



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:41 am BST

PDB ID : 4JK2
Title : X-ray crystal structure of Escherichia coli sigma70 holoenzyme in complex with
guanosine pentaphosphate (pppGpp)
Authors : Murakami, K.S.
Deposited on : 2013-03-09
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

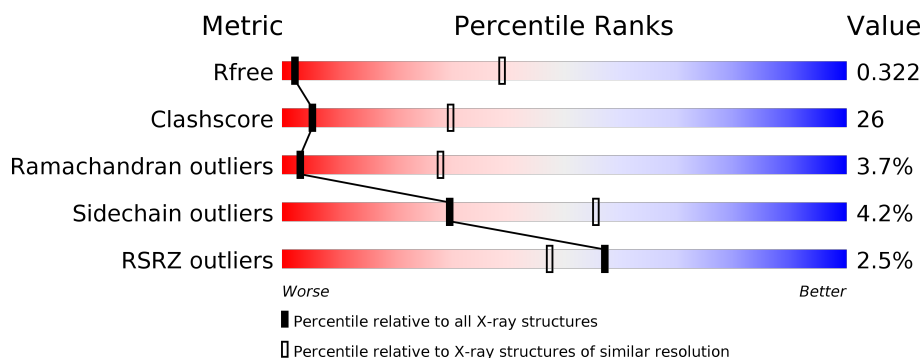
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 59%, yellow 36%, orange 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 59% 36% • • </div> </div>
1	B	329	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 38%, yellow 27%, orange 3%, grey 33%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 38% 27% • 33% </div> </div>
1	F	329	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, green 46%, yellow 22%, orange 2%, grey 30%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 4% 46% 22% • 30% </div> </div>
1	G	329	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 40%, yellow 24%, orange 1%, grey 34%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 40% 24% • 34% </div> </div>
2	C	1342	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 53%, yellow 41%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 53% 41% 5% • </div> </div>
2	H	1342	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 53%, yellow 41%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 53% 41% 5% • </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	
3	I	1407	
4	E	91	
4	J	91	
5	X	613	
5	Y	613	

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
7	0O2	D	1503	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 56129 atoms, of which 10 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 Escherichia coli RNA polymerase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

- Molecule 2 is a protein called Escherichia coli RNA polymerase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

- Molecule 3 is a protein called Escherichia coli RNA polymerase beta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

- Molecule 4 is a protein called Escherichia coli RNA polymerase omega subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

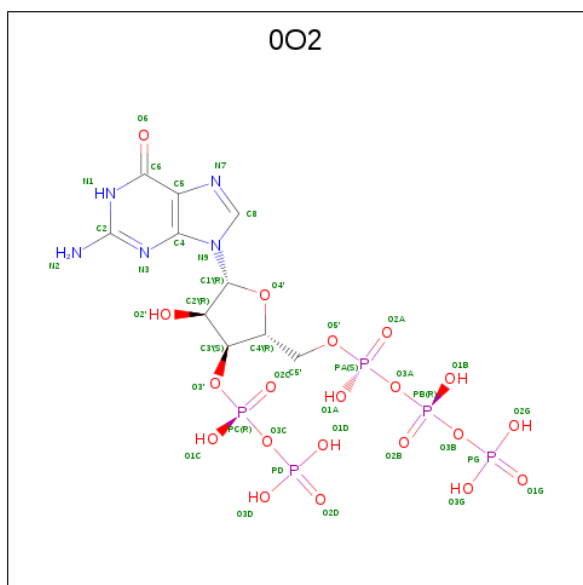
- Molecule 5 is a protein called Escherichia coli RNA polymerase sigma70 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

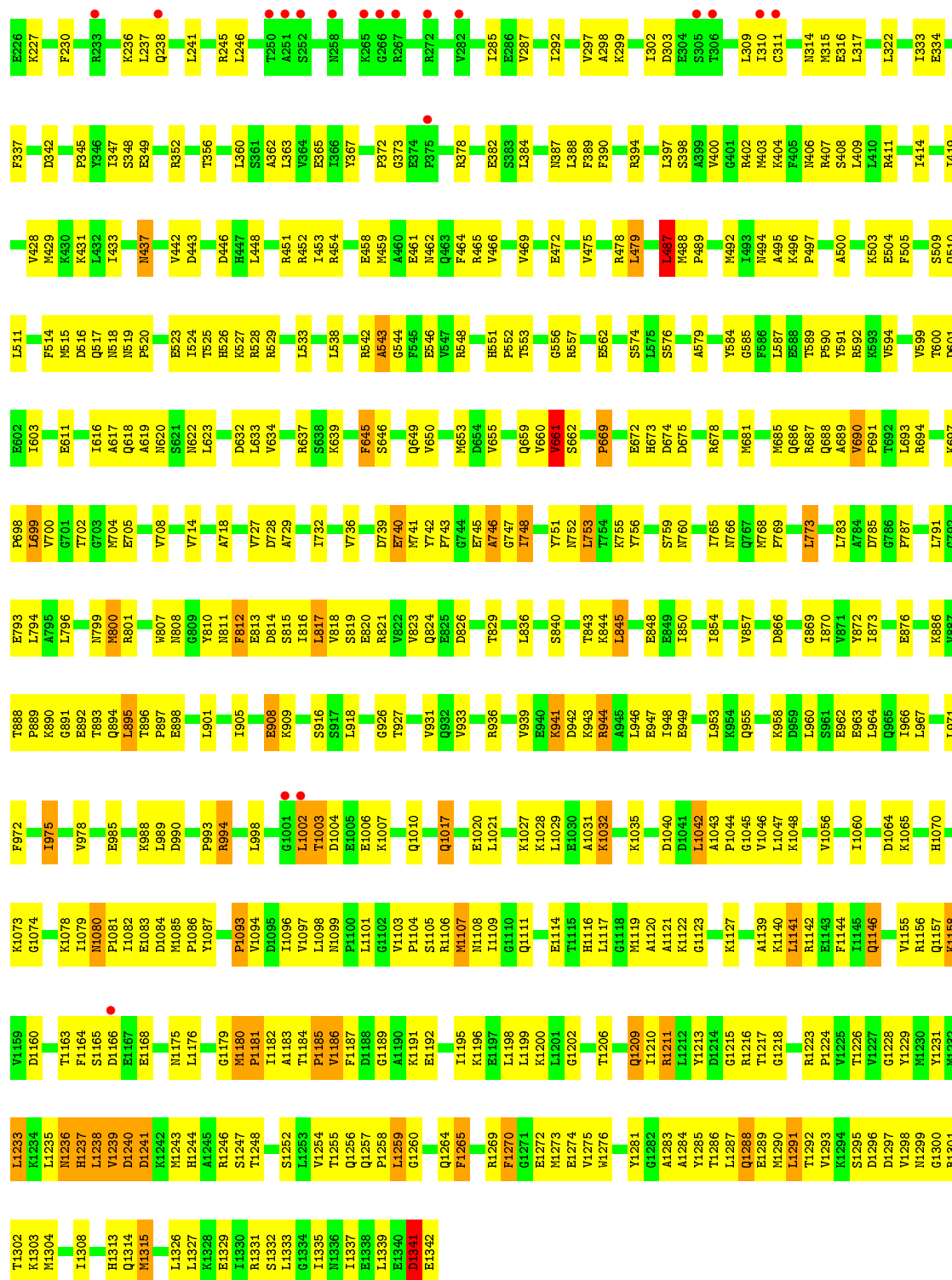
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	2	Total	Zn	0	0
			2	2		
6	D	2	Total	Zn	0	0
			2	2		

- Molecule 7 is guanosine 5'-(tetrahydrogen triphosphate) 3'-(trihydrogen diphosphate) (three-letter code: 0O2) (formula: C₁₀H₁₈N₅O₂₀P₅).



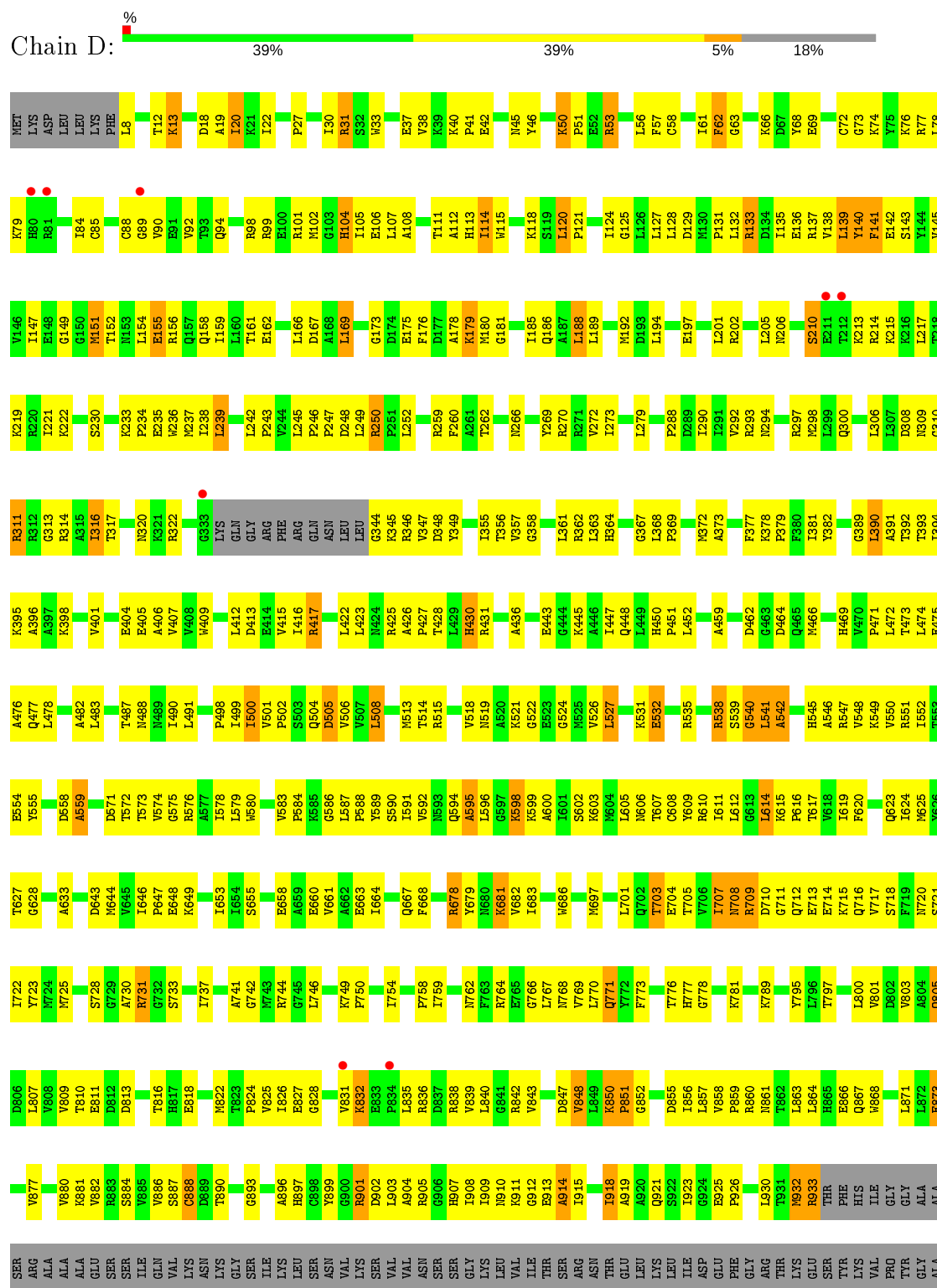
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	H	N	O	0	0
			50	10	10	5	20		

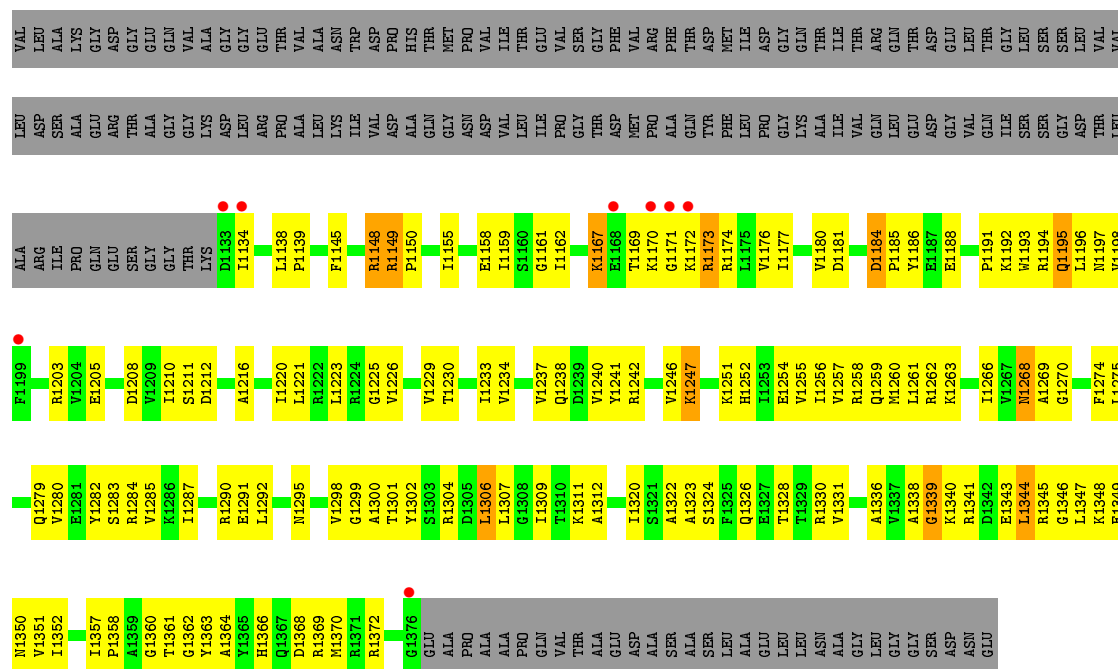


L68	Q69	Y70	V71	S72	W73	R74	P78	V79	F80	D81	V82	Q83	E84	R88	T91	Y92	S93	A94	P95	L96	R97	V98	K99	L100	R101	L102	V103	I104	Y105	E106	R107	A108	E109	P110	T113	V114	K115	E119	Q120	E121	V122	Y123	E126	I127	P128	L129	M130	T131	D132	N133	G134	T135																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
I138	N139	E142	R143	L149	N150	R151	P153	F156	K161	G162	K163	S166	S167	G168	K169	V170	L171	Y172	R175	I176	I177	P178	Y179	D185	D189	P190	N193	R197	R202	K203	L204	P205	I208	T216	T217	E218	Q219	S361	I452	A362	L223	E365	I366	R367	R368	F230	K236	L237																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
Q238	G373	E374	P375	P376	T377	R378	L384	N387	L388	R394	Y395	L397	V400	M403	K404	F405	N406	R407	R411	I414	L420	V428	M429	K431	I432	I433	D434	I435	N437	K438	K439	V442	P443	D444	I347	D446	H447	L448	R452	I453	R454	E458	M459	N462																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
Q463	F464	V469	E472	V475	R478	L479	S480	L481	L484	D485	T486	L487	M488	P489	Q490	D491	M492	I493	M494	A495	K496	P497	E504	F505	S508	S509	Q510	L511	S512	Q513	F514	N515	D516	Q517	N518	P520	L521	I524	R528	S531	A532	L533	G534	P535	A543																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
E546	V547	R548	D549	V550	H551	T552	H554	V555	G556	R557	P560	T562	T563	P564	P567	S574	L575	S576	V577	Y578	A579	N582	G585	F586	L587	T588	P590	Y591	K592	K593	T600	D601	H604	S607	E611	I616	A617	Q618	A619	M622	L623	H628																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
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Q797	Q798	N799	M800	R801	M807	N808	G809	Y810	N811	F812	R813	D814	S815	L816	L817	V818	S819	E820	R821	Q824	R828	T829	V839	K941	D942	K943	R944	A945	L946	E947	I948	E949	Q955	L960	S961	E962	E963	L964	Q965	L966	L967	L971	F972	I975	A976	A977	Y978	L979	E982	R983	T984	P985	E986	E987	E988																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
E899	F900	L901	L902	R903	A904	L905	E908	K909	P912	K913	K914	G923	G926	T927	V933	F934	T935	R936	K941	D942	K943	R944	A945	L946	E947	I948	E949	Q955	L960	S961	E962	E963	L964	Q965	L966	L967	L971	F972	I975	A976	A977	Y978	L979	E982	R983	T984	P985	E986	E987	E988																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
A986	E987	K988	L989	D990	K991	L992	P993	R994	D995	R996	R997	L998	E999	L1000	L1001	L1002	D1003	D1004	E1005	E1006	K1007	Q1008	N1009	Q1010	L1011	E1012	Q1013	L1014	Q1017	Y1018	D1019	E1020	F1025	E1026	K1027	K1028	K1032	L1042	A1043	P1044	G1045	V1046	L1047	K1048	V1056	R1059	I1060	Y980	Q981	R982	G983	V984	E985																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
R1069	H1070	K1073	G1074	K1078	L1079	N1080	P1081	I1082	E1083	D1084	M1085	P1086	Y1087	T1092	P1093	V1094	D1095	I1096	V1097	L1098	N1099	P1100	L1101	G1102	P1103	P1104	S1105	R1106	M1107	N1108	Q1111	E1114	T1115	H1116	L1117	G1118	M1119	A1120	A1121	K1122	G1123	K1127	I1128	N1129	K1133	Q1134	V1138	A1139	L1140	L1141	R1142																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
E1143	F1144	Q1146	R1147	A1148	K1158	V1159	D1160	L1161	S1162	T1163	F1164	S1165	D1166	E1167	E1168	L1172	M1175	L1176	R1177	K1178	G1179	M1180	P1181	I1182	A1183	T1184	P1185	V1186	F1187	D1188	G1189	L1198	L1199	K1200	L1201	G1202	T1206	Q1209	R1210	R1211	L1212	Y1213	D1214	G1215	R1216	T1217	G1218	R1223	P1224	V1225	T1226																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
V1227	G1228	Y1229	M1230	Y1231	M1232	L1233	K1234	L1235	N1236	H1237	L1238	V1239	D1240	D1241	S1247	T1248	S1282	L1283	V1284	T1285	Q1286	Q1287	F1288	E1289	M1290	L1291	T1292	V1293	D1297	V1298	N1299	G1300	R1301	T1302	V1303	L1304	T1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960	L1961	L1962	L1963	L1964	L1965	L1966	L1967	L1968	L1969	L1970	L1971	L1972	L1973	L1974	L1975	L1976	L1977	L1978	L1979	L1980	L1981	L1982	L1983	L1984	L1985	L1986	L1987	L1988	L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000	L2001	L2002	L2003	L2004	L2005	L2006	L2007	L2008	L2009	L2010	L2011	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L2025	L2026	L2027	L2028	L2029	L2030	L2031	L2032	L2033	L2034	L2035	L2036	L2037	L2038	L2039	L2040	L2041	L2042	L2043	L2044	L2045	L2046	L2047	L2048	L2049	L2050	L2051	L2052	L2053	L2054	L2055	L2056	L2057	L2058	L2059	L2060	L2061	L2062	L2063	L2064	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2

