU
2	B	530	GLY
2	B	752	ALA
2	B	824	ILE
3	C	126	GLY
4	D	196	PRO
11	K	41	THR
12	L	54	ARG
1	A	196	GLU
2	B	1018	PRO
2	B	1214	PRO
1	A	55	ASP
1	A	1158	PRO
1	A	1164	PRO
2	B	364	ILE
2	B	611	PRO
2	B	729	ILE

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Mol	Chain	Res	Type
2	B	901	PRO
7	G	34	VAL
1	A	357	PRO
1	A	364	VAL
1	A	410	GLY
1	A	492	PRO
1	A	718	VAL
3	C	212	PRO
3	C	255	VAL
1	A	35	ILE
1	A	99	ILE
1	A	842	VAL
2	B	758	PHE
2	B	867	GLY
3	C	139	GLY
1	A	652	VAL
1	A	653	VAL
2	B	636	PRO

### 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	1244/1520 (82%)	1138 (92%)	106 (8%)	12	48
2	B	967/1061 (91%)	890 (92%)	77 (8%)	14	50
3	C	235/274 (86%)	215 (92%)	20 (8%)	12	48
4	D	159/200 (80%)	136 (86%)	23 (14%)	4	24
5	E	196/197 (100%)	191 (97%)	5 (3%)	51	78
6	F	77/137 (56%)	68 (88%)	9 (12%)	6	33
7	G	152/152 (100%)	140 (92%)	12 (8%)	14	51
8	H	119/128 (93%)	112 (94%)	7 (6%)	23	60
9	I	110/116 (95%)	97 (88%)	13 (12%)	6	32
10	J	60/65 (92%)	53 (88%)	7 (12%)	6	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	99/102 (97%)	86 (87%)	13 (13%)	5	28
12	L	40/57 (70%)	36 (90%)	4 (10%)	9	39
All	All	3458/4009 (86%)	3162 (91%)	296 (9%)	12	47

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	5	GLN
1	A	11	LEU
1	A	34	LYS
1	A	37	PHE
1	A	38	PRO
1	A	62	ASP
1	A	67	CYS
1	A	83	HIS
1	A	93	VAL
1	A	108	MET
1	A	122	MET
1	A	130	ASP
1	A	142	CYS
1	A	198	GLU
1	A	200	ARG
1	A	215	SER
1	A	245	PRO
1	A	270	LEU
1	A	302	THR
1	A	312	PRO
1	A	320	ARG
1	A	326	ARG
1	A	335	ARG
1	A	344	ARG
1	A	350	ARG
1	A	381	THR
1	A	385	ILE
1	A	404	TYR
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	412	ARG
1	A	418	SER

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Mol	Chain	Res	Type
1	A	425	GLN
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	462	VAL
1	A	466	SER
1	A	470	LEU
1	A	475	THR
1	A	481	ASP
1	A	493	GLN
1	A	515	GLN
1	A	527	THR
1	A	560	ILE
1	A	562	THR
1	A	577	ILE
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	666	ILE
1	A	670	ILE
1	A	711	ARG
1	A	768	GLN
1	A	774	ARG
1	A	779	PHE
1	A	821	ARG
1	A	831	THR
1	A	845	LEU
1	A	858	ASN
1	A	859	SER
1	A	886	ILE
1	A	890	ASP
1	A	903	ASN
1	A	906	HIS
1	A	907	THR
1	A	929	LEU
1	A	940	ARG
1	A	969	GLN
1	A	992	ASP
1	A	1029	ARG
1	A	1030	ARG
1	A	1035	TYR

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Mol	Chain	Res	Type
1	A	1052	GLN
1	A	1067	LEU
1	A	1110	ASN
1	A	1116	LEU
1	A	1122	PRO
1	A	1127	ASP
1	A	1170	ILE
1	A	1187	GLN
1	A	1206	ASP
1	A	1264	GLU
1	A	1271	ILE
1	A	1291	VAL
1	A	1295	THR
1	A	1309	ASP
1	A	1332	PHE
1	A	1333	ILE
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1385	THR
1	A	1386	ARG
1	A	1389	PHE
1	A	1405	THR
1	A	1432	GLN
1	A	1442	ASP
1	A	1443	VAL
1	A	1444	MET
1	A	1445	ILE
2	B	30	SER
2	B	35	SER
2	B	37	PHE
2	B	57	TYR
2	B	106	ASP
2	B	128	LEU
2	B	175	ARG
2	B	180	TYR
2	B	188	ASP
2	B	194	GLU
2	B	199	MET
2	B	217	ARG