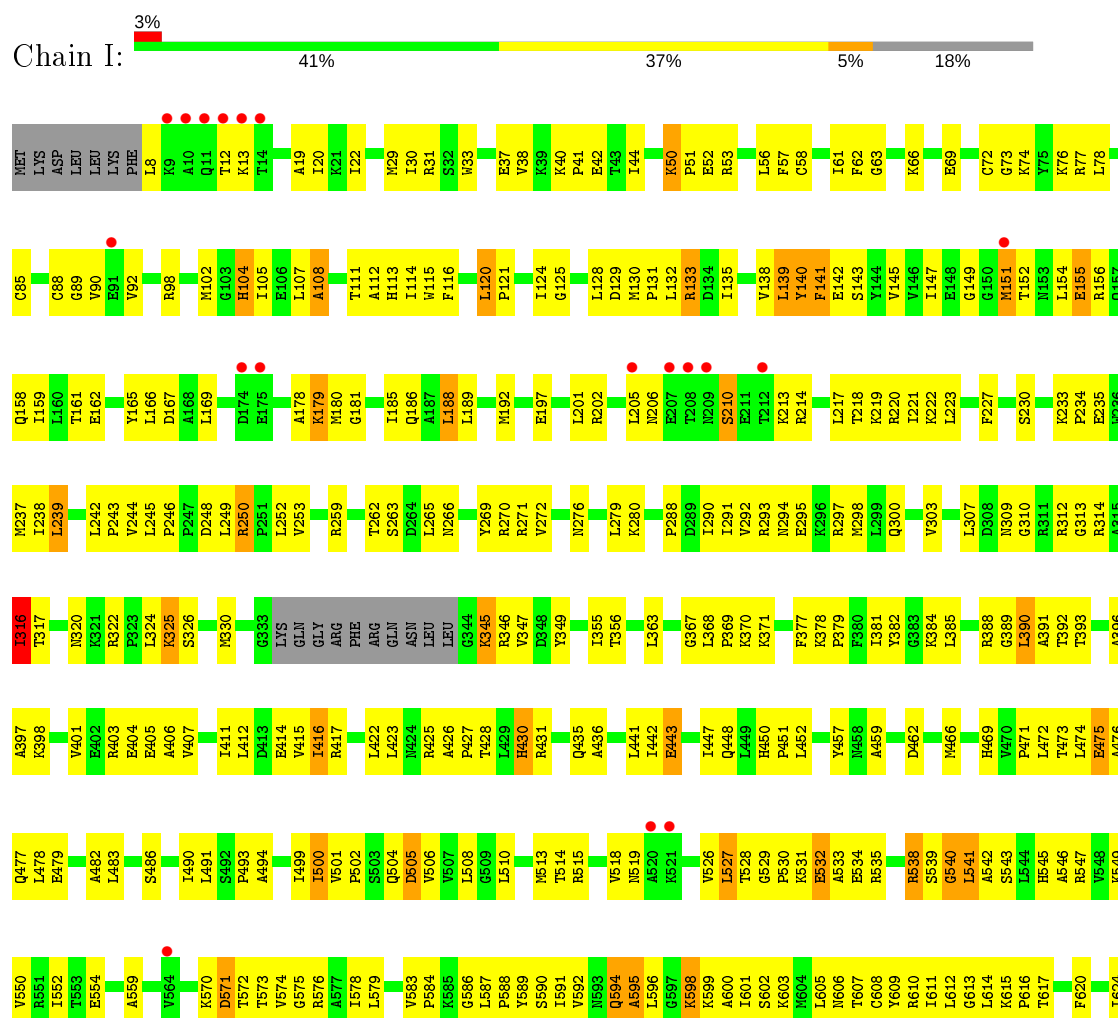


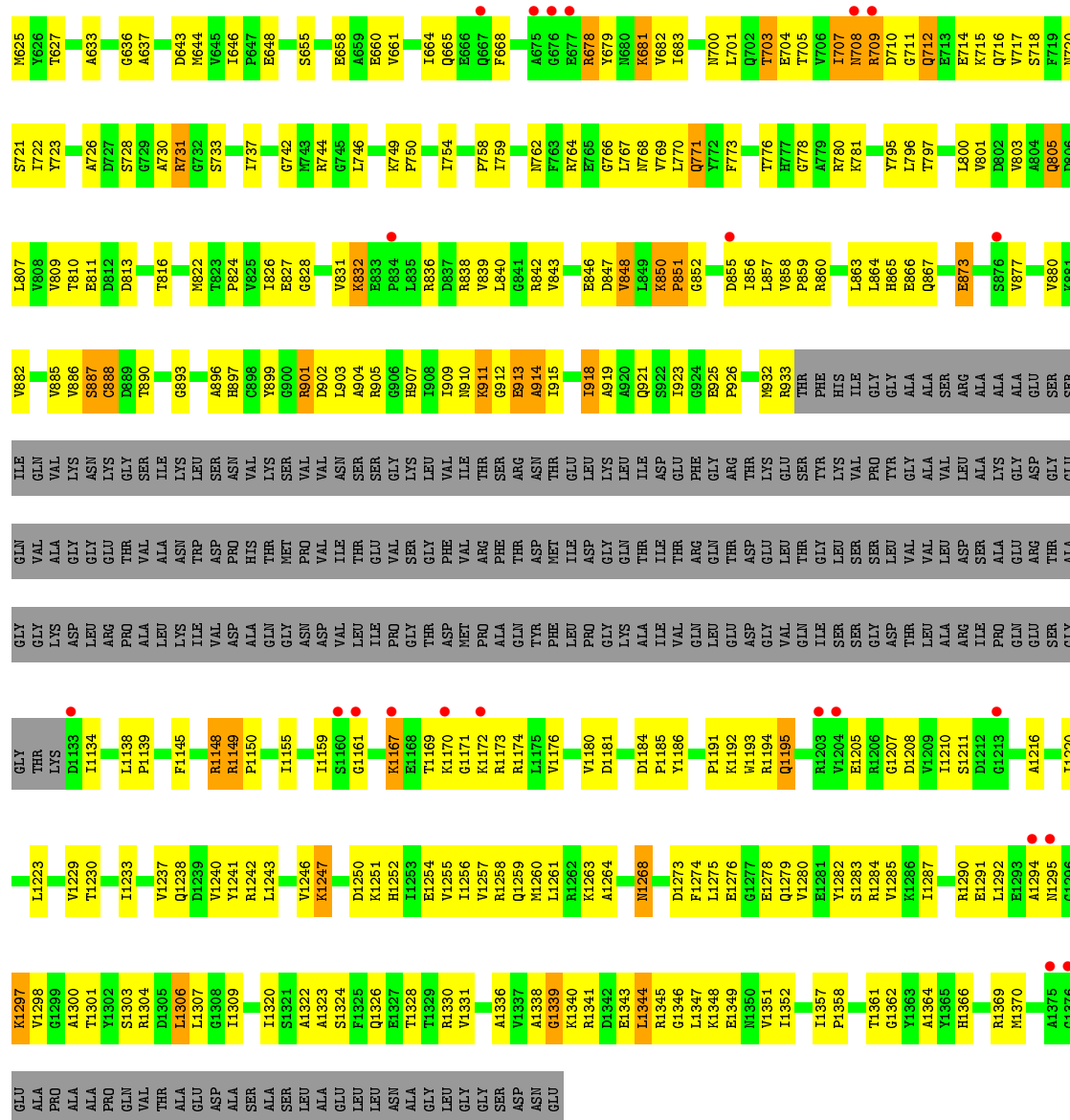
● Molecule 3: Escherichia coli RNA polymerase beta' subunit





• Molecule 3: Escherichia coli RNA polymerase beta' subunit





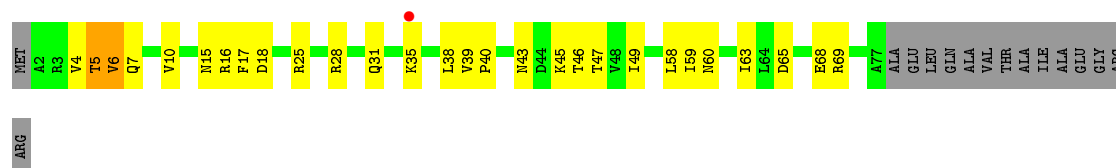
- Molecule 4: Escherichia coli RNA polymerase omega subunit

Chain E: 59% 35%

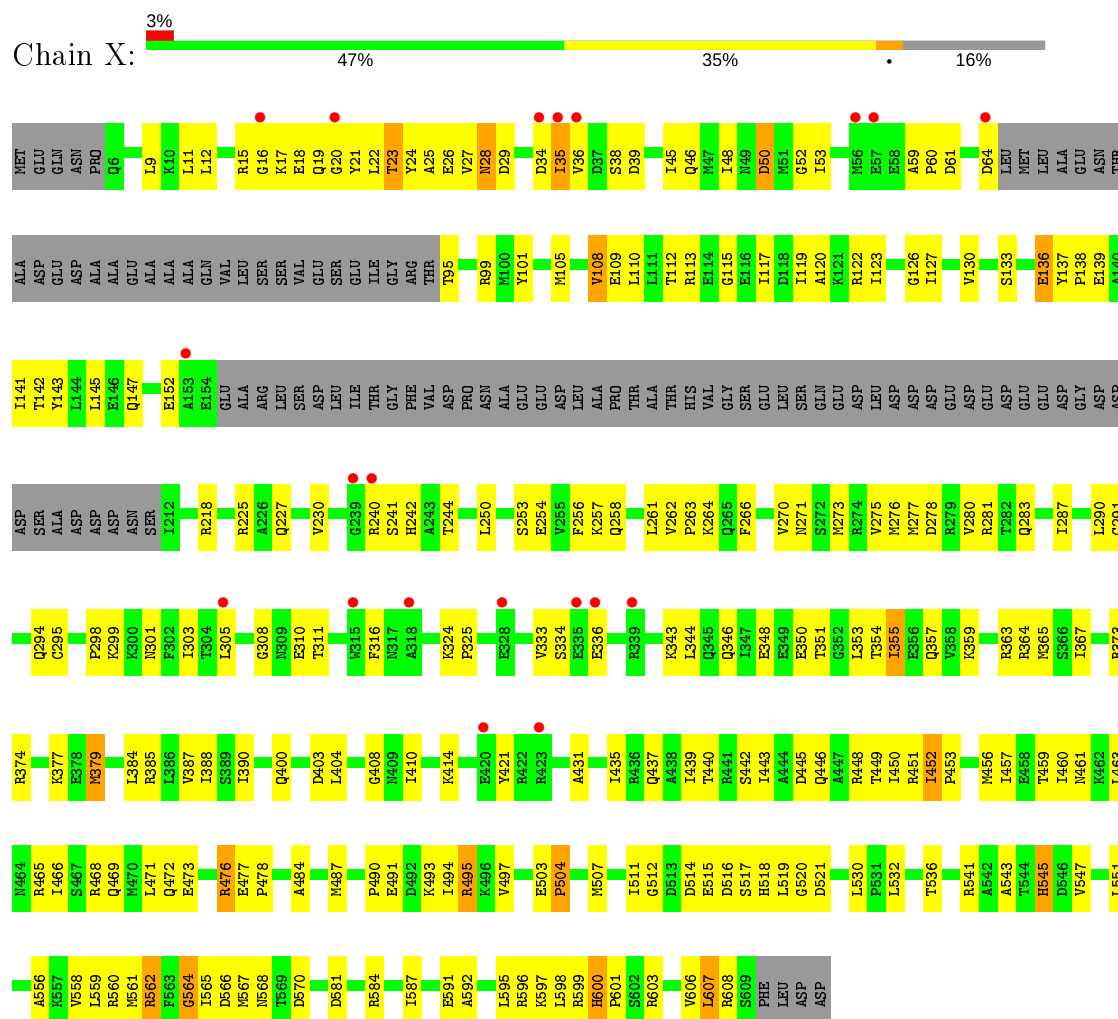


- Molecule 4: Escherichia coli RNA polymerase omega subunit

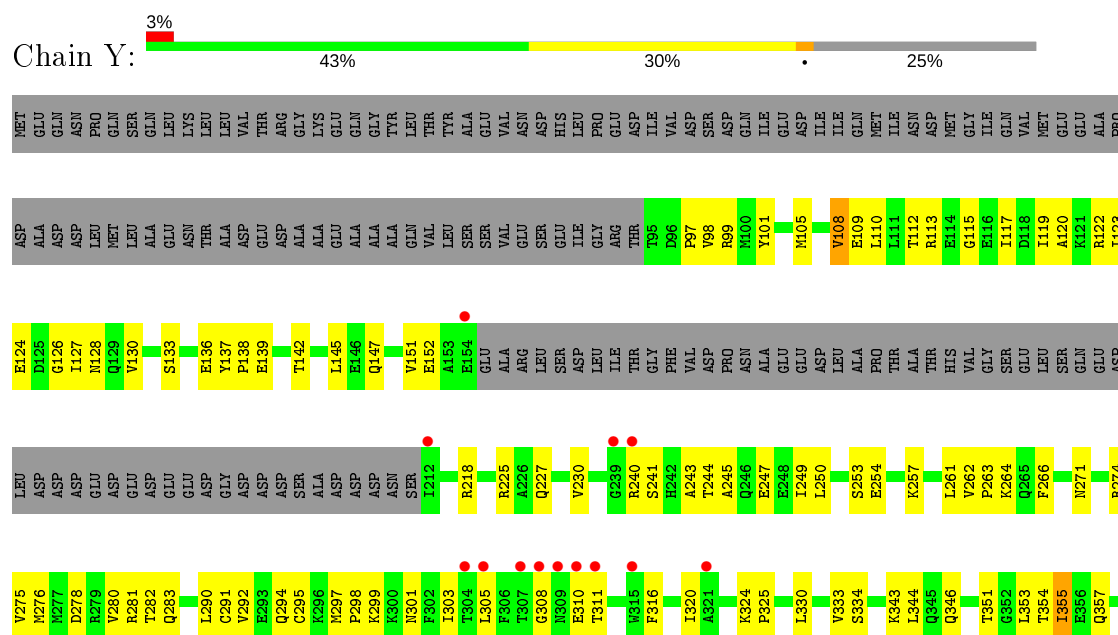
Chain J: 53% 29% 16%

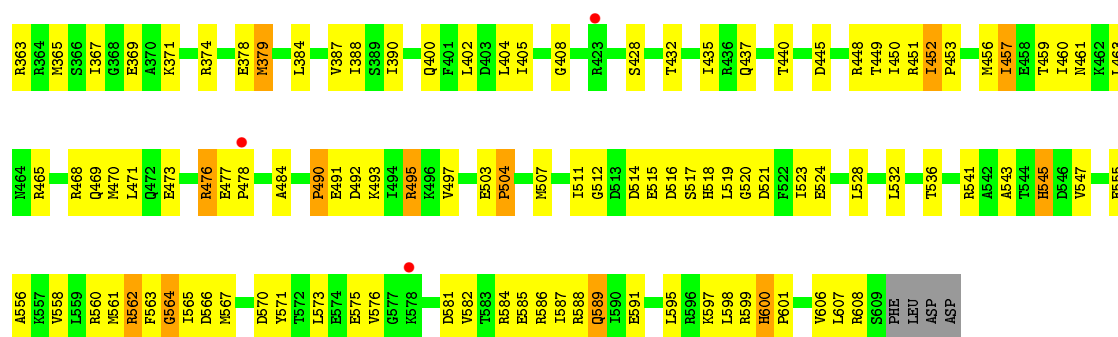


Chain X:



Chain Y:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.32Å 205.41Å 309.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 4.20 30.04 – 4.20	Depositor EDS
% Data completeness (in resolution range)	80.4 (29.94-4.20) 70.4 (30.04-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 4.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.244 , 0.322 0.244 , 0.322	Depositor DCC
R_{free} test set	3506 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	155.9	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	56129	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 0O2

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	0.19	0/2548	0.36	0/3454
1	B	0.19	0/1725	0.39	0/2337
1	F	0.19	0/1797	0.38	0/2436
1	G	0.19	0/1690	0.37	0/2290
2	C	0.20	0/10690	0.38	0/14423
2	H	0.20	0/10690	0.37	0/14423
3	D	0.20	0/9198	0.38	0/12413
3	I	0.20	0/9198	0.38	0/12413
4	E	0.19	0/710	0.38	0/956
4	J	0.19	0/607	0.37	0/817
5	X	0.19	0/4253	0.36	0/5719
5	Y	0.20	0/3783	0.36	0/5083
All	All	0.20	0/56889	0.38	0/76764

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2514	0	2566	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1706	0	1738	91	0
1	F	1775	0	1800	79	0
1	G	1671	0	1706	91	0
2	C	10523	0	10546	600	0
2	H	10523	0	10546	574	0
3	D	9060	0	9257	658	0
3	I	9060	0	9257	591	0
4	E	708	0	719	52	0
4	J	605	0	612	33	0
5	X	4198	0	4250	197	0
5	Y	3732	0	3809	157	0
6	D	2	0	0	0	0
6	I	2	0	0	0	0
7	D	40	10	16	9	0
All	All	56119	10	56822	2973	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 26.

All (2973) 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)
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.23	1.20
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.24	1.18
2:H:488:MET:HB2	2:H:490:GLN:H	1.07	1.11
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.30	1.09
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.28	1.08
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.21	1.08
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.33	1.07
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.34	1.06
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.38	1.03
2:C:54:ARG:H	2:C:55:SER:HB2	1.21	1.02
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.41	1.01
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.42	1.01
2:H:54:ARG:H	2:H:55:SER:HB2	1.19	1.01
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.42	1.01
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.41	1.01
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.40	1.00
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.38	1.00
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.44	1.00
1:F:10:LYS:HE3	1:G:226:GLU:HB3	1.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.40	0.99
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.44	0.99
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.45	0.99
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.44	0.98
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.41	0.98
2:H:1101:LEU:HD21	3:I:508:LEU:HD12	1.46	0.98
2:H:487:LEU:HB3	2:H:488:MET:HA	1.47	0.96
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.48	0.95
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.46	0.95
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.47	0.94
1:B:12:ARG:H	1:B:30:PRO:HG2	1.30	0.94
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.47	0.94
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.47	0.94
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.50	0.93
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.50	0.93
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.48	0.93
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.49	0.93
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.50	0.92
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.50	0.92
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.49	0.92
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.51	0.91
2:C:163:LYS:HD3	2:C:163:LYS:H	1.34	0.91
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.53	0.91
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.52	0.91
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.52	0.90
2:H:488:MET:HB2	2:H:490:GLN:N	1.85	0.90
3:D:546:ALA:H	3:D:547:ARG:HA	1.34	0.90
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.54	0.90
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.54	0.89
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.54	0.89
2:C:131:THR:HG21	2:C:135:THR:HG22	1.55	0.89
3:D:128:LEU:HD11	3:D:188:LEU:HD22	1.53	0.88
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.55	0.88
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	1.53	0.88
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.03	0.88
3:I:546:ALA:H	3:I:547:ARG:HA	1.37	0.88
1:F:163:GLU:HG3	1:F:170:ARG:HH12	1.38	0.88
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.55	0.87
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.56	0.87
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.57	0.87
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.57	0.87
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.57	0.86
2:H:908:GLU:HG2	2:H:909:LYS:H	1.38	0.86
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.39	0.86
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.58	0.86
2:H:876:GLU:HG3	2:H:927:THR:HG22	1.56	0.86
3:D:643:ASP:O	3:D:720:ASN:ND2	2.09	0.85
5:X:448:ARG:HD2	5:X:452:ILE:HD12	1.58	0.85
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.57	0.85
2:H:38:PHE:HE2	2:H:49:LEU:HD12	1.41	0.85
1:F:221:ALA:HB1	1:G:228:LEU:HD12	1.57	0.85
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.59	0.85
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.58	0.85
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.57	0.85
3:I:1247:LYS:HD3	3:I:1247:LYS:H	1.41	0.85
5:X:35:ILE:HG13	5:X:36:VAL:H	1.41	0.85
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.58	0.84
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.58	0.84
5:Y:448:ARG:HH12	5:Y:457:ILE:HD11	1.42	0.84
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.60	0.84
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.57	0.84
2:C:690:VAL:HG22	2:C:691:PRO:HD2	1.59	0.84
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.60	0.84
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.58	0.84
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.60	0.84
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.03	0.84
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.58	0.84
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.57	0.83
2:H:487:LEU:CB	2:H:488:MET:HA	2.07	0.83
3:D:1149:ARG:H	3:D:1149:ARG:HD3	1.43	0.83
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.59	0.83
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.59	0.83
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.60	0.83
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.59	0.82
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.04	0.82
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.62	0.82
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.60	0.82
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.61	0.82
2:H:513:GLN:HA	2:H:513:GLN:HE21	1.44	0.82
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.44	0.82
5:X:240:ARG:HD3	5:X:244:THR:HB	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.61	0.82
5:Y:453:PRO:HD2	5:Y:456:MET:HB2	1.61	0.82
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.60	0.81
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.63	0.81
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.62	0.81
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.62	0.81
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.61	0.81
3:D:487:THR:HG21	4:E:4:VAL:HG12	1.60	0.81
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.63	0.81
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.44	0.81
3:D:1247:LYS:H	3:D:1247:LYS:HD3	1.45	0.81
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.46	0.81
2:H:487:LEU:HB3	2:H:488:MET:CA	2.10	0.81
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.61	0.81
4:J:5:THR:HA	4:J:6:VAL:CB	2.11	0.81
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.17	0.80
3:I:230:SER:HB2	3:I:1339:GLY:H	1.46	0.80
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	1.60	0.80
3:D:541:LEU:H	3:D:541:LEU:HD23	1.46	0.80
3:D:828:GLY:HA2	3:D:832:LYS:H	1.45	0.80
2:H:54:ARG:N	2:H:55:SER:HB2	1.96	0.80
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.64	0.80
3:I:541:LEU:H	3:I:541:LEU:HD23	1.46	0.80
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	1.64	0.80
4:E:5:THR:HA	4:E:6:VAL:CB	2.11	0.80
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.64	0.80
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.64	0.80
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.63	0.79
2:H:163:LYS:HD3	2:H:163:LYS:H	1.48	0.79
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.64	0.79
3:D:128:LEU:HD21	3:D:188:LEU:HD13	1.65	0.79
2:C:54:ARG:N	2:C:55:SER:HB2	1.98	0.78
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.65	0.78
3:D:259:ARG:HH21	5:X:504:PRO:HB2	1.49	0.78
2:C:37:LYS:HE3	2:C:37:LYS:HA	1.65	0.78
1:F:150:ARG:HH12	1:G:8:PHE:HA	1.45	0.78
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.66	0.78
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.66	0.78
3:I:610:ARG:CG	3:I:864:LEU:HD13	2.12	0.78
3:I:259:ARG:HH21	5:Y:504:PRO:HB2	1.49	0.77
2:C:131:THR:CG2	2:C:135:THR:HG22	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.67	0.77
2:C:1304:MET:HE1	3:D:472:LEU:HD13	1.66	0.77
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.49	0.77
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.65	0.77
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.49	0.77
2:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.50	0.77
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.67	0.77
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.67	0.77
3:I:643:ASP:O	3:I:720:ASN:ND2	2.16	0.76
3:I:828:GLY:HA2	3:I:832:LYS:H	1.48	0.76
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.67	0.76
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.67	0.76
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.67	0.76
5:Y:448:ARG:HD2	5:Y:452:ILE:HD12	1.66	0.76
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.16	0.76
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.49	0.76
1:B:29:GLU:HA	1:B:200:LYS:CB	2.16	0.75
2:C:170:VAL:HG23	2:C:171:LEU:H	1.50	0.75
3:D:545:HIS:HB2	3:D:546:ALA:HB2	1.66	0.75
1:G:12:ARG:H	1:G:30:PRO:HG2	1.51	0.75
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.68	0.75
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.68	0.75
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.65	0.75
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.68	0.75
3:I:850:LYS:O	3:I:852:GLY:N	2.20	0.75
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.69	0.75
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.67	0.75
2:H:131:THR:CG2	2:H:135:THR:HG22	2.16	0.75
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.68	0.74
3:I:1261:LEU:HD21	3:I:1306:LEU:HD22	1.67	0.74
2:C:800:MET:HE2	2:C:800:MET:HA	1.67	0.74
3:I:20:ILE:HD11	3:I:1320:ILE:CD1	2.15	0.74
2:C:127:ILE:HD13	2:C:127:ILE:H	1.52	0.74
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.68	0.74
3:D:836:ARG:HH12	3:D:839:VAL:HB	1.53	0.74
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.67	0.74
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.69	0.74
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.51	0.74
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.70	0.74
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.69	0.74
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.68	0.74
3:I:422:LEU:HA	3:I:436:ALA:HA	1.69	0.74
3:I:864:LEU:HD11	3:I:901:ARG:HH12	1.53	0.74
2:H:800:MET:HE2	2:H:800:MET:HA	1.69	0.73
4:E:5:THR:HA	4:E:6:VAL:HB	1.68	0.73
2:H:1141:LEU:HD13	2:H:1141:LEU:H	1.52	0.73
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.70	0.73
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.71	0.73
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.70	0.73
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.69	0.73
4:J:5:THR:HA	4:J:6:VAL:HB	1.68	0.73
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.70	0.73
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.53	0.73
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.71	0.73
2:C:660:VAL:HG22	2:C:661:VAL:H	1.53	0.73
5:X:108:VAL:HG23	5:X:109:GLU:H	1.53	0.73
1:B:41:ASN:HD21	2:C:1217:THR:HG22	1.54	0.73
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.70	0.73
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.71	0.73
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.69	0.73
2:H:600:THR:HG22	2:H:601:ASP:H	1.53	0.73
5:X:511:ILE:HG23	5:X:512:GLY:H	1.53	0.73
3:D:546:ALA:H	3:D:547:ARG:CA	2.02	0.73
4:E:10:VAL:CG2	4:E:16:ARG:HG2	2.18	0.73
4:E:5:THR:HB	4:E:7:GLN:HB2	1.71	0.73
2:H:660:VAL:HG22	2:H:661:VAL:H	1.53	0.73
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.70	0.72
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.71	0.72
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.54	0.72
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.71	0.72
2:H:127:ILE:HD13	2:H:127:ILE:H	1.53	0.72
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.71	0.72
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.71	0.72
3:D:828:GLY:HA2	3:D:832:LYS:N	2.05	0.72
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.71	0.72
4:J:15:ASN:HD21	4:J:17:PHE:HB2	1.53	0.72
2:C:600:THR:HG22	2:C:601:ASP:H	1.53	0.72
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.71	0.72
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.70	0.72
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.71	0.72
4:J:5:THR:CA	4:J:6:VAL:HB	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.70	0.72
2:H:616:ILE:HB	2:H:637:ARG:HB2	1.71	0.72
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.71	0.72
3:D:230:SER:HB2	3:D:1339:GLY:H	1.55	0.72
3:I:1268:ASN:HB3	3:I:1300:ALA:CB	2.19	0.72
2:C:54:ARG:H	2:C:55:SER:CB	2.01	0.71
3:D:615:LYS:HD2	7:D:1503:O2:H16	1.55	0.71
2:H:54:ARG:H	2:H:55:SER:CB	1.98	0.71
1:F:11:PRO:HG2	1:G:228:LEU:H	1.55	0.71
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.21	0.71
4:E:5:THR:HB	4:E:7:GLN:H	1.54	0.71
3:I:828:GLY:HA2	3:I:832:LYS:N	2.04	0.71
2:C:1117:LEU:HD21	2:C:1182:ILE:HD13	1.72	0.71
2:H:131:THR:HG23	2:H:133:ASN:H	1.54	0.71
2:H:21:VAL:HG13	2:H:22:LEU:H	1.56	0.71
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.23	0.71
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.25	0.71
3:I:139:LEU:HD21	3:I:185:ILE:HD13	1.73	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.71	0.71
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.19	0.71
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.56	0.71
3:D:546:ALA:N	3:D:547:ARG:HA	2.04	0.71
3:I:546:ALA:N	3:I:547:ARG:HA	2.05	0.71
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.72	0.71
1:F:52:PRO:HG2	1:F:219:ARG:HH21	1.54	0.71
5:X:112:THR:HG22	5:X:113:ARG:H	1.55	0.71
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.72	0.71
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.25	0.71
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.54	0.71
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.21	0.71
3:D:423:LEU:HD21	3:D:447:ILE:HD11	1.71	0.71
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.54	0.71
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.71	0.70
2:H:131:THR:HG21	2:H:135:THR:HG22	1.71	0.70
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.73	0.70
2:C:1042:LEU:H	2:C:1042:LEU:HD13	1.56	0.70
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.73	0.70
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.74	0.70
1:B:49:SER:HA	1:B:151:GLY:HA2	1.74	0.70
2:C:360:LEU:HD13	2:C:378:ARG:HH11	1.56	0.70
2:H:142:GLU:HG2	2:H:515:MET:SD	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.22	0.70
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.72	0.70
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.26	0.70
3:I:412:LEU:O	3:I:416:ILE:HD12	1.92	0.70
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.21	0.70
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.74	0.70
2:H:91:THR:HG22	2:H:139:ASN:H	1.57	0.70
2:H:309:LEU:HD23	2:H:309:LEU:H	1.55	0.70
2:H:684:ASN:HA	2:H:687:ARG:HD3	1.74	0.70
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.74	0.70
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.56	0.70
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.21	0.70
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.27	0.70
3:I:546:ALA:H	3:I:547:ARG:CA	2.04	0.70
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.21	0.69
2:H:241:LEU:HD22	2:H:285:ILE:HD13	1.73	0.69
2:H:68:LEU:HG	2:H:100:LEU:HD23	1.73	0.69
5:X:457:ILE:O	5:X:461:ASN:ND2	2.25	0.69
2:C:302:ILE:HA	2:C:309:LEU:HA	1.73	0.69
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.27	0.69
5:X:101:TYR:HE2	5:X:388:ILE:HD11	1.57	0.69
1:B:83:LEU:HD21	3:D:551:ARG:HG3	1.72	0.69
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.72	0.69
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.74	0.69
3:D:316:ILE:HG23	3:D:317:THR:H	1.57	0.69
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.72	0.69
1:G:65:LEU:H	1:G:65:LEU:HD23	1.55	0.69
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.73	0.69
3:I:1173:ARG:HB3	3:I:1174:ARG:O	1.92	0.69
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.57	0.69
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.28	0.69
2:C:131:THR:HG23	2:C:133:ASN:H	1.57	0.69
3:D:850:LYS:O	3:D:852:GLY:N	2.25	0.69
2:H:1239:VAL:O	2:H:1241:ASP:N	2.26	0.69
5:X:139:GLU:HA	5:X:142:THR:HG22	1.74	0.69
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.75	0.69
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.74	0.69
3:I:545:HIS:HB2	3:I:546:ALA:HB2	1.74	0.69
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.74	0.69
3:I:836:ARG:HH12	3:I:839:VAL:HB	1.56	0.69
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:905:ARG:HE	3:I:907:HIS:HB2	1.56	0.69
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.28	0.69
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.75	0.69
5:X:476:ARG:H	5:X:476:ARG:HD2	1.57	0.69
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.75	0.69
2:C:309:LEU:HD23	2:C:309:LEU:H	1.56	0.68
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	1.74	0.68
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.23	0.68
3:D:932:MET:O	3:D:933:ARG:HG3	1.93	0.68
2:H:151:ARG:HH22	2:H:175:ARG:HH11	1.40	0.68
2:C:845:LEU:H	2:C:845:LEU:HD13	1.58	0.68
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.28	0.68
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.73	0.68
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.26	0.68
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.75	0.68
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.24	0.68
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.25	0.68
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.74	0.68
5:Y:573:LEU:HD21	5:Y:588:ARG:HD3	1.74	0.68
2:C:528:ARG:NH2	2:C:576:SER:O	2.27	0.68
3:D:905:ARG:HB2	4:E:16:ARG:HH12	1.59	0.68
3:D:778:GLY:HA2	3:D:781:LYS:HE3	1.75	0.68
2:H:170:VAL:HG23	2:H:171:LEU:H	1.58	0.68
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.76	0.68
5:X:298:PRO:HB2	5:X:301:ASN:HD22	1.58	0.68
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.26	0.68
3:D:142:GLU:HG2	3:D:293:ARG:HB2	1.74	0.68
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.74	0.68
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.76	0.68
1:F:192:VAL:HG21	1:F:198:LEU:HD12	1.74	0.68
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.74	0.68
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.76	0.68
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.27	0.68
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.24	0.67
2:C:488:MET:N	2:C:489:PRO:HD3	2.09	0.67
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.58	0.67
3:D:609:TYR:HE2	3:D:614:LEU:HD22	1.57	0.67
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.75	0.67
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.76	0.67
2:C:1239:VAL:O	2:C:1241:ASP:N	2.27	0.67
2:C:557:ARG:HB3	2:C:587:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:SER:CB	2:H:56:VAL:HG22	2.24	0.67