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Mol	Chain	Res	Type
2	B	218	SER
2	B	223	VAL
2	B	268	THR
2	B	298	LEU
2	B	365	THR
2	B	371	GLU
2	B	393	LYS
2	B	396	ASP
2	B	399	ASP
2	B	427	ASP
2	B	429	PHE
2	B	463	THR
2	B	465	ASN
2	B	466	TRP
2	B	485	ARG
2	B	496	ARG
2	B	498	THR
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	557	PHE
2	B	582	VAL
2	B	593	PRO
2	B	603	LEU
2	B	615	MET
2	B	635	ARG
2	B	644	GLU
2	B	682	SER
2	B	684	LEU
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	790	ASP
2	B	811	TYR
2	B	830	TYR
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	857	ARG
2	B	878	GLN
2	B	901	PRO
2	B	909	ASP

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Mol	Chain	Res	Type
2	B	935	ARG
2	B	939	THR
2	B	953	LEU
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1022	THR
2	B	1047	PHE
2	B	1069	PHE
2	B	1084	GLN
2	B	1087	PHE
2	B	1092	TYR
2	B	1095	LEU
2	B	1099	VAL
2	B	1106	ARG
2	B	1108	ARG
2	B	1159	ARG
2	B	1160	VAL
2	B	1170	THR
2	B	1176	ASN
2	B	1183	LYS
2	B	1202	LEU
2	B	1216	LEU
3	C	22	LEU
3	C	48	SER
3	C	56	THR
3	C	58	LEU
3	C	62	PHE
3	C	77	ILE
3	C	99	LEU
3	C	104	PHE
3	C	108	GLU
3	C	129	ILE
3	C	140	ASN
3	C	145	CYS
3	C	147	LEU
3	C	151	GLN
3	C	163	ILE
3	C	193	TYR
3	C	214	ASN
3	C	240	VAL
3	C	259	LEU

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Mol	Chain	Res	Type
3	C	266	ASP
4	D	8	PHE
4	D	13	ARG
4	D	16	LYS
4	D	17	LYS
4	D	19	GLU
4	D	22	GLU
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	156	ASP
4	D	159	THR
4	D	170	THR
4	D	174	PRO
4	D	182	SER
4	D	187	THR
4	D	192	LYS
4	D	193	THR
4	D	208	GLU
4	D	221	TYR
5	E	60	PHE
5	E	74	ASP
5	E	104	ASN
5	E	114	ASN
5	E	183	PRO
6	F	79	ARG
6	F	90	ARG
6	F	99	LEU
6	F	111	LEU
6	F	119	ARG
6	F	123	LYS
6	F	143	PHE
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	13	LEU
7	G	17	PHE
7	G	74	TYR

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Mol	Chain	Res	Type
7	G	78	VAL
7	G	80	LYS
7	G	88	ASP
7	G	96	GLN
7	G	115	MET
7	G	118	ASP
7	G	126	ASN
7	G	171	ILE
8	H	86	ASP
8	H	93	TYR
8	H	95	TYR
8	H	102	TYR
8	H	130	ARG
8	H	134	ASN
8	H	143	LEU
9	I	8	ARG
9	I	9	ASP
9	I	15	TYR
9	I	34	TYR
9	I	40	SER
9	I	75	CYS
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	99	LEU
9	I	101	PHE
9	I	106	CYS
10	J	7	CYS
10	J	9	SER
10	J	10	CYS
10	J	28	ASP
10	J	44	TYR
10	J	46	CYS
10	J	48	ARG
11	K	5	ASP
11	K	10	PHE
11	K	25	THR
11	K	42	LEU
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR

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Mol	Chain	Res	Type
11	K	68	PHE
11	K	78	THR
11	K	81	TYR
11	K	111	LEU
11	K	112	GLN
11	K	113	THR
12	L	51	CYS
12	L	55	ILE
12	L	65	VAL
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	64	ASN
1	A	68	GLN
1	A	71	GLN
1	A	83	HIS
1	A	92	HIS
1	A	225	ASN
1	A	339	ASN
1	A	358	ASN
1	A	435	HIS
1	A	479	ASN
1	A	517	ASN
1	A	631	HIS
1	A	654	ASN
1	A	698	GLN
1	A	736	ASN
1	A	741	ASN
1	A	757	ASN
1	A	767	GLN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	965	GLN
1	A	1140	HIS
1	A	1218	GLN
1	A	1364	ASN

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Mol	Chain	Res	Type
1	A	1432	GLN
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	363	HIS
2	B	366	GLN
2	B	449	ASN
2	B	465	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	734	HIS
2	B	744	HIS
2	B	776	GLN
2	B	794	ASN
2	B	821	GLN
2	B	842	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1025	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1141	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	231	ASN
3	C	252	GLN
4	D	39	ASN
4	D	40	HIS
4	D	137	ASN
5	E	8	ASN
5	E	101	GLN
5	E	104	ASN

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Mol	Chain	Res	Type
5	E	114	ASN
5	E	147	HIS
7	G	53	ASN
7	G	97	HIS
7	G	122	ASN
7	G	126	ASN
9	I	12	ASN
9	I	90	GLN
10	J	53	HIS
10	J	64	ASN
11	K	44	ASN
11	K	65	HIS
11	K	76	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/11 (81%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	7	A
14	P	8	G
14	P	9	A

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues 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
15	TT	T	19	15	39,43,44	4.95	11 (28%)	59,69,72	2.36	18 (30%)
15	BRU	T	22	15,14	13,21,22	1.61	2 (15%)	16,30,33	4.13	3 (18%)