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.77	0.67
2:H:845:LEU:H	2:H:845:LEU:HD13	1.57	0.67
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.74	0.67
2:C:20:GLN:O	2:C:22:LEU:N	2.27	0.67
3:D:1173:ARG:HB3	3:D:1174:ARG:O	1.93	0.67
2:H:1042:LEU:H	2:H:1042:LEU:HD13	1.59	0.67
3:I:133:ARG:O	3:I:133:ARG:NH2	2.26	0.67
1:A:90:VAL:HG13	1:A:121:VAL:HG13	1.76	0.67
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.76	0.67
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.30	0.67
3:D:590:SER:O	3:D:594:GLN:N	2.27	0.67
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.76	0.67
1:G:45:ARG:O	3:I:538:ARG:NH2	2.27	0.67
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.77	0.67
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.27	0.67
3:D:362:ARG:HH12	7:D:1503:O2:H7	1.58	0.67
3:D:711:GLY:O	3:D:712:GLN:HG2	1.94	0.67
3:I:573:THR:HG22	3:I:576:ARG:HG3	1.77	0.67
2:H:1211:ARG:O	2:H:1211:ARG:NE	2.27	0.67
2:H:99:LYS:N	2:H:99:LYS:HD3	2.09	0.67
2:C:843:THR:HG22	2:C:844:LYS:H	1.60	0.67
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.28	0.67
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.74	0.67
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.59	0.67
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.77	0.67
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.09	0.67
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.58	0.67
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.27	0.67
2:C:403:MET:HG3	2:C:414:ILE:HB	1.77	0.67
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.76	0.67
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.77	0.66
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.60	0.66
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.77	0.66
2:C:55:SER:CB	2:C:56:VAL:HG22	2.25	0.66
2:C:533:LEU:HD23	2:C:533:LEU:H	1.60	0.66
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.76	0.66
3:D:588:PRO:HG2	3:D:591:ILE:HD11	1.76	0.66
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.26	0.66
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.24	0.66
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.76	0.66
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.60	0.66
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	1.77	0.66
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.61	0.66
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.78	0.66
2:C:106:GLU:N	2:C:107:ARG:HA	2.08	0.66
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.77	0.66
3:D:822:MET:SD	3:D:838:ARG:NH1	2.69	0.66
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.78	0.66
2:H:403:MET:HG2	2:H:407:ARG:NH1	2.10	0.66
2:H:528:ARG:NH2	2:H:576:SER:O	2.29	0.66
2:H:55:SER:CB	2:H:56:VAL:HG13	2.25	0.66
3:I:1167:LYS:HB3	3:I:1170:LYS:HD2	1.77	0.66
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.77	0.66
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.26	0.66
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.61	0.66
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.78	0.66
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.25	0.66
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.26	0.66
2:H:923:GLY:HA2	3:I:371:LYS:HE3	1.78	0.66
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.78	0.66
2:C:756:TYR:H	2:C:766:ASN:HB3	1.61	0.66
2:H:152:SER:HG	2:H:404:LYS:HZ2	1.42	0.66
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.61	0.65
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.78	0.65
3:D:139:LEU:HD21	3:D:185:ILE:HD13	1.76	0.65
5:Y:298:PRO:HB2	5:Y:301:ASN:HD22	1.60	0.65
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.77	0.65
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.77	0.65
2:H:488:MET:CB	2:H:490:GLN:H	1.95	0.65
3:I:527:LEU:HD13	3:I:531:LYS:HB3	1.78	0.65
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.29	0.65
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.78	0.65
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.79	0.65
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.76	0.65
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.79	0.65
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.60	0.65
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.78	0.65
3:I:644:MET:O	3:I:764:ARG:NH1	2.29	0.65
2:C:202:ARG:HD3	5:X:35:ILE:HB	1.77	0.65
4:E:5:THR:CA	4:E:6:VAL:HB	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:PRO:CG	1:G:228:LEU:H	2.10	0.65
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.24	0.65
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.10	0.65
3:I:827:GLU:O	3:I:831:VAL:HG12	1.96	0.65
3:I:708:ASN:OD1	3:I:712:GLN:HB2	1.97	0.65
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.78	0.65
2:C:1273:MET:HB3	3:D:428:THR:HB	1.79	0.65
2:H:1140:LYS:HE2	2:H:1166:ASP:HB3	1.78	0.65
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.62	0.65
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	1.79	0.65
3:D:588:PRO:CG	3:D:591:ILE:HD11	2.27	0.65
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.78	0.65
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.60	0.65
3:D:527:LEU:HD13	3:D:531:LYS:HB3	1.79	0.65
3:I:504:GLN:HA	3:I:730:ALA:HA	1.78	0.65
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.78	0.65
2:H:106:GLU:N	2:H:107:ARG:HA	2.10	0.64
2:H:1288:GLN:HE21	2:H:1288:GLN:HA	1.62	0.64
2:H:484:LEU:HD22	2:H:484:LEU:H	1.62	0.64
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.78	0.64
3:I:145:VAL:HG22	3:I:180:MET:SD	2.37	0.64
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.28	0.64
2:C:189:ASP:OD1	2:C:193:ASN:N	2.24	0.64
2:H:360:LEU:HD13	2:H:378:ARG:HH11	1.62	0.64
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.33	0.64
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.12	0.64
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.11	0.64
2:H:667:LEU:O	2:H:1069:ARG:NH2	2.31	0.64
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.13	0.64
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.78	0.64
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.79	0.64
3:I:711:GLY:O	3:I:712:GLN:HG2	1.97	0.64
3:I:905:ARG:HH22	4:J:10:VAL:HG11	1.63	0.64
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.63	0.64
2:C:897:PRO:HB3	5:X:564:GLY:O	1.97	0.64
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.79	0.64
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.32	0.64
1:B:227:GLN:O	1:B:228:LEU:HG	1.96	0.64
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.80	0.64
2:H:504:GLU:O	2:H:508:SER:HB3	1.98	0.64
2:C:1237:HIS:O	2:C:1238:LEU:HG	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:514:THR:HG23	3:I:576:ARG:HE	1.63	0.64
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.13	0.64
3:D:405:GLU:O	3:D:407:VAL:N	2.30	0.64
3:I:1297:LYS:NZ	3:I:1297:LYS:HA	2.13	0.64
3:I:590:SER:O	3:I:594:GLN:N	2.30	0.64
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.30	0.64
2:C:55:SER:CB	2:C:56:VAL:HG13	2.26	0.64
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.79	0.64
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.62	0.64
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.63	0.64
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.79	0.63
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.77	0.63
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.80	0.63
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.80	0.63
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.80	0.63
4:J:15:ASN:HD22	4:J:18:ASP:H	1.44	0.63
3:D:614:LEU:HG	4:E:5:THR:HG21	1.79	0.63
3:I:809:VAL:HG13	3:I:912:GLY:H	1.64	0.63
2:H:1237:HIS:O	2:H:1238:LEU:HG	1.99	0.63
3:I:1155:ILE:HG13	3:I:1210:ILE:CG2	2.28	0.63
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.78	0.63
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.80	0.63
3:D:932:MET:SD	3:D:932:MET:N	2.67	0.63
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.32	0.63
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.79	0.63
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.81	0.63
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.29	0.63
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.81	0.63
3:I:598:LYS:NZ	3:I:726:ALA:O	2.32	0.63
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.80	0.63
1:A:284:ARG:NH1	1:A:288:GLU:HG3	2.13	0.63
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.81	0.63
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.30	0.63
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.29	0.63
2:H:1273:MET:HB3	3:I:428:THR:HB	1.81	0.63
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.80	0.63
3:D:149:GLY:HA2	3:D:156:ARG:HG2	1.81	0.63
3:D:27:PRO:O	3:D:31:ARG:HD3	1.98	0.63
1:F:231:PHE:CZ	1:G:39:LEU:HD13	2.26	0.63
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.30	0.63
2:H:727:VAL:HG22	2:H:773:LEU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.63	0.63
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.33	0.62
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.29	0.62
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.32	0.62
3:I:513:MET:HE2	3:I:579:LEU:HB2	1.81	0.62
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.63	0.62
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.17	0.62
2:C:11:ILE:HG21	2:C:697:LYS:NZ	2.13	0.62
1:A:11:PRO:HD3	1:B:227:GLN:HG3	1.80	0.62
2:C:21:VAL:HG13	2:C:22:LEU:H	1.63	0.62
3:D:573:THR:HG22	3:D:576:ARG:CG	2.29	0.62
2:H:176:ILE:HD11	2:H:428:VAL:HG21	1.81	0.62
3:I:850:LYS:HD2	3:I:851:PRO:CD	2.19	0.62
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.34	0.62
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.82	0.62
2:C:634:VAL:H	2:C:645:PHE:HE2	1.47	0.62
2:C:714:VAL:HG23	2:C:787:PRO:HD2	1.82	0.62
2:H:678:ARG:HE	2:H:1106:ARG:HG2	1.65	0.62
2:H:1252:SER:OG	2:H:1255:THR:O	2.17	0.62
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.82	0.62
3:D:107:LEU:HD12	3:D:107:LEU:H	1.64	0.62
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.15	0.62
2:H:91:THR:HG22	2:H:139:ASN:N	2.14	0.62
2:H:20:GLN:O	2:H:22:LEU:N	2.32	0.62
2:H:562:GLU:HG2	2:H:574:SER:CB	2.29	0.62
3:I:579:LEU:HD23	3:I:627:THR:HG21	1.81	0.62
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.30	0.62
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.65	0.62
3:D:77:ARG:HG3	3:D:78:LEU:H	1.62	0.62
4:E:5:THR:HA	4:E:6:VAL:CG1	2.30	0.62
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.14	0.62
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.64	0.62
2:C:241:LEU:HD22	2:C:285:ILE:HD13	1.82	0.62
2:C:901:LEU:O	2:C:905:ILE:HG13	2.00	0.62
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.82	0.62
2:H:660:VAL:O	2:H:661:VAL:HG22	2.00	0.62
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.32	0.62
3:I:262:THR:OG1	3:I:266:ASN:ND2	2.25	0.62
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.14	0.62
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.64	0.62
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.82	0.62
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.82	0.62
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.81	0.61
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.81	0.61
1:B:49:SER:OG	3:D:538:ARG:NH2	2.33	0.61
4:E:5:THR:HA	4:E:6:VAL:HG12	1.82	0.61
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.81	0.61
2:C:1244:HIS:HB3	2:C:1265:PHE:CD2	2.34	0.61
3:D:205:LEU:HD22	3:D:217:LEU:CD2	2.29	0.61
3:D:768:ASN:O	3:D:771:GLN:NE2	2.34	0.61
2:H:1078:LYS:HG2	2:H:1079:ILE:H	1.65	0.61
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.33	0.61
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.82	0.61
3:I:213:LYS:O	3:I:217:LEU:HG	1.99	0.61
1:B:227:GLN:O	1:B:229:GLU:N	2.30	0.61
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.82	0.61
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.81	0.61
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.01	0.61
2:H:908:GLU:HG2	2:H:909:LYS:N	2.14	0.61
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.29	0.61
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.34	0.61
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.27	0.61
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.31	0.61
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.81	0.61
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.01	0.61
1:F:9:LEU:O	1:G:227:GLN:NE2	2.33	0.61
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.33	0.61
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.23	0.61
3:D:720:ASN:O	3:D:722:ILE:N	2.34	0.61
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.65	0.61
2:H:152:SER:OG	2:H:404:LYS:NZ	2.25	0.61
3:I:139:LEU:HD13	3:I:140:TYR:N	2.16	0.61
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.16	0.61
3:I:77:ARG:HG3	3:I:78:LEU:H	1.64	0.61
4:J:5:THR:HA	4:J:6:VAL:CG1	2.30	0.61
2:H:487:LEU:HB3	2:H:488:MET:CG	2.30	0.61
3:I:107:LEU:HD12	3:I:107:LEU:H	1.65	0.61
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.82	0.61
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.82	0.61
3:D:1191:PRO:O	3:D:1193:TRP:N	2.32	0.61
3:D:1362:GLY:O	3:D:1364:ALA:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:422:LEU:HA	3:D:436:ALA:HA	1.83	0.61
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.29	0.61
3:I:1191:PRO:O	3:I:1193:TRP:N	2.33	0.61
1:B:65:LEU:HD23	1:B:65:LEU:H	1.65	0.61
2:C:91:THR:HG22	2:C:139:ASN:H	1.65	0.61
3:D:139:LEU:HD13	3:D:140:TYR:N	2.16	0.61
3:D:527:LEU:HD12	3:D:535:ARG:NE	2.15	0.61
3:D:827:GLU:O	3:D:831:VAL:HG12	2.00	0.61
2:H:517:GLN:HE21	2:H:760:ASN:H	1.48	0.61
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.83	0.61
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.83	0.61
2:H:714:VAL:HG23	2:H:787:PRO:HD2	1.83	0.61
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.66	0.60
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.65	0.60
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.83	0.60
3:D:1338:ALA:O	3:D:1340:LYS:N	2.34	0.60
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.36	0.60
2:H:55:SER:HB3	2:H:56:VAL:CB	2.31	0.60
2:H:618:GLN:OE1	2:H:637:ARG:NH1	2.33	0.60
3:I:1297:LYS:HA	3:I:1297:LYS:HZ3	1.66	0.60
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.32	0.60
1:G:49:SER:OG	3:I:538:ARG:NH2	2.33	0.60
2:C:747:GLY:O	2:C:748:ILE:HG13	2.00	0.60
2:C:752:ASN:O	2:C:753:LEU:HG	2.01	0.60
4:E:13:ILE:HD11	4:E:19:LEU:HD23	1.82	0.60
1:G:191:ARG:NH2	3:I:442:ILE:HA	2.17	0.60
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.67	0.60
2:H:892:GLU:O	2:H:893:THR:OG1	2.19	0.60
3:I:233:LYS:HD2	3:I:234:PRO:HD2	1.83	0.60
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.83	0.60
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.36	0.60
2:C:517:GLN:HE21	2:C:760:ASN:H	1.49	0.60
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.01	0.60
3:D:202:ARG:O	3:D:206:ASN:ND2	2.34	0.60
2:H:1304:MET:HE1	3:I:472:LEU:HD13	1.83	0.60
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.82	0.60
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.82	0.60
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.82	0.60
3:I:252:LEU:HD23	3:I:252:LEU:H	1.66	0.60
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.34	0.60
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:584:ARG:O	5:X:587:ILE:HG22	2.01	0.60
5:X:595:LEU:O	5:X:599:ARG:NH1	2.35	0.60
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.35	0.60
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.83	0.60
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.84	0.60
1:G:191:ARG:HH22	3:I:442:ILE:HA	1.67	0.60
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.82	0.60
1:G:181:GLU:HG2	3:I:531:LYS:HD3	1.83	0.60
4:J:5:THR:HB	4:J:7:GLN:HB2	1.83	0.60
2:C:1252:SER:OG	2:C:1255:THR:O	2.19	0.60
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.16	0.60
2:C:963:GLU:O	2:C:966:ILE:HG22	2.02	0.60
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.35	0.60
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.66	0.60
5:X:240:ARG:O	5:X:242:HIS:N	2.34	0.60
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.84	0.60
2:C:562:GLU:HG2	2:C:574:SER:CB	2.31	0.60
3:D:500:ILE:H	3:D:500:ILE:HD13	1.65	0.60
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.65	0.60
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.35	0.60
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.02	0.60
5:X:9:LEU:HD22	5:X:60:PRO:HB3	1.82	0.60
3:D:145:VAL:HG22	3:D:180:MET:SD	2.41	0.60
3:D:85:CYS:HB3	3:D:88:CYS:O	2.02	0.60
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.17	0.60
2:H:800:MET:HA	2:H:800:MET:CE	2.32	0.60
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.32	0.60
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.37	0.60
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.17	0.60
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.35	0.60
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.65	0.60
3:D:128:LEU:CD1	3:D:192:MET:HE3	2.28	0.60
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.84	0.60
3:D:579:LEU:HD23	3:D:627:THR:HG21	1.82	0.60
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.17	0.60
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.83	0.60
3:D:151:MET:N	3:D:151:MET:SD	2.74	0.60
3:D:252:LEU:HD23	3:D:252:LEU:H	1.67	0.60
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.66	0.60
3:I:1338:ALA:O	3:I:1340:LYS:N	2.35	0.60
3:I:554:GLU:HA	3:I:589:TYR:HD2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:894:GLN:HE21	3:I:77:ARG:HD3	1.66	0.60
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.83	0.60
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.67	0.59
2:C:660:VAL:O	2:C:661:VAL:HG22	2.01	0.59
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.36	0.59
3:D:546:ALA:HB3	3:D:547:ARG:O	2.02	0.59
2:H:646:SER:HB2	2:H:649:GLN:HG3	1.84	0.59
3:I:681:LYS:NZ	3:I:681:LYS:HB2	2.17	0.59
3:I:863:LEU:HB2	3:I:866:GLU:HB2	1.83	0.59
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.83	0.59
3:D:473:THR:HB	3:D:476:ALA:HB2	1.83	0.59
3:D:66:LYS:HG3	3:D:69:GLU:OE2	2.01	0.59
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.30	0.59
3:D:583:VAL:CG1	3:D:587:LEU:HD22	2.31	0.59
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.32	0.59
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.83	0.59
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.32	0.59
2:C:619:ALA:HA	2:C:653:MET:HE2	1.84	0.59
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.68	0.59
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.84	0.59
2:H:543:ALA:HB1	2:H:548:ARG:HD2	1.85	0.59
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.85	0.59
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.84	0.59
3:I:720:ASN:O	3:I:722:ILE:N	2.35	0.59
4:J:5:THR:HA	4:J:6:VAL:HG12	1.82	0.59
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.17	0.59
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.33	0.59
2:C:163:LYS:HD3	2:C:163:LYS:N	2.14	0.59
3:D:316:ILE:HG23	3:D:317:THR:N	2.17	0.59
1:F:158:ARG:NH2	1:F:162:GLU:HB3	2.18	0.59
2:H:130:MET:SD	2:H:134:GLY:HA2	2.42	0.59
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.85	0.59
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.68	0.59
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.85	0.59
2:C:372:PRO:CB	5:X:34:ASP:HB3	2.31	0.59
5:X:442:SER:OG	5:X:446:GLN:NE2	2.34	0.59
3:D:125:GLY:O	3:D:129:ASP:N	2.36	0.59
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.83	0.59
3:D:858:VAL:HB	3:D:859:PRO:CD	2.26	0.59
4:E:45:LYS:O	4:E:49:ILE:HG12	2.03	0.59
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:50:LYS:NZ	3:I:50:LYS:HB3	2.18	0.59
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.84	0.59
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.83	0.59
2:C:801:ARG:NH1	2:C:1093:PRO:O	2.36	0.59
1:G:176:CYS:O	1:G:178:SER:N	2.33	0.59
2:H:1141:LEU:CD1	2:H:1141:LEU:H	2.15	0.59
2:H:94:ALA:N	2:H:126:GLU:OE2	2.27	0.59
2:C:91:THR:HG22	2:C:138:ILE:HA	1.85	0.59
3:D:213:LYS:O	3:D:217:LEU:HG	2.01	0.59
3:D:389:GLY:O	3:D:391:ALA:N	2.36	0.59
3:D:589:TYR:O	3:D:591:ILE:N	2.34	0.59
2:H:69:GLN:HE22	2:H:101:ARG:HH21	1.50	0.59
3:I:1261:LEU:CD2	3:I:1306:LEU:HD22	2.32	0.59
3:I:588:PRO:CG	3:I:591:ILE:HD11	2.33	0.59
3:D:313:GLY:H	5:X:38:SER:HB3	1.67	0.59
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.32	0.59
2:C:1288:GLN:HE21	2:C:1288:GLN:HA	1.68	0.59
4:E:14:GLY:O	4:E:15:ASN:ND2	2.36	0.59
1:F:234:LEU:HD22	1:G:214:GLU:OE2	2.03	0.59
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.85	0.59
2:H:302:ILE:HG22	2:H:309:LEU:HB3	1.85	0.59
3:I:128:LEU:HD11	3:I:188:LEU:HD22	1.84	0.59
3:I:704:GLU:HB2	3:I:718:SER:HG	1.67	0.59
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.85	0.59
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.02	0.59
5:X:515:GLU:N	5:X:516:ASP:HA	2.18	0.59
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	1.84	0.59
5:Y:119:ILE:HG21	5:Y:379:MET:HG2	1.85	0.58
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.18	0.58
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.86	0.58
3:D:186:GLN:CB	3:D:238:ILE:HD11	2.28	0.58
3:D:554:GLU:HA	3:D:589:TYR:HD2	1.67	0.58
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.86	0.58
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.37	0.58
3:I:85:CYS:HB3	3:I:88:CYS:O	2.02	0.58
3:D:114:ILE:HG21	3:D:308:ASP:HB3	1.83	0.58
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.39	0.58
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.39	0.58
2:H:99:LYS:H	2:H:99:LYS:HD3	1.68	0.58
3:I:707:ILE:HG22	3:I:708:ASN:H	1.68	0.58
2:C:42:ASP:O	2:C:44:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.85	0.58
3:D:809:VAL:HG13	3:D:912:GLY:H	1.66	0.58
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.18	0.58
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.04	0.58
2:C:1314:GLN:HG3	4:E:28:ARG:NH1	2.18	0.58
2:C:387:ASN:HB3	2:C:394:ARG:HG3	1.86	0.58
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.33	0.58
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.36	0.58
2:H:747:GLY:O	2:H:748:ILE:HG13	2.03	0.58
3:I:142:GLU:HG2	3:I:293:ARG:HB2	1.84	0.58
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.84	0.58
3:I:768:ASN:O	3:I:771:GLN:NE2	2.37	0.58
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.34	0.58
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.84	0.58
5:Y:355:ILE:HD13	5:Y:355:ILE:O	2.03	0.58
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.02	0.58
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.85	0.58
3:I:550:VAL:HG23	3:I:552:ILE:HD11	1.86	0.58
5:X:517:SER:O	5:X:518:HIS:ND1	2.37	0.58
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.68	0.58
2:C:800:MET:HA	2:C:800:MET:CE	2.34	0.58
3:D:19:ALA:HA	3:D:1344:LEU:HD12	1.86	0.58
3:D:504:GLN:HA	3:D:730:ALA:HA	1.84	0.58
3:I:120:LEU:HD22	3:I:1330:ARG:CD	2.34	0.58
3:I:246:PRO:HB2	3:I:249:LEU:HD13	1.85	0.58
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.86	0.58
1:A:104:LYS:HD3	1:A:105:SER:N	2.19	0.58
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.37	0.58
2:C:1200:LYS:O	2:C:1202:GLY:N	2.34	0.58
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.85	0.58
2:C:166:SER:O	2:C:168:GLY:N	2.34	0.58
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.84	0.58
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.86	0.58
3:I:701:LEU:HD23	3:I:723:TYR:HB2	1.86	0.58
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.19	0.58
1:B:149:GLY:HA3	1:B:177:TYR:CE2	2.39	0.58
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.68	0.58
3:D:709:ARG:O	3:D:711:GLY:N	2.37	0.58
1:G:49:SER:HA	1:G:151:GLY:HA2	1.86	0.58
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.39	0.58
2:H:1101:LEU:CD1	3:I:504:GLN:HB2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:591:ILE:HA	3:I:594:GLN:HB2	1.86	0.58
3:I:478:LEU:HD12	4:J:47:THR:HG23	1.86	0.58
2:C:845:LEU:HD23	2:C:889:PRO:HG2	1.85	0.58
2:H:237:LEU:HD13	2:H:292:ILE:HD12	1.85	0.58
3:I:125:GLY:O	3:I:129:ASP:N	2.37	0.58
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.85	0.57
2:C:54:ARG:HG2	2:C:55:SER:CB	2.34	0.57
2:C:898:GLU:N	2:C:898:GLU:OE1	2.34	0.57
3:D:610:ARG:CG	3:D:864:LEU:HD13	2.27	0.57
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.19	0.57
3:I:389:GLY:O	3:I:391:ALA:N	2.37	0.57
1:B:176:CYS:C	1:B:178:SER:H	2.08	0.57
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.33	0.57
2:C:55:SER:HB3	2:C:56:VAL:CB	2.34	0.57
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.86	0.57
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.29	0.57
2:H:189:ASP:OD1	2:H:193:ASN:N	2.31	0.57
5:X:35:ILE:HG23	5:X:36:VAL:HG13	1.86	0.57
5:Y:457:ILE:HG23	5:Y:461:ASN:HD21	1.69	0.57
1:B:64:VAL:HG13	1:B:69:SER:OG	2.04	0.57
3:D:179:LYS:H	3:D:179:LYS:HD3	1.69	0.57
2:H:564:PRO:HA	2:H:684:ASN:HD21	1.69	0.57
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.86	0.57
5:Y:283:GLN:NE2	5:Y:343:LYS:HD2	2.19	0.57
2:C:94:ALA:N	2:C:126:GLU:OE2	2.25	0.57
2:C:406:ASN:HB3	2:C:411:ARG:HB2	1.85	0.57
3:D:1237:VAL:O	3:D:1240:VAL:HG22	2.04	0.57
1:F:181:GLU:OE1	1:F:181:GLU:N	2.38	0.57
2:H:1200:LYS:O	2:H:1202:GLY:N	2.36	0.57
3:I:1297:LYS:CE	3:I:1297:LYS:HA	2.34	0.57
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.19	0.57
3:D:395:LYS:HG3	5:X:536:THR:CG2	2.34	0.57
3:D:393:THR:HG21	5:X:607:LEU:HD22	1.86	0.57
2:C:24:VAL:HG11	2:C:704:MET:HE1	1.87	0.57
3:D:120:LEU:CB	3:D:121:PRO:CD	2.81	0.57
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.05	0.57
3:D:131:PRO:HG2	3:D:135:ILE:HD13	1.87	0.57
3:D:619:ILE:HD13	7:D:1503:O2:O3D	2.05	0.57
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.86	0.57
3:D:423:LEU:CD2	3:D:447:ILE:HD11	2.35	0.57
3:D:744:ARG:HB2	3:D:759:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:VAL:O	1:G:20:SER:OG	2.17	0.57
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	1.86	0.57
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.37	0.57
5:X:17:LYS:N	5:X:18:GLU:HA	2.19	0.57
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.40	0.57
3:I:202:ARG:O	3:I:206:ASN:ND2	2.33	0.57
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.39	0.57
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.86	0.57
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.34	0.57
3:I:704:GLU:HB2	3:I:718:SER:OG	2.05	0.57
5:Y:119:ILE:HD12	5:Y:122:ARG:HH21	1.69	0.57
1:A:318:LEU:O	1:A:320:ASN:N	2.33	0.57
3:D:1343:GLU:HA	3:D:1344:LEU:CB	2.31	0.57
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.86	0.57
2:H:533:LEU:HD23	2:H:533:LEU:H	1.69	0.57
3:I:1280:VAL:HA	3:I:1283:SER:HB2	1.87	0.57
3:I:824:PRO:O	3:I:826:ILE:HG13	2.05	0.57
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.86	0.57
2:C:106:GLU:H	2:C:107:ARG:HA	1.70	0.57
3:D:886:VAL:CG1	3:D:1230:THR:HG21	2.35	0.57
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.85	0.57
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.40	0.57
2:H:753:LEU:HD12	2:H:753:LEU:O	2.05	0.57
3:I:905:ARG:HG2	3:I:907:HIS:H	1.70	0.57
5:X:503:GLU:N	5:X:504:PRO:HA	2.20	0.57
2:C:403:MET:HG2	2:C:407:ARG:HH12	1.70	0.57
4:E:15:ASN:HD21	4:E:18:ASP:HB2	1.70	0.57
3:I:88:CYS:O	3:I:90:VAL:N	2.38	0.57
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.85	0.56
1:B:42:ALA:O	1:B:46:ILE:HG12	2.04	0.56
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.34	0.56
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.70	0.56
3:D:417:ARG:HH12	4:E:3:ARG:HH22	1.53	0.56
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.05	0.56
5:Y:600:HIS:HB2	5:Y:601:PRO:HD3	1.87	0.56
1:A:227:GLN:HE22	1:B:11:PRO:HD3	1.71	0.56
1:B:65:LEU:HA	1:B:169:GLY:HA2	1.87	0.56
2:C:542:ARG:O	2:C:544:GLY:N	2.34	0.56
3:D:141:PHE:O	3:D:297:ARG:HD3	2.04	0.56
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.35	0.56
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:496:LYS:N	2:H:497:PRO:HD2	2.20	0.56
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.05	0.56
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.05	0.56
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.04	0.56
2:H:1111:GLN:HG3	2:H:1230:MET:HE2	1.87	0.56
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.38	0.56
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.70	0.56
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.35	0.56
2:C:13:LYS:CE	2:C:1183:ALA:HB2	2.31	0.56
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.05	0.56
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.88	0.56
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.35	0.56
2:H:548:ARG:NH2	2:H:567:PRO:O	2.39	0.56
3:I:546:ALA:HB3	3:I:547:ARG:O	2.06	0.56
3:I:919:ALA:O	3:I:923:ILE:HG12	2.05	0.56
5:X:503:GLU:HB3	5:X:504:PRO:O	2.05	0.56
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.87	0.56
1:A:232:VAL:HA	1:B:218:ARG:HG3	1.87	0.56
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.25	0.56
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.36	0.56
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.86	0.56
3:D:316:ILE:HG13	3:D:317:THR:N	2.21	0.56
3:D:905:ARG:NH2	4:E:10:VAL:HG11	2.20	0.56
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.41	0.56
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.70	0.56
5:X:390:ILE:HD11	5:X:435:ILE:CG2	2.35	0.56
3:D:545:HIS:HB2	3:D:546:ALA:CB	2.35	0.56
3:D:850:LYS:HD2	3:D:851:PRO:CD	2.26	0.56
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.87	0.56
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.86	0.56
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.17	0.56
3:D:51:PRO:HB3	3:D:57:PHE:O	2.05	0.56
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.26	0.56
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.40	0.56
2:H:488:MET:H	2:H:489:PRO:HA	1.70	0.56
3:I:478:LEU:CD1	4:J:47:THR:HG23	2.36	0.56
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.87	0.56
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.85	0.56
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.87	0.56
3:D:1155:ILE:HG13	3:D:1210:ILE:CG2	2.30	0.56
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1341:ARG:NH2	3:D:1343:GLU:OE1	2.37	0.56
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.70	0.56
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.20	0.56
2:H:367:TYR:CD1	2:H:384:LEU:HD13	2.40	0.56
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.41	0.56
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.87	0.56
3:D:1148:ARG:HB2	3:D:1148:ARG:NH2	2.21	0.56
3:D:1369:ARG:NH1	3:D:1369:ARG:HB3	2.19	0.56
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.06	0.56
3:D:488:ASN:HD21	4:E:6:VAL:CG1	2.19	0.56
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.36	0.56
3:D:905:ARG:HH22	4:E:10:VAL:HG11	1.71	0.56
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.87	0.56
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.88	0.56
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.41	0.56
5:X:22:LEU:HD13	5:X:48:ILE:HD12	1.88	0.56
2:C:753:LEU:O	2:C:753:LEU:HD12	2.06	0.56
3:D:166:LEU:HD12	3:D:167:ASP:N	2.21	0.56
2:H:810:TYR:CE1	2:H:1078:LYS:HD2	2.41	0.56
3:I:1362:GLY:O	3:I:1364:ALA:N	2.37	0.56
5:X:363:ARG:O	5:X:367:ILE:HG12	2.05	0.56
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.87	0.56
3:I:1280:VAL:HG11	3:I:1304:ARG:NE	2.19	0.56
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.36	0.56
5:Y:476:ARG:HD2	5:Y:476:ARG:H	1.71	0.56
2:C:487:LEU:HD13	2:C:488:MET:H	1.71	0.55
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	1.88	0.55
3:I:914:ALA:O	3:I:918:ILE:HG22	2.05	0.55
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.88	0.55
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.35	0.55
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.21	0.55
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.88	0.55
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.41	0.55
2:H:505:PHE:O	2:H:512:SER:OG	2.23	0.55
2:H:531:SER:OG	2:H:533:LEU:HD23	2.06	0.55
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.88	0.55
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.27	0.55
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.39	0.55
3:D:919:ALA:O	3:D:923:ILE:HG12	2.06	0.55
1:F:10:LYS:HD2	1:G:226:GLU:O	2.06	0.55
2:H:9:LYS:HD3	2:H:9:LYS:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1344:LEU:H	3:I:1345:ARG:HG3	1.71	0.55
3:I:166:LEU:HD12	3:I:167:ASP:N	2.20	0.55
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.87	0.55
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.36	0.55
3:D:813:ASP:OD1	3:D:896:ALA:HB3	2.06	0.55
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.05	0.55
2:H:639:LYS:HE2	2:H:639:LYS:HA	1.88	0.55
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.89	0.55
3:I:573:THR:HG22	3:I:576:ARG:CG	2.37	0.55
5:X:120:ALA:CB	5:X:421:TYR:HB3	2.36	0.55
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.37	0.55
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.69	0.55
2:C:681:MET:O	2:C:685:MET:HG2	2.06	0.55
3:D:368:LEU:HG	3:D:373:ALA:HB2	1.88	0.55
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.89	0.55
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.37	0.55
2:C:646:SER:HB2	2:C:649:GLN:HG3	1.89	0.55
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.89	0.55
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.72	0.55
2:H:178:PRO:HA	2:H:397:LEU:HD23	1.89	0.55
2:H:263:VAL:HG22	2:H:273:HIS:CD2	2.40	0.55
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.87	0.55
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.71	0.55
4:J:4:VAL:O	4:J:5:THR:OG1	2.23	0.55
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.42	0.55
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.42	0.55
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.27	0.55
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.88	0.55
3:D:473:THR:HB	3:D:476:ALA:CB	2.37	0.55
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.40	0.55
1:F:158:ARG:HH11	1:F:172:LEU:HD11	1.70	0.55
3:I:120:LEU:CB	3:I:121:PRO:CD	2.85	0.55
2:C:817:LEU:HD21	2:C:1080:ASN:HB2	1.87	0.55
1:G:42:ALA:O	1:G:46:ILE:HG12	2.07	0.55
2:H:664:GLY:O	2:H:686:GLN:NE2	2.39	0.55
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.06	0.55
5:X:379:MET:CE	5:X:379:MET:HA	2.36	0.55
5:Y:387:VAL:HG13	5:Y:408:GLY:HA3	1.88	0.55
1:A:282:VAL:HG22	1:A:316:MET:HE2	1.89	0.55
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.42	0.55
2:C:496:LYS:N	2:C:497:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:894:GLN:O	2:C:895:LEU:HB2	2.06	0.55
3:D:905:ARG:HG2	3:D:907:HIS:H	1.72	0.55
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.24	0.55
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.88	0.55
1:A:11:PRO:HB3	1:A:31:LEU:CD2	2.35	0.55
2:C:142:GLU:HG2	2:C:515:MET:SD	2.47	0.55
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.89	0.55
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.88	0.55
1:G:86:LYS:NZ	3:I:526:VAL:O	2.39	0.55
2:H:106:GLU:HG2	2:H:109:ALA:H	1.71	0.55
2:H:1284:ALA:HB3	3:I:1361:THR:HB	1.88	0.55
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.07	0.55
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.35	0.55
3:I:500:ILE:HD13	3:I:500:ILE:H	1.72	0.55
2:C:163:LYS:H	2:C:163:LYS:CD	2.10	0.54
3:D:1262:ARG:HH22	3:D:1312:ALA:HB1	1.72	0.54
3:D:609:TYR:CE2	3:D:614:LEU:HD22	2.41	0.54
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.07	0.54
1:G:37:HIS:CE1	2:H:1216:ARG:HD3	2.42	0.54
2:H:453:ILE:HG22	2:H:585:GLY:O	2.07	0.54
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.71	0.54
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.42	0.54
2:H:459:MET:SD	2:H:511:LEU:HD22	2.47	0.54
2:H:524:ILE:HD12	2:H:708:VAL:HG13	1.88	0.54
2:H:936:ARG:HH11	5:Y:495:ARG:HH11	1.53	0.54
2:C:639:LYS:HA	2:C:639:LYS:HE2	1.89	0.54
3:D:514:THR:HG21	3:D:595:ALA:O	2.07	0.54
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.38	0.54
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.08	0.54
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.88	0.54
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.89	0.54
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.89	0.54
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.88	0.54
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.07	0.54
2:H:38:PHE:CE2	2:H:49:LEU:HD12	2.32	0.54
2:H:740:GLU:HB2	2:H:741:MET:SD	2.47	0.54
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.35	0.54
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.37	0.54
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.07	0.54
1:A:243:LYS:NZ	1:A:243:LYS:HB2	2.23	0.54
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.88	0.54
2:H:1255:THR:O	2:H:1257:GLN:N	2.38	0.54
2:H:1293:VAL:HG23	2:H:1301:ARG:HA	1.90	0.54
3:I:120:LEU:HD22	3:I:1330:ARG:HD3	1.89	0.54
3:I:128:LEU:HD12	3:I:192:MET:CE	2.37	0.54
3:I:589:TYR:O	3:I:591:ILE:N	2.37	0.54
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.89	0.54
2:C:678:ARG:HD3	2:C:681:MET:HG3	1.90	0.54
3:I:253:VAL:HG11	5:Y:523:ILE:HG21	1.90	0.54
3:I:297:ARG:HH22	5:Y:101:TYR:HB2	1.71	0.54
4:J:15:ASN:ND2	4:J:18:ASP:H	2.06	0.54
1:A:219:ARG:O	1:A:223:ILE:HG13	2.08	0.54
2:C:91:THR:HG22	2:C:139:ASN:N	2.23	0.54
1:F:150:ARG:NH1	1:G:8:PHE:HA	2.20	0.54
2:H:660:VAL:HG22	2:H:661:VAL:N	2.22	0.54
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.07	0.54
3:D:474:LEU:HA	3:D:477:GLN:HE21	1.73	0.54
4:E:5:THR:CA	4:E:6:VAL:CB	2.85	0.54
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.08	0.54
2:H:54:ARG:HG2	2:H:55:SER:CB	2.36	0.54
2:H:704:MET:HA	2:H:704:MET:HE2	1.90	0.54
3:I:405:GLU:O	3:I:407:VAL:N	2.41	0.54
3:I:40:LYS:HB3	3:I:42:GLU:HG2	1.90	0.54
3:I:42:GLU:HG3	5:Y:451:ARG:HH21	1.73	0.54
3:I:549:LYS:HE2	3:I:571:ASP:OD2	2.07	0.54
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.34	0.54
3:D:450:HIS:NE2	3:D:625:MET:SD	2.81	0.54
1:F:118:ASP:OD1	1:F:119:GLY:N	2.41	0.54
1:G:118:ASP:OD1	1:G:119:GLY:N	2.41	0.54
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.90	0.54
3:I:151:MET:N	3:I:151:MET:SD	2.81	0.54