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
15	TT	T	19	15	-	0/18/105/106	0/3/6/6
15	BRU	T	22	15,14	-	0/3/21/22	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	19	TT	C5-C6	-21.02	1.31	1.55
15	T	19	TT	C5T-C6T	-20.02	1.32	1.55
15	T	19	TT	C6-N1	-5.01	1.38	1.46
15	T	19	TT	C6T-N1T	-3.45	1.40	1.46
15	T	19	TT	C4-N3	2.01	1.40	1.37
15	T	19	TT	O4-C4	2.20	1.26	1.22
15	T	19	TT	C1R-N1T	2.53	1.49	1.45
15	T	19	TT	C2-N1	2.58	1.41	1.36
15	T	19	TT	O3'-C3'	2.59	1.48	1.43
15	T	22	BRU	C4-N3	2.64	1.37	1.33
15	T	19	TT	O5'-C5'	3.50	1.49	1.44
15	T	19	TT	C1'-N1	4.04	1.50	1.45
15	T	22	BRU	C4-C5	4.86	1.44	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	-7.01	115.24	123.64
15	T	19	TT	C5-C6-C6T	-5.71	79.91	89.28
15	T	19	TT	C5-C5T-C6T	-5.45	81.59	88.38
15	T	19	TT	N3T-C2T-N1T	-2.94	113.64	116.69
15	T	19	TT	N3-C2-N1	-2.55	114.04	116.69
15	T	19	TT	O3'-C3'-C4'	-2.41	105.32	113.93
15	T	19	TT	C2R-C1R-N1T	-2.31	112.47	115.59
15	T	19	TT	C5A-C5-C6	-2.30	107.08	114.16
15	T	19	TT	C5-C4-N3	-2.13	114.20	116.06
15	T	19	TT	O3R-C3R-C4R	-2.01	102.21	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	19	TT	O4T-C4T-C5T	2.14	124.58	122.88
15	T	19	TT	C5T-C6T-C6	2.26	92.99	89.28
15	T	19	TT	C6-C6T-N1T	2.46	128.06	118.20
15	T	19	TT	O4R-C4R-C5R	2.74	118.67	109.40
15	T	22	BRU	C5-C6-N1	2.84	123.71	119.56
15	T	19	TT	C5'-C4'-C3'	3.05	121.57	114.57
15	T	19	TT	O4-C4-C5	3.62	125.77	122.88
15	T	19	TT	C5T-C5-C6	6.02	95.86	88.38
15	T	19	TT	C5T-C6T-N1T	6.14	124.22	115.61
15	T	19	TT	C5-C6-N1	8.44	127.43	115.61
15	T	22	BRU	C4-N3-C2	14.34	127.70	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	19	TT	26	0
15	T	22	BRU	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1421/1733 (81%)	-0.37	9 (0%) 89 85	17, 78, 152, 199	0
2	B	1115/1224 (91%)	-0.28	12 (1%) 80 72	20, 91, 167, 200	0
3	C	267/318 (83%)	-0.41	0 100 100	39, 77, 139, 165	0
4	D	177/221 (80%)	-0.17	2 (1%) 80 72	61, 111, 160, 175	0
5	E	214/215 (99%)	-0.28	2 (0%) 84 77	50, 133, 184, 188	0
6	F	87/155 (56%)	-0.52	0 100 100	27, 56, 100, 138	0
7	G	171/171 (100%)	-0.28	0 100 100	57, 80, 126, 137	0
8	H	135/146 (92%)	0.24	3 (2%) 62 53	95, 138, 173, 183	0
9	I	116/122 (95%)	-0.12	1 (0%) 84 77	75, 134, 166, 186	0
10	J	65/70 (92%)	-0.61	0 100 100	42, 73, 117, 125	0
11	K	114/120 (95%)	-0.33	2 (1%) 69 60	38, 83, 112, 167	0
12	L	46/70 (65%)	0.16	2 (4%) 36 28	78, 156, 175, 181	0
13	N	8/14 (57%)	0.52	0 100 100	129, 140, 153, 155	0
14	P	10/11 (90%)	0.12	1 (10%) 8 7	115, 126, 152, 158	0
15	T	17/25 (68%)	0.36	0 100 100	125, 138, 151, 153	0
All	All	3963/4615 (85%)	-0.29	34 (0%) 84 77	17, 89, 165, 200	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	114	LEU	7.5
2	B	471	LYS	6.3
11	K	113	THR	5.0
2	B	882	THR	4.0
2	B	883	LEU	3.4
1	A	1257	ASP	3.3
2	B	334	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	472	ALA	3.1
5	E	110	PHE	2.8
2	B	734	HIS	2.6
8	H	139	ASN	2.6
1	A	257	ARG	2.5
2	B	709	ASP	2.5
1	A	253	ASN	2.5
2	B	341	LEU	2.5
2	B	340	ALA	2.4
5	E	82	PHE	2.3
1	A	159	THR	2.3
1	A	171	GLN	2.3
1	A	1455	PRO	2.3
12	L	50	ASP	2.3
12	L	43	THR	2.2
1	A	251	SER	2.2
9	I	55	THR	2.2
14	P	8	G	2.2
2	B	113	TYR	2.2
4	D	9	GLN	2.2
4	D	8	PHE	2.1
1	A	158	PRO	2.1
8	H	112	ILE	2.1
2	B	884	ARG	2.1
1	A	145	LYS	2.1
8	H	140	ALA	2.1
2	B	133	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	BRU	T	22	20/21	0.78	0.24	-	112,118,124,128	0
15	TT	T	19	38/39	0.84	0.27	-	130,144,163,166	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	ZN	A	2460	1/1	0.99	0.14	-0.32	88,88,88,88	0
17	ZN	A	2463	1/1	0.99	0.14	-0.78	47,47,47,47	0
17	ZN	A	2461	1/1	0.95	0.11	-1.05	200,200,200,200	0
17	ZN	A	2462	1/1	0.99	0.07	-1.19	39,39,39,39	0
17	ZN	A	2465	1/1	0.99	0.06	-1.99	39,39,39,39	0
17	ZN	A	2458	1/1	0.99	0.16	-2.31	57,57,57,57	0
17	ZN	A	2459	1/1	0.98	0.03	-2.38	125,125,125,125	0
17	ZN	A	2464	1/1	0.98	0.07	-2.76	87,87,87,87	0
16	MG	A	2457	1/1	0.98	0.16	-	35,35,35,35	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.