3:I:842:ARG:HD2	3:I:882:VAL:HG21	1.90	0.54
1:B:176:CYS:O	1:B:178:SER:N	2.41	0.54
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.89	0.54
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.23	0.54
3:D:88:CYS:O	3:D:90:VAL:N	2.41	0.54
1:F:102:LEU:HG	1:F:115:ILE:HG12	1.90	0.54
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.08	0.54
3:I:810:THR:HG22	3:I:893:GLY:HA3	1.90	0.54
5:X:556:ALA:O	5:X:560:ARG:HB2	2.08	0.54
5:X:600:HIS:H	5:X:601:PRO:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASP:OD1	1:B:119:GLY:N	2.41	0.53
2:C:1141:LEU:H	2:C:1141:LEU:CD1	2.20	0.53
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.08	0.53
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.40	0.53
3:D:128:LEU:HA	3:D:192:MET:HE3	1.90	0.53
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.30	0.53
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.90	0.53
2:H:442:VAL:HG12	2:H:443:ASP:H	1.74	0.53
3:I:571:ASP:N	3:I:571:ASP:OD1	2.39	0.53
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.90	0.53
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.89	0.53
2:C:494:ASN:OD1	2:C:495:ALA:N	2.41	0.53
2:C:134:GLY:O	2:C:527:LYS:NZ	2.40	0.53
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.31	0.53
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.89	0.53
2:H:728:ASP:OD2	2:H:729:ALA:N	2.41	0.53
2:H:752:ASN:O	2:H:753:LEU:HG	2.08	0.53
3:I:205:LEU:HD22	3:I:217:LEU:CD2	2.34	0.53
2:C:1303:LYS:HA	2:C:1303:LYS:HE2	1.89	0.53
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.39	0.53
3:D:450:HIS:CE1	3:D:452:LEU:HD12	2.43	0.53
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.90	0.53
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	1.90	0.53
2:C:31:GLN:HG3	2:C:130:MET:HE1	1.90	0.53
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.08	0.53
3:D:393:THR:HG23	3:D:396:ALA:H	1.73	0.53
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.90	0.53
1:G:29:GLU:HA	1:G:200:LYS:CB	2.38	0.53
5:X:437:GLN:HA	5:X:440:THR:HG22	1.89	0.53
5:Y:585:GLU:HB3	5:Y:589:GLN:HE22	1.74	0.53
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.07	0.53
2:C:756:TYR:H	2:C:766:ASN:CB	2.22	0.53
3:D:584:PRO:HG2	3:D:587:LEU:CD1	2.33	0.53
3:D:591:ILE:HD12	3:D:592:VAL:N	2.24	0.53
3:D:746:LEU:CD1	3:D:758:PRO:HG3	2.28	0.53
2:H:1332:SER:O	3:I:243:PRO:HG2	2.09	0.53
2:H:387:ASN:HB3	2:H:394:ARG:HG3	1.89	0.53
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.90	0.53
3:I:1357:ILE:H	3:I:1357:ILE:HD12	1.73	0.53
3:I:363:LEU:O	3:I:486:SER:OG	2.20	0.53
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1119:MET:O	2:C:1123:GLY:N	2.40	0.53
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.44	0.53
2:C:728:ASP:OD2	2:C:729:ALA:N	2.41	0.53
3:D:294:ASN:ND2	3:D:298:MET:SD	2.81	0.53
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.28	0.53
2:H:1274:GLU:N	2:H:1274:GLU:OE1	2.41	0.53
2:H:494:ASN:OD1	2:H:495:ALA:N	2.40	0.53
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.91	0.53
3:I:709:ARG:O	3:I:711:GLY:N	2.42	0.53
1:A:80:GLU:HB2	2:C:694:ARG:NH2	2.19	0.53
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.44	0.53
1:B:19:VAL:O	1:B:20:SER:HB3	2.08	0.53
1:B:185:TYR:HB2	1:B:201:LEU:HD11	1.91	0.53
2:C:106:GLU:HG2	2:C:109:ALA:H	1.73	0.53
2:C:122:VAL:HG22	5:X:472:GLN:HE21	1.72	0.53
2:C:360:LEU:HD13	2:C:378:ARG:NH1	2.23	0.53
2:C:818:VAL:HG22	2:C:819:SER:H	1.74	0.53
3:D:1241:TYR:HB3	3:D:1246:VAL:HG23	1.91	0.53
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.30	0.53
3:D:41:PRO:HB3	3:D:270:ARG:HG3	1.90	0.53
3:D:425:ARG:CD	3:D:459:ALA:HB2	2.39	0.53
3:D:490:ILE:O	3:D:499:ILE:HG22	2.09	0.53
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.91	0.53
5:X:355:ILE:HD13	5:X:355:ILE:O	2.08	0.53
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.09	0.53
5:Y:576:VAL:HG12	5:Y:587:ILE:HG12	1.90	0.53
1:A:42:ALA:O	1:A:46:ILE:HG12	2.08	0.53
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.39	0.53
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.91	0.53
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.43	0.53
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.90	0.53
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.44	0.53
1:F:79:LEU:O	1:F:83:LEU:HD13	2.09	0.53
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.43	0.53
3:I:591:ILE:HD12	3:I:592:VAL:N	2.23	0.53
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.08	0.53
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.74	0.53
3:D:1159:ILE:HD12	3:D:1186:TYR:HE2	1.74	0.53
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.90	0.53
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.24	0.53
2:H:1327:LEU:HA	2:H:1337:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:664:ILE:HD12	3:I:681:LYS:HE3	1.91	0.53
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.90	0.53
5:X:301:ASN:O	5:X:305:LEU:HD13	2.09	0.53
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.44	0.53
2:C:367:TYR:CD1	2:C:384:LEU:HD13	2.44	0.53
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.90	0.53
1:G:182:ARG:CG	1:G:206:GLU:HB3	2.38	0.53
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.90	0.53
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.90	0.53
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.90	0.53
5:Y:584:ARG:O	5:Y:587:ILE:HG22	2.09	0.53
2:C:1335:ILE:HD11	3:D:22:ILE:HG13	1.91	0.52
2:C:205:PRO:O	2:C:208:ILE:HG22	2.10	0.52
2:C:402:ARG:NH2	2:C:419:ILE:O	2.43	0.52
3:D:152:THR:O	3:D:154:LEU:N	2.38	0.52
2:H:106:GLU:H	2:H:107:ARG:HA	1.74	0.52
2:H:37:LYS:HE3	2:H:37:LYS:HA	1.91	0.52
2:H:844:LYS:NZ	2:H:844:LYS:HB2	2.23	0.52
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.45	0.52
3:I:679:TYR:CZ	3:I:683:ILE:HD11	2.44	0.52
4:J:45:LYS:O	4:J:49:ILE:HG12	2.09	0.52
5:Y:598:LEU:O	5:Y:599:ARG:HD2	2.08	0.52
1:A:195:ARG:HH21	1:A:198:LEU:HD21	1.73	0.52
2:C:311:CYS:SG	2:C:315:MET:HB2	2.49	0.52
2:C:946:LEU:O	2:C:949:GLU:HG3	2.09	0.52
3:D:1171:GLY:N	3:D:1172:LYS:O	2.41	0.52
3:D:413:ASP:O	3:D:417:ARG:HG2	2.10	0.52
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.44	0.52
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.91	0.52
3:I:197:GLU:O	3:I:201:LEU:HD23	2.09	0.52
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.74	0.52
5:X:264:LYS:HD2	5:X:264:LYS:H	1.73	0.52
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.22	0.52
2:C:96:LEU:HD22	2:C:127:ILE:HD12	1.92	0.52
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.35	0.52
4:E:5:THR:HB	4:E:7:GLN:N	2.24	0.52
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.44	0.52
3:I:1251:LYS:O	3:I:1255:VAL:HG23	2.10	0.52
3:I:797:THR:O	3:I:801:VAL:HG23	2.09	0.52
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.23	0.52
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:264:LYS:H	5:Y:264:LYS:HD2	1.74	0.52
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.09	0.52
2:C:1244:HIS:HB3	2:C:1265:PHE:CG	2.45	0.52
1:A:134:THR:HG21	2:C:727:VAL:O	2.09	0.52
4:E:77:ALA:O	4:E:80:LEU:HD22	2.10	0.52
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.42	0.52
2:H:992:LEU:HD23	2:H:996:ARG:HG3	1.91	0.52
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.09	0.52
3:I:393:THR:HG23	3:I:396:ALA:H	1.73	0.52
3:I:648:GLU:N	3:I:648:GLU:OE2	2.43	0.52
5:X:484:ALA:CB	5:X:494:ILE:HD12	2.39	0.52
5:X:466:ILE:HD12	5:X:487:MET:HE2	1.91	0.52
5:X:493:LYS:O	5:X:497:VAL:HG23	2.09	0.52
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.39	0.52
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.39	0.52
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.75	0.52
3:D:118:LYS:HE3	5:X:39:ASP:OD2	2.09	0.52
5:X:541:ARG:O	5:X:545:HIS:HB2	2.10	0.52
3:D:615:LYS:HD2	7:D:1503:O2:N2	2.23	0.52
3:D:655:SER:O	3:D:658:GLU:HG2	2.09	0.52
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.45	0.52
4:E:82:ALA:O	4:E:86:ILE:HG13	2.10	0.52
2:H:131:THR:HG22	2:H:135:THR:HG22	1.91	0.52
2:H:888:THR:O	2:H:914:LYS:N	2.36	0.52
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.92	0.52
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.91	0.52
2:C:127:ILE:HD13	2:C:127:ILE:N	2.25	0.52
2:C:302:ILE:HG22	2:C:309:LEU:CB	2.39	0.52
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.92	0.52
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.91	0.52
2:C:975:ILE:HD13	2:C:975:ILE:O	2.09	0.52
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.91	0.52
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.91	0.52
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.45	0.52
3:D:709:ARG:HD2	3:D:714:GLU:HB2	1.91	0.52
3:D:746:LEU:HB3	3:D:754:ILE:HG21	1.91	0.52
4:E:5:THR:CB	4:E:7:GLN:H	2.20	0.52
2:H:18:ARG:HD3	2:H:619:ALA:O	2.09	0.52
2:H:694:ARG:O	2:H:798:GLN:NE2	2.37	0.52
2:H:699:LEU:H	2:H:799:ASN:HD21	1.56	0.52
2:H:741:MET:N	2:H:741:MET:SD	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:598:LEU:O	5:X:599:ARG:HD2	2.08	0.52
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.39	0.52
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.92	0.52
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.90	0.52
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.33	0.52
3:D:646:ILE:HG22	3:D:741:ALA:O	2.09	0.52
3:D:810:THR:OG1	3:D:811:GLU:N	2.42	0.52
3:I:504:GLN:HG3	3:I:505:ASP:H	1.75	0.52
5:X:119:ILE:O	5:X:123:ILE:HG13	2.10	0.52
2:C:179:TYR:HE2	2:C:462:ASN:HD21	1.58	0.52
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.40	0.52
2:C:755:LYS:HZ1	2:C:756:TYR:HE2	1.58	0.52
2:C:843:THR:HG22	2:C:844:LYS:N	2.24	0.52
2:C:891:GLY:O	2:C:893:THR:HG23	2.10	0.52
3:D:767:LEU:HB3	3:D:771:GLN:HE22	1.75	0.52
3:D:63:GLY:O	3:D:98:ARG:NH2	2.42	0.52
1:G:31:LEU:HB2	1:G:199:ASP:O	2.10	0.52
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.09	0.52
2:C:80:PHE:O	2:C:84:GLU:HB3	2.10	0.52
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.10	0.52
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.91	0.52
3:D:504:GLN:HG3	3:D:505:ASP:H	1.75	0.52
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.91	0.52
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.24	0.52
2:H:403:MET:HG3	2:H:414:ILE:HB	1.91	0.52
2:H:446:ASP:OD1	2:H:547:VAL:N	2.29	0.52
3:I:451:PRO:HG2	3:I:625:MET:SD	2.50	0.52
1:B:33:ARG:NE	1:B:197:ASP:HB2	2.26	0.51
2:C:487:LEU:CD1	2:C:488:MET:H	2.23	0.51
3:D:703:THR:HA	3:D:717:VAL:HA	1.90	0.51
3:D:767:LEU:HB3	3:D:771:GLN:NE2	2.24	0.51
2:H:21:VAL:HG13	2:H:22:LEU:N	2.23	0.51
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.10	0.51
3:I:858:VAL:HB	3:I:859:PRO:CD	2.26	0.51
5:X:400:GLN:O	5:X:404:LEU:HD13	2.11	0.51
2:C:699:LEU:H	2:C:799:ASN:HD21	1.56	0.51
1:G:192:VAL:CG1	1:G:194:GLN:HG2	2.40	0.51
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.51
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.93	0.51
2:H:496:LYS:HE2	5:Y:471:LEU:CD2	2.39	0.51
3:I:807:LEU:O	3:I:807:LEU:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:430:HIS:HA	3:I:921:GLN:HB3	1.92	0.51
5:Y:379:MET:CE	5:Y:379:MET:HA	2.41	0.51
1:B:107:ILE:HD11	1:B:136:GLU:HG2	1.91	0.51
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.09	0.51
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.93	0.51
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.45	0.51
3:D:133:ARG:NH2	3:D:133:ARG:HB2	2.25	0.51
3:D:664:ILE:CD1	3:D:681:LYS:HE3	2.40	0.51
2:C:1104:PRO:HG3	3:D:725:MET:SD	2.51	0.51
2:H:829:THR:HG22	2:H:1059:ARG:HG2	1.92	0.51
2:H:800:MET:HG2	2:H:1096:ILE:HD13	1.91	0.51
2:H:1281:TYR:CZ	3:I:431:ARG:HG2	2.45	0.51
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.10	0.51
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.44	0.51
5:X:484:ALA:HB2	5:X:494:ILE:HD12	1.92	0.51
2:C:1106:ARG:O	2:C:1108:ASN:N	2.40	0.51
2:C:21:VAL:HG13	2:C:22:LEU:N	2.26	0.51
3:D:20:ILE:CD1	3:D:1320:ILE:HD11	2.41	0.51
3:D:68:TYR:OH	3:D:94:GLN:NE2	2.44	0.51
1:G:41:ASN:HD21	2:H:1217:THR:HG22	1.76	0.51
2:H:1336:ASN:HB2	3:I:33:TRP:HH2	1.75	0.51
2:H:634:VAL:H	2:H:645:PHE:HE2	1.59	0.51
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.40	0.51
5:Y:99:ARG:HD3	5:Y:99:ARG:O	2.11	0.51
1:B:77:ASP:O	1:B:81:ILE:HG13	2.10	0.51
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.92	0.51
2:C:59:ILE:CG2	2:C:479:LEU:HB3	2.41	0.51
2:C:936:ARG:HD2	2:C:1047:LEU:H	1.74	0.51
2:C:989:LEU:HG	2:C:990:ASP:H	1.76	0.51
2:C:9:LYS:N	2:C:9:LYS:HD3	2.25	0.51
2:H:153:PRO:HD2	2:H:452:ARG:HD3	1.92	0.51
2:H:989:LEU:HG	2:H:990:ASP:H	1.76	0.51
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.92	0.51
3:I:482:ALA:C	3:I:483:LEU:HD12	2.31	0.51
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.92	0.51
1:A:207:THR:OG1	1:A:208:ASN:N	2.44	0.51
1:A:248:GLU:N	1:A:248:GLU:OE1	2.42	0.51
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.39	0.51
4:E:5:THR:HB	4:E:7:GLN:CB	2.38	0.51
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.76	0.51
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1256:GLN:HB3	2:H:1301:ARG:HH22	1.76	0.51
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.24	0.51
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.92	0.51
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.30	0.51
2:H:1335:ILE:HD11	3:I:22:ILE:CG1	2.41	0.51
3:I:245:LEU:O	3:I:250:ARG:NH1	2.43	0.51
1:B:41:ASN:ND2	2:C:1217:THR:HG22	2.23	0.51
1:B:45:ARG:O	3:D:538:ARG:NH2	2.44	0.51
3:D:648:GLU:N	3:D:648:GLU:OE2	2.42	0.51
3:D:899:TYR:CE1	3:D:915:ILE:HD12	2.46	0.51
4:E:4:VAL:O	4:E:5:THR:OG1	2.24	0.51
2:H:1247:SER:O	2:H:1248:THR:HG23	2.11	0.51
5:X:311:THR:HG21	5:X:348:GLU:CD	2.31	0.51
5:X:545:HIS:NE2	5:X:566:ASP:OD2	2.44	0.51
5:X:600:HIS:H	5:X:601:PRO:CD	2.23	0.51
2:C:576:SER:HB3	2:C:579:ALA:HB2	1.93	0.51
3:D:316:ILE:O	3:D:317:THR:OG1	2.20	0.51
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.75	0.51
3:I:1174:ARG:HA	3:I:1192:LYS:HG3	1.92	0.51
3:I:857:LEU:HB2	3:I:860:ARG:HB2	1.91	0.51
4:J:5:THR:HB	4:J:7:GLN:H	1.75	0.51
5:X:277:MET:HE1	5:X:359:LYS:HE2	1.93	0.51
1:A:118:ASP:OD1	1:A:119:GLY:N	2.44	0.51
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.44	0.51
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.93	0.51
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.30	0.51
2:C:844:LYS:NZ	2:C:844:LYS:HB2	2.26	0.51
3:D:1254:GLU:HA	3:D:1257:VAL:HG12	1.93	0.51
2:C:1105:SER:HB2	3:D:731:ARG:HD3	1.93	0.51
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.75	0.51
2:H:901:LEU:O	2:H:905:ILE:HG13	2.11	0.51
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.10	0.51
1:A:303:ILE:O	1:A:307:LEU:HD13	2.10	0.51
1:B:129:VAL:HG11	1:B:132:HIS:HE1	1.76	0.51
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	1.93	0.51
2:C:49:LEU:HD21	2:C:464:PHE:HB3	1.93	0.51
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.10	0.51
3:D:886:VAL:HG11	3:D:1230:THR:HG21	1.92	0.51
2:H:1335:ILE:HD11	3:I:22:ILE:HG13	1.92	0.51
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.92	0.51
2:H:681:MET:O	2:H:685:MET:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:140:TYR:OH	3:I:312:ARG:NH1	2.42	0.51
3:I:473:THR:HB	3:I:476:ALA:HB2	1.93	0.51
1:A:256:PRO:HA	1:A:277:TYR:HA	1.92	0.50
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.46	0.50
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.41	0.50
7:D:1503:O2:O2'	7:D:1503:O2:O1C	2.29	0.50
3:D:396:ALA:CB	5:X:606:VAL:HG11	2.41	0.50
1:G:179:PRO:O	1:G:207:THR:OG1	2.25	0.50
3:I:822:MET:HG2	3:I:839:VAL:HG22	1.93	0.50
5:Y:437:GLN:HA	5:Y:440:THR:HG22	1.93	0.50
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.10	0.50
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.92	0.50
3:D:262:THR:HG1	3:D:266:ASN:HD22	1.58	0.50
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.41	0.50
3:D:701:LEU:HD23	3:D:723:TYR:HB2	1.93	0.50
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.37	0.50
1:F:42:ALA:O	1:F:46:ILE:HG12	2.11	0.50
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.46	0.50
2:H:36:GLN:O	2:H:39:ILE:HG22	2.11	0.50
2:H:812:PHE:CD2	2:H:813:GLU:HG3	2.46	0.50
5:Y:449:THR:HG23	5:Y:503:GLU:OE1	2.12	0.50
1:A:263:THR:HG23	1:A:266:SER:H	1.76	0.50
2:C:149:LEU:HD12	2:C:452:ARG:O	2.11	0.50
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.92	0.50
3:D:1174:ARG:HA	3:D:1192:LYS:HG3	1.92	0.50
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.11	0.50
3:D:910:ASN:HB3	4:E:15:ASN:HA	1.92	0.50
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.12	0.50
2:H:818:VAL:HG22	2:H:819:SER:H	1.76	0.50
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.24	0.50
5:X:384:LEU:O	5:X:384:LEU:HD13	2.10	0.50
2:C:1285:TYR:HA	2:C:1288:GLN:HB3	1.92	0.50
2:C:442:VAL:HG12	2:C:443:ASP:H	1.77	0.50
3:D:205:LEU:HD13	3:D:217:LEU:HA	1.93	0.50
3:D:482:ALA:C	3:D:483:LEU:HD12	2.32	0.50
3:D:840:LEU:O	3:D:840:LEU:HD12	2.11	0.50
3:D:478:LEU:CD1	4:E:47:THR:HG23	2.41	0.50
2:H:707:ALA:O	2:H:710:VAL:HG12	2.11	0.50
3:I:1260:MET:HE2	3:I:1306:LEU:HD11	1.92	0.50
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.32	0.50
3:I:152:THR:O	3:I:154:LEU:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:LEU:HB2	2:C:389:PHE:CE1	2.46	0.50
2:C:873:ILE:HG13	2:C:944:ARG:NH2	2.26	0.50
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.46	0.50
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.93	0.50
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.27	0.50
2:H:38:PHE:O	2:H:39:ILE:HB	2.10	0.50
3:I:513:MET:CE	3:I:579:LEU:HB2	2.41	0.50
5:X:561:MET:HA	5:X:567:MET:SD	2.50	0.50
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.26	0.50
1:A:47:LEU:HD23	1:A:51:MET:SD	2.52	0.50
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.46	0.50
1:A:80:GLU:HA	2:C:694:ARG:HH12	1.77	0.50
3:D:545:HIS:O	3:D:573:THR:OG1	2.18	0.50
3:D:57:PHE:HB3	3:D:98:ARG:HH11	1.76	0.50
1:F:52:PRO:HG2	1:F:219:ARG:NH2	2.24	0.50
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.92	0.50
2:H:487:LEU:CB	2:H:488:MET:HG3	2.39	0.50
2:H:946:LEU:O	2:H:949:GLU:HG3	2.11	0.50
3:I:355:ILE:HG21	3:I:466:MET:SD	2.52	0.50
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.77	0.50
2:C:1335:ILE:HD11	3:D:22:ILE:CG1	2.41	0.50
3:D:245:LEU:O	3:D:250:ARG:NH1	2.44	0.50
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.93	0.50
3:D:546:ALA:N	3:D:547:ARG:CA	2.69	0.50
1:F:151:GLY:O	1:F:177:TYR:HB2	2.12	0.50
3:I:1171:GLY:N	3:I:1172:LYS:O	2.44	0.50
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.40	0.50
3:I:842:ARG:HB3	3:I:882:VAL:HG21	1.94	0.50
5:X:101:TYR:OH	5:X:384:LEU:HD11	2.11	0.50
5:X:354:THR:HG23	5:X:357:GLN:HB3	1.93	0.50
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.44	0.50
2:C:131:THR:HG22	2:C:135:THR:N	2.27	0.50
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.93	0.50
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.93	0.50
2:C:697:LYS:HZ3	2:C:791:LEU:HD11	1.77	0.50
3:D:173:GLY:O	3:D:175:GLU:HG3	2.11	0.50
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.46	0.50
3:D:478:LEU:HD12	4:E:47:THR:HG23	1.93	0.50
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.45	0.50
3:I:316:ILE:N	3:I:316:ILE:HD13	2.27	0.50
3:I:608:CYS:O	3:I:612:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:644:MET:HG3	3:I:764:ARG:HD3	1.92	0.50
3:D:515:ARG:HH22	3:D:717:VAL:C	2.15	0.50
3:D:614:LEU:CD1	4:E:5:THR:HG21	2.42	0.50
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.12	0.50
2:H:1335:ILE:HD12	3:I:1336:ALA:HB2	1.94	0.50
3:I:1255:VAL:O	3:I:1258:ARG:HB3	2.11	0.50
3:I:370:LYS:HA	3:I:441:LEU:HD12	1.94	0.50
3:I:513:MET:O	3:I:575:GLY:HA3	2.12	0.50
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.45	0.50
3:I:660:GLU:O	3:I:664:ILE:HG12	2.12	0.50
5:X:283:GLN:NE2	5:X:343:LYS:HD2	2.26	0.50
5:Y:283:GLN:CD	5:Y:343:LYS:HD2	2.32	0.50
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.12	0.50
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.76	0.50
2:C:1087:TYR:O	2:C:1213:TYR:N	2.28	0.49
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.93	0.49
2:C:38:PHE:CE2	2:C:49:LEU:HD12	2.35	0.49
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.12	0.49
3:D:392:THR:HG22	5:X:603:ARG:HG2	1.94	0.49
2:C:813:GLU:HG2	3:D:504:GLN:NE2	2.26	0.49
3:D:899:TYR:CZ	3:D:915:ILE:HD12	2.47	0.49
2:H:384:LEU:O	2:H:388:LEU:HG	2.12	0.49
2:H:698:PRO:HD3	2:H:795:ALA:HB2	1.94	0.49
3:I:546:ALA:N	3:I:547:ARG:CA	2.70	0.49
3:I:678:ARG:O	3:I:681:LYS:HG3	2.11	0.49
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.26	0.49
5:X:290:LEU:O	5:X:294:GLN:HB3	2.12	0.49
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.93	0.49
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.94	0.49
5:Y:519:LEU:O	5:Y:519:LEU:HD13	2.11	0.49
1:B:9:LEU:H	1:B:9:LEU:HD23	1.77	0.49
3:D:57:PHE:CD1	3:D:247:PRO:HB3	2.46	0.49
2:H:794:LEU:HD21	2:H:796:LEU:CG	2.39	0.49
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.12	0.49
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.95	0.49
3:I:579:LEU:HD13	3:I:579:LEU:O	2.12	0.49
3:I:810:THR:OG1	3:I:811:GLU:N	2.42	0.49
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.11	0.49
1:A:310:ARG:HA	1:A:310:ARG:NE	2.28	0.49
1:G:185:TYR:HB2	1:G:201:LEU:HD11	1.92	0.49
2:H:1042:LEU:N	2:H:1042:LEU:HD13	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:ILE:HD13	2:H:127:ILE:N	2.26	0.49
2:H:138:ILE:HB	2:H:143:ARG:HD2	1.94	0.49
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.12	0.49
2:H:735:LYS:HA	2:H:748:ILE:HA	1.94	0.49
3:I:526:VAL:HG12	3:I:549:LYS:HB2	1.92	0.49
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.26	0.49
2:C:1288:GLN:CA	2:C:1288:GLN:HE21	2.26	0.49
2:C:475:VAL:O	2:C:479:LEU:HB2	2.12	0.49
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.13	0.49
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.48	0.49
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.42	0.49
3:D:550:VAL:HG23	3:D:552:ILE:HD11	1.92	0.49
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.93	0.49
3:I:840:LEU:O	3:I:840:LEU:HD12	2.11	0.49
5:X:278:ASP:OD1	5:X:281:ARG:NH2	2.45	0.49
1:A:88:LEU:HD22	1:A:90:VAL:HG23	1.95	0.49
3:D:589:TYR:O	3:D:591:ILE:HG13	2.13	0.49
2:H:1119:MET:O	2:H:1123:GLY:N	2.45	0.49
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.42	0.49
2:H:895:LEU:HD21	2:H:903:ARG:CZ	2.41	0.49
2:H:998:LEU:O	2:H:998:LEU:HD13	2.12	0.49
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.78	0.49
5:X:108:VAL:HB	5:X:110:LEU:HG	1.94	0.49
5:X:115:GLY:O	5:X:119:ILE:HG12	2.13	0.49
5:X:310:GLU:O	5:X:344:LEU:HD23	2.12	0.49
2:C:12:ARG:O	2:C:13:LYS:HG2	2.11	0.49
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.28	0.49
2:C:818:VAL:HG22	2:C:819:SER:N	2.28	0.49
3:D:1346:GLY:HA3	3:D:1349:GLU:CD	2.33	0.49
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.77	0.49
2:H:590:PRO:O	2:H:659:GLN:NE2	2.46	0.49
2:H:975:ILE:HD13	2:H:975:ILE:O	2.12	0.49
3:I:1161:GLY:HA2	3:I:1181:ASP:HB2	1.95	0.49
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.47	0.49
2:C:510:GLN:O	2:C:511:LEU:HB2	2.13	0.49
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.48	0.49
2:C:998:LEU:HD13	2:C:998:LEU:O	2.13	0.49
3:D:807:LEU:O	3:D:807:LEU:HD12	2.12	0.49
3:D:614:LEU:CG	4:E:5:THR:HG21	2.42	0.49
2:H:395:TYR:CE2	2:H:420:LEU:HG	2.48	0.49
2:H:484:LEU:HB3	2:H:486:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:SER:O	2:H:98:VAL:HG23	2.12	0.49
3:I:205:LEU:CD2	3:I:217:LEU:HD22	2.36	0.49
3:I:186:GLN:CB	3:I:238:ILE:HD11	2.32	0.49
5:X:35:ILE:HG23	5:X:36:VAL:N	2.28	0.49
2:C:971:LEU:HD21	2:C:1017:GLN:HE22	1.78	0.49
2:C:119:GLU:HG2	2:C:120:GLN:N	2.28	0.49
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.27	0.49
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.12	0.49
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.43	0.49
2:C:808:ASN:H	3:D:633:ALA:HB2	1.78	0.49
1:G:9:LEU:H	1:G:9:LEU:HD23	1.78	0.49
2:H:1066:MET:HG3	2:H:1234:LYS:HA	1.94	0.49
2:H:1252:SER:HA	5:Y:524:GLU:HA	1.95	0.49
2:H:1270:PHE:CE2	2:H:1274:GLU:HB3	2.48	0.49
2:H:840:SER:HB3	2:H:850:ILE:HD11	1.94	0.49
3:I:227:PHE:O	3:I:230:SER:OG	2.24	0.49
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.94	0.49
5:X:379:MET:HE2	5:X:379:MET:HA	1.95	0.49
3:D:120:LEU:CG	5:X:46:GLN:HB2	2.42	0.49
5:X:511:ILE:HG23	5:X:512:GLY:N	2.25	0.49
1:A:158:ARG:HH21	1:A:158:ARG:HB2	1.77	0.49
1:A:79:LEU:O	1:A:83:LEU:HD13	2.13	0.49
2:C:1335:ILE:HD12	3:D:1336:ALA:HB2	1.95	0.49
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.39	0.49
2:C:741:MET:SD	2:C:741:MET:N	2.85	0.49
2:C:751:TYR:HE1	2:C:783:LEU:HD12	1.76	0.49
3:D:452:LEU:HG	3:D:625:MET:SD	2.53	0.49
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.43	0.49
3:D:531:LYS:HB3	3:D:531:LYS:NZ	2.28	0.49
3:D:803:VAL:HG13	3:D:1259:GLN:HE22	1.77	0.49
1:F:60:GLU:HG3	1:F:169:GLY:O	2.12	0.49
2:H:119:GLU:HG2	2:H:120:GLN:N	2.26	0.49
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.94	0.49
2:H:843:THR:HG22	2:H:844:LYS:H	1.78	0.49
1:B:227:GLN:C	1:B:229:GLU:H	2.16	0.49
3:D:918:ILE:HD11	3:D:1252:HIS:NE2	2.27	0.49
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.93	0.49
3:D:644:MET:O	3:D:764:ARG:NH1	2.46	0.49
2:H:12:ARG:O	2:H:13:LYS:HG2	2.12	0.49
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.94	0.49
3:I:245:LEU:CD1	3:I:246:PRO:HD2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:317:THR:H	3:I:324:LEU:HD21	1.77	0.49
3:I:543:SER:O	3:I:574:VAL:HB	2.13	0.49
1:A:310:ARG:HA	1:A:310:ARG:HE	1.77	0.48
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.28	0.48
2:C:740:GLU:HB2	2:C:741:MET:SD	2.53	0.48
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.13	0.48
2:C:812:PHE:H	2:C:815:SER:HB2	1.78	0.48
2:C:866:ASP:HA	2:C:872:TYR:OH	2.12	0.48
3:D:120:LEU:HA	5:X:46:GLN:OE1	2.13	0.48
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.95	0.48
3:D:824:PRO:O	3:D:826:ILE:HG13	2.12	0.48
3:D:914:ALA:O	3:D:918:ILE:HG22	2.13	0.48
1:G:152:TYR:OH	3:I:535:ARG:NH1	2.38	0.48
3:I:1261:LEU:HD21	3:I:1306:LEU:CD2	2.38	0.48
3:I:128:LEU:HD12	3:I:192:MET:HE3	1.94	0.48
3:I:519:ASN:HD21	3:I:707:ILE:HG21	1.78	0.48
5:X:126:GLY:O	5:X:130:VAL:HG23	2.13	0.48
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.95	0.48
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.26	0.48
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.48	0.48
2:C:99:LYS:HG2	2:C:121:GLU:HB3	1.94	0.48
2:C:660:VAL:HG22	2:C:661:VAL:N	2.23	0.48
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.12	0.48
1:F:182:ARG:HH11	2:H:1092:THR:HG22	1.78	0.48
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.43	0.48
5:X:123:ILE:O	5:X:127:ILE:HG12	2.13	0.48
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.43	0.48
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.13	0.48
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.26	0.48
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.77	0.48
2:C:727:VAL:CG2	2:C:773:LEU:HB3	2.40	0.48
3:D:124:ILE:HA	3:D:237:MET:HE2	1.95	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.13	0.48
3:D:873:GLU:OE2	3:D:877:VAL:HB	2.12	0.48
3:D:8:LEU:HD23	3:D:8:LEU:N	2.29	0.48
1:F:44:ARG:HG3	1:F:183:ILE:HG22	1.96	0.48
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.95	0.48
3:I:221:ILE:HG13	3:I:222:LYS:N	2.28	0.48
3:I:233:LYS:CD	3:I:234:PRO:HD2	2.43	0.48
3:I:531:LYS:HB3	3:I:531:LYS:NZ	2.28	0.48
3:I:701:LEU:HD21	3:I:723:TYR:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.95	0.48
2:C:529:ARG:HH22	2:C:687:ARG:NH2	2.12	0.48
2:C:747:GLY:C	2:C:748:ILE:HG13	2.34	0.48
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.48	0.48
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.13	0.48
2:H:1339:LEU:N	2:H:1339:LEU:HD12	2.28	0.48
3:I:1216:ALA:O	3:I:1220:ILE:HG13	2.13	0.48
3:I:1343:GLU:CA	3:I:1344:LEU:HB2	2.39	0.48
5:X:143:TYR:O	5:X:147:GLN:HG2	2.13	0.48
1:B:192:VAL:HG12	1:B:194:GLN:H	1.78	0.48
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.12	0.48
3:D:1254:GLU:O	3:D:1257:VAL:HG12	2.13	0.48
3:D:398:LYS:HD2	5:X:532:LEU:HD11	1.95	0.48
3:D:450:HIS:HE2	3:D:625:MET:CE	2.27	0.48
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.95	0.48
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.29	0.48
2:H:1252:SER:HB3	2:H:1259:LEU:HD21	1.94	0.48
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.28	0.48
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.37	0.48
3:I:646:ILE:HD12	3:I:646:ILE:O	2.12	0.48
3:I:746:LEU:HB3	3:I:754:ILE:HG21	1.96	0.48
5:X:519:LEU:O	5:X:519:LEU:HD13	2.12	0.48
5:Y:457:ILE:HG23	5:Y:461:ASN:ND2	2.28	0.48
1:A:243:LYS:N	1:A:243:LYS:HD3	2.29	0.48
2:C:678:ARG:NE	2:C:1106:ARG:HG2	2.24	0.48
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.14	0.48
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.94	0.48
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.48	0.48
3:D:915:ILE:HG22	3:D:1255:VAL:HG11	1.96	0.48
3:D:128:LEU:HD11	3:D:188:LEU:CD2	2.37	0.48
3:D:221:ILE:HG13	3:D:222:LYS:N	2.29	0.48
3:D:608:CYS:O	3:D:612:LEU:HB2	2.13	0.48
3:D:646:ILE:HD12	3:D:646:ILE:O	2.13	0.48
1:G:90:VAL:HG13	1:G:121:VAL:HG13	1.94	0.48
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.95	0.48
2:H:898:GLU:N	2:H:898:GLU:OE1	2.37	0.48
3:I:140:TYR:HA	3:I:181:GLY:HA2	1.95	0.48
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.96	0.48
3:I:703:THR:O	3:I:718:SER:N	2.47	0.48
5:X:11:LEU:HD22	5:X:15:ARG:NH2	2.28	0.48
5:X:227:GLN:HA	5:X:230:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:O	1:A:194:GLN:N	2.45	0.48
3:D:579:LEU:O	3:D:579:LEU:HD13	2.14	0.48
2:H:747:GLY:C	2:H:748:ILE:HG13	2.34	0.48
3:I:572:THR:HG22	3:I:594:GLN:OE1	2.14	0.48
3:I:51:PRO:HB3	3:I:57:PHE:O	2.14	0.48
2:H:808:ASN:H	3:I:633:ALA:HB2	1.79	0.48
3:I:888:CYS:SG	3:I:890:THR:HB	2.54	0.48
2:C:98:VAL:HG11	2:C:124:MET:SD	2.53	0.48
3:D:843:VAL:HG11	3:D:897:HIS:HB3	1.96	0.48
3:D:918:ILE:HD13	3:D:919:ALA:N	2.29	0.48
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.46	0.48
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.14	0.48
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.42	0.48
2:H:72:SER:OG	2:H:99:LYS:HE3	2.13	0.48
3:I:147:ILE:HD12	3:I:178:ALA:HB2	1.96	0.48
3:I:294:ASN:ND2	3:I:298:MET:SD	2.87	0.48
3:I:573:THR:CG2	3:I:576:ARG:HG3	2.43	0.48
5:X:145:LEU:HD11	5:X:225:ARG:HH21	1.78	0.48
2:C:225:PHE:CZ	2:C:347:ILE:HB	2.49	0.48
2:C:59:ILE:HD11	2:C:63:SER:OG	2.14	0.48
3:D:41:PRO:HG3	3:D:273:ILE:HG22	1.95	0.48
3:D:363:LEU:HD12	3:D:450:HIS:ND1	2.29	0.48
1:G:47:LEU:HD13	1:G:205:MET:HE2	1.96	0.48
1:G:82:LEU:O	1:G:86:LYS:HG3	2.14	0.48
2:H:127:ILE:HG12	2:H:127:ILE:O	2.14	0.48
2:H:818:VAL:HG22	2:H:819:SER:N	2.28	0.48
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.49	0.48
3:I:707:ILE:HD11	3:I:716:GLN:HG3	1.96	0.48
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.13	0.48
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.14	0.48
2:C:718:ALA:HB2	2:C:783:LEU:HG	1.96	0.48
3:D:120:LEU:HG	5:X:46:GLN:CB	2.42	0.48
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.95	0.48
1:G:196:THR:OG1	3:I:443:GLU:HG3	2.14	0.48
2:H:356:THR:HG21	2:H:362:ALA:HA	1.95	0.48
3:I:265:LEU:HD11	3:I:330:MET:SD	2.54	0.48
3:I:377:PHE:O	3:I:381:ILE:HG13	2.14	0.48
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.29	0.48
3:I:714:GLU:HG2	3:I:715:LYS:H	1.79	0.48
3:I:899:TYR:CD2	3:I:909:ILE:HG12	2.49	0.48
5:X:119:ILE:HD12	5:X:122:ARG:HH21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:271:ASN:O	5:X:275:VAL:HG23	2.14	0.48
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.14	0.48
5:Y:316:PHE:CZ	5:Y:320:ILE:HD11	2.48	0.48
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.96	0.47
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	1.96	0.47
3:D:1347:LEU:HD22	3:D:1357:ILE:CG2	2.44	0.47
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.49	0.47
2:H:759:SER:HB3	2:H:763:THR:H	1.80	0.47
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.13	0.47
3:I:910:ASN:HB3	4:J:15:ASN:OD1	2.13	0.47
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.30	0.47
1:B:195:ARG:HH21	1:B:198:LEU:HD21	1.79	0.47
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.49	0.47
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.97	0.47
3:D:269:TYR:CD2	3:D:306:LEU:HD11	2.49	0.47
3:D:50:LYS:HB3	3:D:50:LYS:NZ	2.29	0.47
1:F:182:ARG:NH1	2:H:1092:THR:HG22	2.29	0.47
2:H:901:LEU:HD13	5:Y:563:PHE:CE2	2.49	0.47
2:H:750:ILE:HD13	2:H:963:GLU:OE2	2.14	0.47
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.96	0.47
2:H:618:GLN:OE1	3:I:769:VAL:HG13	2.14	0.47
1:A:58:GLU:HG2	1:A:172:LEU:HD23	1.96	0.47
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.95	0.47
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.78	0.47
2:C:699:LEU:HD12	2:C:1121:ALA:HB1	1.95	0.47
2:C:812:PHE:N	2:C:815:SER:HB2	2.28	0.47
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.14	0.47
3:D:487:THR:HG21	4:E:4:VAL:CG1	2.40	0.47
4:E:18:ASP:O	4:E:22:VAL:HG12	2.14	0.47
1:F:28:LEU:HD22	1:G:231:PHE:CZ	2.49	0.47
1:F:45:ARG:NE	1:G:38:THR:OG1	2.46	0.47
2:H:963:GLU:O	2:H:967:LEU:HD13	2.14	0.47
3:I:161:THR:HG22	3:I:162:GLU:H	1.79	0.47
3:I:288:PRO:O	3:I:292:VAL:HG12	2.14	0.47
3:I:679:TYR:O	3:I:683:ILE:HG13	2.14	0.47
1:A:222:THR:O	1:A:226:GLU:HG3	2.13	0.47
2:C:893:THR:O	2:C:895:LEU:N	2.41	0.47
3:D:179:LYS:HD3	3:D:179:LYS:N	2.29	0.47
3:D:358:GLY:HA3	3:D:361:LEU:HD23	1.96	0.47
1:F:28:LEU:HD13	1:G:231:PHE:CE2	2.50	0.47
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:425:ARG:CD	3:I:459:ALA:HB2	2.44	0.47
3:I:591:ILE:HD12	3:I:592:VAL:HG13	1.97	0.47
1:B:33:ARG:HE	1:B:197:ASP:HB2	1.79	0.47
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.79	0.47
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.29	0.47
2:C:131:THR:HG22	2:C:135:THR:H	1.80	0.47
2:C:562:GLU:HG2	2:C:574:SER:HB3	1.95	0.47
2:C:963:GLU:O	2:C:967:LEU:HD13	2.13	0.47
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.14	0.47
3:D:714:GLU:HG2	3:D:715:LYS:H	1.79	0.47
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.30	0.47
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.50	0.47
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.96	0.47
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	1.96	0.47
3:I:201:LEU:HD12	3:I:205:LEU:HD11	1.97	0.47
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.95	0.47
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.14	0.47
1:A:252:ILE:HG22	1:A:278:ILE:HD11	1.96	0.47
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.15	0.47
3:D:364:HIS:HB3	3:D:487:THR:HG23	1.95	0.47
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.76	0.47
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.79	0.47
3:I:514:THR:HG21	3:I:595:ALA:O	2.15	0.47
3:I:8:LEU:N	3:I:8:LEU:HD23	2.30	0.47
3:I:614:LEU:CG	4:J:7:GLN:HG3	2.43	0.47
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.55	0.47
5:Y:428:SER:O	5:Y:432:THR:OG1	2.28	0.47
1:A:234:LEU:N	1:A:234:LEU:HD12	2.29	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.67	0.47
2:C:127:ILE:HG12	2:C:127:ILE:O	2.14	0.47
2:C:237:LEU:HB2	2:C:287:VAL:O	2.14	0.47
3:D:310:GLY:O	3:D:314:ARG:HG2	2.14	0.47
3:D:474:LEU:HD11	4:E:27:ALA:HB3	1.97	0.47
3:D:797:THR:O	3:D:801:VAL:HG23	2.15	0.47
2:H:1106:ARG:O	2:H:1108:ASN:N	2.38	0.47
2:H:1304:MET:O	2:H:1308:ILE:HG13	2.14	0.47
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.49	0.47
2:H:546:GLU:O	2:H:548:ARG:N	2.43	0.47
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.50	0.47
2:H:908:GLU:CD	2:H:908:GLU:H	2.18	0.47
3:I:450:HIS:CE1	3:I:452:LEU:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:349:TYR:CD1	3:I:472:LEU:HD11	2.49	0.47
3:I:473:THR:CG2	3:I:475:GLU:HG2	2.44	0.47
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.30	0.47
1:B:151:GLY:O	1:B:177:TYR:HB2	2.14	0.47
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.95	0.47
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.50	0.47
2:C:153:PRO:HD2	2:C:452:ARG:HD3	1.96	0.47
2:C:702:THR:HA	2:C:1184:THR:O	2.15	0.47
2:C:941:LYS:HD2	2:C:941:LYS:O	2.14	0.47
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.49	0.47
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.96	0.47
3:I:12:THR:O	3:I:13:LYS:HD2	2.14	0.47
2:H:1314:GLN:O	3:I:473:THR:HG23	2.15	0.47
5:X:431:ALA:O	5:X:435:ILE:HG13	2.15	0.47
1:A:166:ARG:HA	1:A:167:PRO:HD2	1.80	0.47
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.97	0.47
3:D:1346:GLY:O	3:D:1350:ASN:HB2	2.15	0.47
3:D:856:ILE:HG13	3:D:857:LEU:O	2.14	0.47
2:H:1233:LEU:O	2:H:1233:LEU:HD12	2.15	0.47
2:H:59:ILE:HB	2:H:480:SER:OG	2.15	0.47
2:H:876:GLU:N	2:H:876:GLU:OE2	2.48	0.47
5:X:457:ILE:HG23	5:X:461:ASN:HD21	1.80	0.47
5:Y:291:CYS:O	5:Y:295:CYS:HB2	2.14	0.47
1:A:12:ARG:HB2	1:A:30:PRO:HG2	1.96	0.47
1:B:19:VAL:O	1:B:20:SER:CB	2.63	0.47
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.15	0.47
2:C:538:LEU:HD12	2:C:538:LEU:N	2.29	0.47
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.77	0.47
3:D:1343:GLU:CA	3:D:1344:LEU:HB2	2.32	0.47
3:D:154:LEU:HD22	3:D:176:PHE:CE1	2.49	0.47
3:I:720:ASN:ND2	3:I:720:ASN:O	2.48	0.47
5:Y:108:VAL:HB	5:Y:110:LEU:HG	1.96	0.47
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.15	0.47
5:Y:545:HIS:NE2	5:Y:566:ASP:OD2	2.29	0.47
3:D:356:THR:O	3:D:448:GLN:HA	2.15	0.47
3:D:539:SER:OG	3:D:540:GLY:N	2.48	0.47
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	1.97	0.47
2:H:845:LEU:CD2	2:H:889:PRO:HG2	2.41	0.47
2:H:966:ILE:HG23	2:H:967:LEU:HD12	1.97	0.47
3:I:1280:VAL:HG21	3:I:1304:ARG:NH2	2.30	0.47
5:Y:253:SER:O	5:Y:257:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.96	0.47
1:B:232:VAL:O	1:B:233:ASP:HB2	2.15	0.46
2:C:216:THR:O	2:C:220:ILE:HG13	2.15	0.46
2:C:41:GLN:CD	2:C:42:ASP:H	2.17	0.46
2:C:28:LEU:HD22	2:C:527:LYS:HD2	1.96	0.46
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.50	0.46
3:D:423:LEU:HB3	3:D:466:MET:CE	2.44	0.46
3:D:524:GLY:HA2	3:D:548:VAL:HG23	1.96	0.46
3:D:607:THR:O	3:D:611:ILE:HG12	2.15	0.46
1:G:190:ALA:N	1:G:198:LEU:O	2.37	0.46
2:H:1017:GLN:HA	2:H:1020:GLU:HB3	1.97	0.46
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.29	0.46
3:I:210:SER:O	3:I:214:ARG:HG3	2.15	0.46
3:I:72:CYS:SG	3:I:73:GLY:N	2.88	0.46
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.15	0.46
3:I:298:MET:HE3	5:Y:402:LEU:HB3	1.96	0.46
5:Y:608:ARG:HB3	5:Y:608:ARG:NH1	2.31	0.46
1:B:179:PRO:O	1:B:207:THR:OG1	2.29	0.46
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.39	0.46
2:C:843:THR:HB	2:C:845:LEU:HD22	1.96	0.46
3:D:33:TRP:HB3	3:D:102:MET:HG3	1.96	0.46
3:D:541:LEU:HB2	3:D:545:HIS:CE1	2.50	0.46
3:D:545:HIS:HA	3:D:546:ALA:HA	1.80	0.46
1:G:36:GLY:O	1:G:201:LEU:HD13	2.14	0.46
1:F:221:ALA:CB	1:G:228:LEU:HD12	2.37	0.46
2:H:516:ASP:OD2	2:H:518:ASN:ND2	2.48	0.46
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.49	0.46
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.29	0.46
2:H:697:LYS:HE2	2:H:793:GLU:HB3	1.97	0.46
3:D:1301:THR:CG2	3:I:1301:THR:HG23	2.45	0.46
3:I:605:LEU:HD13	3:I:605:LEU:O	2.15	0.46
5:X:291:CYS:O	5:X:295:CYS:HB2	2.15	0.46
5:X:448:ARG:NH1	5:X:452:ILE:HD12	2.31	0.46
3:D:260:PHE:O	5:X:504:PRO:HG2	2.15	0.46
5:Y:124:GLU:HG2	5:Y:128:ASN:ND2	2.31	0.46
5:Y:101:TYR:HE2	5:Y:388:ILE:HD11	1.79	0.46
2:C:122:VAL:HG22	2:C:123:TYR:N	2.29	0.46
2:C:356:THR:HG21	2:C:362:ALA:HA	1.97	0.46
3:D:580:TRP:HE1	3:D:589:TYR:HB3	1.80	0.46
3:D:825:VAL:CG2	3:D:835:LEU:HB2	2.45	0.46
3:D:824:PRO:CB	3:D:836:ARG:HD3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1084:ASP:HB2	2:H:1216:ARG:HG2	1.96	0.46
1:F:45:ARG:NH1	2:H:1216:ARG:HA	2.26	0.46
2:H:156:PHE:CE2	2:H:177:ILE:HD13	2.51	0.46
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.96	0.46
3:I:611:ILE:HG13	3:I:612:LEU:HD23	1.97	0.46
3:D:394:ILE:HG21	5:X:536:THR:HA	1.97	0.46
5:Y:278:ASP:OD1	5:Y:281:ARG:NH2	2.48	0.46
5:Y:484:ALA:HB1	5:Y:490:PRO:O	2.15	0.46
1:A:66:HIS:CE1	1:A:69:SER:HB2	2.50	0.46
2:C:1287:LEU:HD23	3:D:1357:ILE:HD11	1.98	0.46
2:C:866:ASP:HA	2:C:872:TYR:CZ	2.50	0.46
2:C:908:GLU:CG	2:C:909:LYS:H	2.27	0.46
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.27	0.46
3:D:233:LYS:HB3	3:D:236:TRP:CE2	2.50	0.46
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.37	0.46
1:G:185:TYR:HA	1:G:202:VAL:O	2.15	0.46
2:H:1006:GLU:CD	2:H:1006:GLU:H	2.19	0.46
2:H:1297:ASP:OD1	2:H:1300:GLY:HA3	2.15	0.46
2:H:59:ILE:HD11	2:H:63:SER:HB3	1.96	0.46
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.49	0.46
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.16	0.46
3:I:911:LYS:O	3:I:911:LYS:HD2	2.15	0.46
5:Y:379:MET:HE2	5:Y:379:MET:HA	1.97	0.46
2:C:843:THR:HB	2:C:845:LEU:CD2	2.46	0.46
3:D:33:TRP:O	3:D:102:MET:HB2	2.15	0.46
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.98	0.46
3:D:868:TRP:HA	3:D:871:LEU:HD23	1.96	0.46
1:F:207:THR:HG23	1:F:209:GLY:H	1.81	0.46
3:I:1180:VAL:HG22	3:I:1185:PRO:HA	1.97	0.46
3:I:1241:TYR:HB3	3:I:1246:VAL:HG23	1.96	0.46
3:I:356:THR:O	3:I:448:GLN:HA	2.16	0.46
3:I:773:PHE:O	3:I:776:THR:HG22	2.15	0.46
2:C:372:PRO:HB3	5:X:34:ASP:HB3	1.98	0.46
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.45	0.46
3:D:12:THR:C	3:D:13:LYS:HD2	2.36	0.46
2:C:1246:ARG:NE	3:D:348:ASP:OD2	2.34	0.46
3:D:73:GLY:O	3:D:76:LYS:HE3	2.15	0.46
3:D:773:PHE:O	3:D:776:THR:HG22	2.16	0.46
3:I:1159:ILE:HD12	3:I:1186:TYR:CE2	2.47	0.46
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.50	0.46
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:138:VAL:O	3:I:143:SER:HB3	2.15	0.46
3:I:382:TYR:HE1	3:I:401:VAL:HG21	1.80	0.46
5:X:139:GLU:HG3	5:X:351:THR:HA	1.97	0.46
2:C:1255:THR:O	2:C:1257:GLN:N	2.42	0.46
2:C:505:PHE:HA	2:C:509:SER:CB	2.46	0.46
3:D:161:THR:HG22	3:D:162:GLU:H	1.79	0.46
3:D:369:PRO:HB2	3:D:372:MET:CB	2.46	0.46
2:H:1032:LYS:NZ	2:H:1032:LYS:HB2	2.30	0.46
1:F:41:ASN:CG	2:H:1218:GLY:HA3	2.36	0.46
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.50	0.46
2:H:714:VAL:CG2	2:H:787:PRO:HD2	2.46	0.46
2:H:1290:MET:SD	3:I:347:VAL:HG11	2.55	0.46
3:I:766:GLY:C	3:I:767:LEU:HD22	2.36	0.46
5:X:276:MET:O	5:X:280:VAL:HG23	2.16	0.46
1:B:18:GLN:C	1:B:20:SER:H	2.19	0.46
1:B:37:HIS:CE1	2:C:1216:ARG:HD3	2.51	0.46
2:C:408:SER:O	2:C:431:LYS:NZ	2.31	0.46
2:C:886:LYS:HD3	2:C:916:SER:O	2.16	0.46
3:D:1195:GLN:N	3:D:1195:GLN:OE1	2.48	0.46
3:D:521:LYS:HB2	3:D:542:ALA:HB2	1.98	0.46
3:D:586:GLY:O	3:D:587:LEU:HB2	2.16	0.46
3:D:72:CYS:SG	3:D:73:GLY:N	2.87	0.46
3:I:1194:ARG:HD2	3:I:1194:ARG:N	2.30	0.46
3:I:217:LEU:O	3:I:221:ILE:HG12	2.15	0.46
3:I:899:TYR:CZ	3:I:915:ILE:HD12	2.51	0.46
5:X:264:LYS:HD2	5:X:264:LYS:N	2.30	0.46
5:Y:585:GLU:O	5:Y:589:GLN:N	2.43	0.46
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.56	0.46
2:C:59:ILE:CG2	2:C:479:LEU:HD13	2.45	0.46
2:C:944:ARG:HD3	2:C:944:ARG:O	2.15	0.46
3:D:1197:ASN:HD22	3:D:1212:ASP:HB3	1.81	0.46
3:D:138:VAL:O	3:D:143:SER:HB3	2.16	0.46
3:D:720:ASN:ND2	3:D:720:ASN:O	2.48	0.46
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.16	0.46
2:H:1269:ARG:N	2:H:1269:ARG:HD3	2.31	0.46
2:H:205:PRO:O	2:H:208:ILE:HG22	2.16	0.46
2:H:453:ILE:HG23	2:H:453:ILE:O	2.16	0.46
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.98	0.46
2:H:895:LEU:HD21	2:H:903:ARG:NH2	2.30	0.46
3:I:129:ASP:HB2	3:I:220:ARG:CZ	2.45	0.46
3:I:19:ALA:HA	3:I:1344:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:539:SER:O	3:I:541:LEU:N	2.49	0.46
5:X:346:GLN:O	5:X:350:GLU:HG3	2.16	0.46
5:X:459:THR:O	5:X:463:LEU:HD13	2.16	0.46
1:A:27:THR:HG22	1:A:202:VAL:HG13	1.98	0.46
1:A:29:GLU:O	1:A:31:LEU:N	2.49	0.46
1:B:74:VAL:HG12	1:B:76:GLU:H	1.81	0.46
2:C:1272:GLU:HG3	2:C:1276:TRP:CZ2	2.51	0.46
2:C:475:VAL:HG23	2:C:492:MET:SD	2.56	0.46
2:C:876:GLU:N	2:C:876:GLU:OE2	2.49	0.46
3:D:1287:ILE:O	3:D:1290:ARG:HG2	2.16	0.46
3:D:573:THR:HG23	3:D:576:ARG:H	1.80	0.46
2:H:40:GLU:O	2:H:73:TYR:OH	2.33	0.46
2:H:500:ALA:O	2:H:504:GLU:HB2	2.16	0.46
3:I:613:GLY:O	3:I:617:THR:OG1	2.22	0.46
5:Y:562:ARG:HG3	5:Y:591:GLU:CD	2.36	0.46
2:C:515:MET:HE2	2:C:523:GLU:HB3	1.97	0.45
2:C:800:MET:HG2	2:C:1096:ILE:HD13	1.98	0.45
2:C:942:ASP:HB2	2:C:1048:LYS:NZ	2.31	0.45
3:D:1226:VAL:HA	3:D:1229:VAL:HG12	1.98	0.45
3:D:111:THR:HG23	3:D:300:GLN:NE2	2.30	0.45
3:D:678:ARG:O	3:D:681:LYS:HG3	2.16	0.45
3:D:832:LYS:HA	3:D:832:LYS:HZ1	1.80	0.45
1:G:218:ARG:HH12	1:G:222:THR:HB	1.81	0.45
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.98	0.45
2:H:337:PHE:O	2:H:338:THR:OG1	2.26	0.45
2:H:510:GLN:NE2	2:H:534:GLY:HA2	2.30	0.45
2:H:600:THR:HG22	2:H:601:ASP:N	2.28	0.45
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.97	0.45
3:I:263:SER:HB2	5:Y:507:MET:HE2	1.98	0.45
3:I:390:LEU:N	3:I:390:LEU:HD12	2.31	0.45
3:I:596:LEU:HD23	3:I:596:LEU:N	2.31	0.45
3:I:620:PHE:O	3:I:624:ILE:HG23	2.16	0.45
3:I:800:LEU:O	3:I:803:VAL:HG12	2.16	0.45
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.16	0.45
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.17	0.45
3:I:44:ILE:HG22	5:Y:450:ILE:HG22	1.97	0.45
1:A:163:GLU:CB	1:A:166:ARG:HB3	2.45	0.45
1:A:300:LEU:HD13	1:A:300:LEU:O	2.17	0.45
1:A:318:LEU:HD13	1:A:318:LEU:N	2.32	0.45
2:C:1006:GLU:H	2:C:1006:GLU:CD	2.19	0.45
2:C:314:ASN:HD21	2:C:348:SER:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.98	0.45
3:D:1198:VAL:HB	3:D:1210:ILE:CD1	2.47	0.45
3:D:127:LEU:HD11	3:D:194:LEU:HD11	1.99	0.45
3:D:1347:LEU:HD23	3:D:1358:PRO:CG	2.30	0.45
3:D:415:VAL:HG23	3:D:416:ILE:HG23	1.97	0.45
3:D:818:GLU:HA	3:D:881:LYS:HE2	1.98	0.45
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.16	0.45
2:H:1117:LEU:HD11	2:H:1182:ILE:CD1	2.47	0.45
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.51	0.45
2:H:1276:TRP:HE3	2:H:1276:TRP:HA	1.81	0.45
2:H:521:LEU:HD22	2:H:667:LEU:HD12	1.99	0.45
3:I:238:ILE:HG13	3:I:238:ILE:O	2.16	0.45
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.81	0.45
3:I:589:TYR:O	3:I:591:ILE:HG13	2.16	0.45
5:X:112:THR:HG22	5:X:113:ARG:N	2.27	0.45
3:D:120:LEU:HG	5:X:46:GLN:CD	2.36	0.45
5:Y:264:LYS:N	5:Y:264:LYS:HD2	2.31	0.45
5:Y:400:GLN:O	5:Y:404:LEU:HD13	2.15	0.45
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.16	0.45
1:A:317:ARG:C	1:A:318:LEU:HD13	2.36	0.45
2:C:1199:LEU:HD13	2:C:1206:THR:HA	1.98	0.45
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.81	0.45
2:C:518:ASN:OD1	2:C:1236:ASN:ND2	2.48	0.45
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.51	0.45
3:D:1269:ALA:N	3:D:1300:ALA:HB2	2.30	0.45
3:D:1307:LEU:HD23	3:D:1307:LEU:H	1.81	0.45
3:D:290:ILE:O	3:D:293:ARG:HG3	2.15	0.45
3:D:605:LEU:O	3:D:605:LEU:HD13	2.17	0.45
3:D:74:LYS:HB3	3:D:74:LYS:NZ	2.31	0.45
3:D:822:MET:HG2	3:D:839:VAL:HG22	1.97	0.45
3:D:909:ILE:O	3:D:909:ILE:HD12	2.16	0.45
3:I:145:VAL:HG21	3:I:165:TYR:CD2	2.52	0.45
3:I:214:ARG:O	3:I:218:THR:HG22	2.16	0.45
3:I:29:MET:HE3	3:I:29:MET:HA	1.98	0.45
3:I:813:ASP:OD1	3:I:896:ALA:HB3	2.16	0.45
5:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.98	0.45
1:B:129:VAL:HG11	1:B:132:HIS:CE1	2.51	0.45
2:C:1141:LEU:HD22	2:C:1141:LEU:O	2.16	0.45
2:C:131:THR:HG23	2:C:133:ASN:N	2.30	0.45
2:C:620:ASN:HD21	3:D:769:VAL:HG12	1.80	0.45
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:362:ARG:HH22	7:D:1503:O02:H7	1.82	0.45
3:D:514:THR:HG23	3:D:576:ARG:HE	1.80	0.45
4:E:15:ASN:ND2	4:E:18:ASP:HB2	2.31	0.45
1:F:45:ARG:HD3	1:G:34:GLY:HA3	1.97	0.45
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.98	0.45
2:H:1103:VAL:H	2:H:1104:PRO:HD2	1.80	0.45
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.31	0.45
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.46	0.45
3:I:501:VAL:HG21	3:I:602:SER:HB2	1.99	0.45
3:I:586:GLY:O	3:I:587:LEU:HB2	2.17	0.45
5:X:101:TYR:CE2	5:X:388:ILE:HD11	2.45	0.45
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	1.97	0.45
2:C:1191:LYS:O	2:C:1195:ILE:HG13	2.16	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:N	2.31	0.45
2:C:96:LEU:HB2	2:C:127:ILE:CD1	2.47	0.45
2:C:22:LEU:HD13	2:C:23:ASP:O	2.17	0.45
2:C:845:LEU:N	2:C:845:LEU:HD13	2.27	0.45
3:D:1148:ARG:HB2	3:D:1148:ARG:HH21	1.81	0.45
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.42	0.45
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.16	0.45
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.99	0.45
2:H:143:ARG:NH1	2:H:512:SER:O	2.50	0.45
2:H:88:ARG:NH1	2:H:88:ARG:HB3	2.30	0.45
3:I:33:TRP:O	3:I:102:MET:HB2	2.16	0.45
3:I:846:GLU:HA	3:I:858:VAL:HA	1.98	0.45
5:X:445:ASP:N	5:X:445:ASP:OD1	2.38	0.45
5:Y:445:ASP:N	5:Y:445:ASP:OD1	2.39	0.45
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.98	0.45
1:B:48:LEU:HB3	3:D:538:ARG:HD3	1.99	0.45
2:C:446:ASP:OD1	2:C:546:GLU:HB3	2.17	0.45
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.80	0.45
2:C:699:LEU:HD11	2:C:1179:GLY:CA	2.43	0.45
3:D:246:PRO:HB2	3:D:249:LEU:HD13	1.98	0.45
3:D:513:MET:O	3:D:575:GLY:HA3	2.17	0.45
2:H:169:LYS:HD3	2:H:169:LYS:HA	1.76	0.45
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.46	0.45
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.98	0.45
3:I:583:VAL:HG13	3:I:587:LEU:HD22	1.98	0.45
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.38	0.45
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.81	0.45
5:X:543:ALA:O	5:X:547:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:592:ALA:O	5:X:596:ARG:HG2	2.16	0.45
1:A:241:GLU:OE2	1:A:243:LYS:HE3	2.17	0.45
2:C:1272:GLU:HA	2:C:1275:VAL:HG22	1.99	0.45
2:C:49:LEU:CD1	2:C:461:GLU:HA	2.47	0.45
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.52	0.45
2:C:958:LYS:O	2:C:962:GLU:HG2	2.17	0.45
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.32	0.45
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	1.97	0.45
3:D:1357:ILE:N	3:D:1357:ILE:HD12	2.32	0.45
3:D:238:ILE:HG13	3:D:238:ILE:O	2.15	0.45
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.46	0.45
2:H:994:ARG:N	2:H:994:ARG:HD3	2.31	0.45
3:I:1297:LYS:HE2	3:I:1297:LYS:HA	1.97	0.45
3:I:1345:ARG:HG2	3:I:1370:MET:HE1	1.98	0.45
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.82	0.45
4:J:60:ASN:H	4:J:63:ILE:HB	1.82	0.45
5:Y:448:ARG:NH1	5:Y:452:ILE:HD12	2.32	0.45
2:C:1122:LYS:HG2	2:C:1229:TYR:CE2	2.51	0.45
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.98	0.45
2:C:462:ASN:O	2:C:466:VAL:HG23	2.17	0.45
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.51	0.45
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.16	0.45
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.98	0.45
3:D:611:ILE:HG13	3:D:612:LEU:HD23	1.99	0.45
3:D:619:ILE:HD11	3:D:623:GLN:HE21	1.82	0.45
2:H:1238:LEU:HD12	2:H:1239:VAL:O	2.16	0.45
2:H:297:VAL:HB	2:H:317:LEU:HD21	1.98	0.45
2:H:634:VAL:HG22	2:H:645:PHE:CZ	2.52	0.45
3:I:113:HIS:CE1	3:I:115:TRP:HB2	2.51	0.45
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.80	0.45
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.99	0.45
5:X:240:ARG:HD3	5:X:244:THR:CB	2.40	0.45
5:X:451:ARG:O	5:X:452:ILE:HG13	2.17	0.45
5:X:449:THR:HG23	5:X:503:GLU:OE1	2.16	0.45
5:Y:276:MET:O	5:Y:280:VAL:HG23	2.17	0.45
2:C:1017:GLN:HA	2:C:1020:GLU:HB3	1.98	0.45
2:C:453:ILE:HG23	2:C:453:ILE:O	2.17	0.45
2:C:821:ARG:HB2	2:C:1082:ILE:CD1	2.47	0.45
3:D:1307:LEU:HD23	3:D:1307:LEU:N	2.32	0.45
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.99	0.45
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:733:SER:O	3:D:737:ILE:HG12	2.17	0.45
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.82	0.45
2:H:149:LEU:HD12	2:H:452:ARG:O	2.17	0.45
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.82	0.45
3:I:704:GLU:O	3:I:705:THR:OG1	2.28	0.45
5:Y:354:THR:HG23	5:Y:357:GLN:HB3	1.97	0.45
1:A:181:GLU:OE2	1:A:181:GLU:N	2.50	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.17	0.45
3:D:210:SER:O	3:D:214:ARG:HG3	2.17	0.45
2:C:1258:PRO:HG2	3:D:346:ARG:CB	2.47	0.45
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.82	0.45
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.99	0.45
2:H:669:PRO:HG2	2:H:1070:HIS:CE1	2.51	0.45
2:H:1081:PRO:O	2:H:1085:MET:HG3	2.17	0.45
2:H:475:VAL:O	2:H:479:LEU:HB2	2.16	0.45
2:H:756:TYR:H	2:H:766:ASN:HB3	1.82	0.45
3:I:120:LEU:HD22	3:I:1330:ARG:HD2	1.99	0.45
3:I:1247:LYS:N	3:I:1247:LYS:HD3	2.22	0.45
3:I:527:LEU:HD12	3:I:535:ARG:NE	2.32	0.45
3:I:856:ILE:HG13	3:I:857:LEU:O	2.16	0.45
3:D:395:LYS:HD3	5:X:607:LEU:HD13	1.99	0.45
5:Y:310:GLU:O	5:Y:344:LEU:HD23	2.17	0.45
3:D:527:LEU:HD13	3:D:531:LYS:CB	2.45	0.44
3:D:596:LEU:HD23	3:D:596:LEU:N	2.32	0.44
3:D:663:GLU:O	3:D:667:GLN:HG3	2.17	0.44
3:D:66:LYS:HB2	3:D:69:GLU:HG2	1.99	0.44
3:D:701:LEU:HD21	3:D:723:TYR:HB2	1.99	0.44
3:D:915:ILE:O	3:D:918:ILE:HG23	2.16	0.44
2:H:1291:LEU:HD13	3:I:345:LYS:NZ	2.31	0.44
2:H:489:PRO:HB2	2:H:492:MET:CB	2.37	0.44
2:H:961:SER:O	2:H:965:GLN:HG3	2.17	0.44
3:I:1357:ILE:N	3:I:1357:ILE:HD12	2.32	0.44
3:I:515:ARG:HH22	3:I:717:VAL:C	2.19	0.44
3:I:74:LYS:HB3	3:I:74:LYS:NZ	2.32	0.44
5:X:113:ARG:O	5:X:117:ILE:HD13	2.18	0.44
5:Y:119:ILE:CG2	5:Y:379:MET:HG2	2.45	0.44
5:Y:555:GLU:OE2	5:Y:597:LYS:NZ	2.33	0.44
1:B:126:PRO:HG2	1:B:127:GLN:OE1	2.18	0.44
2:C:310:ILE:O	2:C:311:CYS:HB3	2.18	0.44
3:D:1161:GLY:HA2	3:D:1181:ASP:CB	2.47	0.44
3:D:239:LEU:HD12	3:D:239:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.82	0.44
1:F:61:ILE:HG12	1:F:142:MET:HB3	1.98	0.44
2:H:1027:LYS:HB2	2:H:1027:LYS:NZ	2.32	0.44
2:H:593:LYS:HD2	2:H:604:HIS:NE2	2.32	0.44
3:I:384:LYS:HD2	3:I:384:LYS:HA	1.88	0.44
4:J:65:ASP:O	4:J:69:ARG:HG3	2.16	0.44
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.98	0.44
5:Y:561:MET:HA	5:Y:567:MET:SD	2.57	0.44
2:C:1027:LYS:NZ	2:C:1027:LYS:HB2	2.33	0.44
2:C:823:VAL:HG22	2:C:1060:ILE:HG13	1.99	0.44
2:C:88:ARG:HB3	2:C:88:ARG:NH1	2.33	0.44
3:D:316:ILE:CG2	3:D:317:THR:H	2.25	0.44
3:D:526:VAL:HG12	3:D:549:LYS:O	2.17	0.44
3:D:664:ILE:HG21	3:D:681:LYS:CD	2.44	0.44
4:E:30:MET:O	4:E:35:LYS:HG2	2.17	0.44
1:G:178:SER:HA	1:G:179:PRO:HD3	1.87	0.44
2:H:1133:LYS:HG3	2:H:1134:GLN:HG3	1.99	0.44
2:H:1120:ALA:HB1	2:H:1198:LEU:HB3	1.99	0.44
2:H:807:TRP:HH2	2:H:1216:ARG:HE	1.65	0.44
2:H:1111:GLN:CG	2:H:1230:MET:HE2	2.48	0.44
2:H:484:LEU:HD22	2:H:484:LEU:N	2.31	0.44
2:H:820:GLU:O	2:H:824:GLN:HG3	2.18	0.44
3:I:161:THR:HG22	3:I:162:GLU:N	2.33	0.44
3:I:490:ILE:O	3:I:499:ILE:HG22	2.18	0.44
3:I:539:SER:OG	3:I:540:GLY:N	2.50	0.44
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.98	0.44
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.17	0.44
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.98	0.44
3:D:217:LEU:O	3:D:221:ILE:HG12	2.16	0.44
3:D:703:THR:O	3:D:718:SER:N	2.50	0.44
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.53	0.44
3:D:825:VAL:HG23	3:D:835:LEU:HB2	1.99	0.44
7:D:1503:O2:O2G	4:E:3:ARG:NH2	2.50	0.44
1:F:185:TYR:HB2	1:F:201:LEU:HD11	1.98	0.44
2:H:1238:LEU:HD12	2:H:1239:VAL:N	2.32	0.44
2:H:429:MET:O	2:H:433:ILE:HG13	2.17	0.44
2:H:702:THR:HA	2:H:1184:THR:O	2.16	0.44
2:H:943:LYS:O	2:H:947:GLU:HG2	2.17	0.44
3:I:378:LYS:HD2	3:I:382:TYR:OH	2.16	0.44
3:I:909:ILE:O	3:I:909:ILE:HD12	2.18	0.44
5:X:23:THR:HG22	5:X:26:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HG3	2:C:694:ARG:HH12	1.83	0.44
2:C:1298:VAL:HG23	2:C:1299:ASN:N	2.29	0.44
2:C:985:GLU:HG2	2:C:989:LEU:HD13	2.00	0.44
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.48	0.44
3:D:1184:ASP:HA	3:D:1185:PRO:HD3	1.80	0.44
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.31	0.44
3:D:1344:LEU:H	3:D:1345:ARG:HG3	1.83	0.44
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.35	0.44
1:G:65:LEU:HD23	1:G:65:LEU:N	2.30	0.44
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.30	0.44
2:H:161:LYS:HB3	2:H:161:LYS:NZ	2.33	0.44
2:H:821:ARG:NE	2:H:1082:ILE:HD13	2.33	0.44
2:H:839:VAL:HG11	2:H:841:ARG:HE	1.83	0.44
3:I:416:ILE:HG13	3:I:441:LEU:CD2	2.48	0.44
3:I:700:ASN:O	3:I:704:GLU:HG2	2.17	0.44
2:H:1276:TRP:CD2	3:I:801:VAL:HG11	2.53	0.44
5:X:61:ASP:HA	5:X:64:ASP:OD2	2.17	0.44
2:C:68:LEU:HG	2:C:100:LEU:HD23	2.00	0.44
2:C:1108:ASN:O	2:C:1108:ASN:ND2	2.51	0.44
2:C:177:ILE:HD12	2:C:177:ILE:N	2.33	0.44
2:C:892:GLU:O	2:C:893:THR:OG1	2.22	0.44
2:C:812:PHE:HB2	3:D:357:VAL:HG21	2.00	0.44
3:D:704:GLU:HB2	3:D:718:SER:OG	2.18	0.44
4:E:15:ASN:ND2	4:E:18:ASP:OD1	2.51	0.44
4:E:5:THR:CA	4:E:7:GLN:H	2.30	0.44
1:G:81:ILE:HG23	1:G:131:CYS:SG	2.58	0.44
1:F:234:LEU:HD21	1:G:217:ILE:HD11	1.98	0.44
1:G:67:GLU:O	1:G:78:ILE:HB	2.18	0.44
1:G:33:ARG:HD3	2:H:1081:PRO:HG3	1.98	0.44
2:H:179:TYR:HE2	2:H:462:ASN:HD21	1.64	0.44
2:H:736:VAL:HG11	2:H:740:GLU:HA	1.98	0.44
3:I:1195:GLN:N	3:I:1195:GLN:OE1	2.48	0.44
3:I:1284:ARG:HA	3:I:1287:ILE:CG1	2.46	0.44
3:I:412:LEU:O	3:I:415:VAL:HG22	2.18	0.44
3:I:899:TYR:CE1	3:I:915:ILE:HG23	2.53	0.44
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.51	0.44
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.47	0.44
1:A:88:LEU:HD22	1:A:90:VAL:CG2	2.48	0.44
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.53	0.44
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.83	0.44
3:D:161:THR:HG22	3:D:162:GLU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:233:LYS:CD	3:D:234:PRO:HD2	2.48	0.44
3:D:382:TYR:HE1	3:D:401:VAL:CG2	2.31	0.44
2:H:1086:PRO:HA	2:H:1213:TYR:O	2.18	0.44
2:H:1103:VAL:HB	2:H:1104:PRO:HD3	2.00	0.44
2:H:202:ARG:NE	2:H:369:MET:HG2	2.33	0.44
2:H:845:LEU:HD13	2:H:845:LEU:N	2.30	0.44
3:I:664:ILE:HG21	3:I:681:LYS:HD2	2.00	0.44
4:J:10:VAL:CG2	4:J:16:ARG:HG2	2.47	0.44
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.99	0.44
1:A:45:ARG:NE	1:B:38:THR:OG1	2.46	0.44
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.32	0.44
2:C:11:ILE:HG21	2:C:697:LYS:HZ1	1.80	0.44
2:C:1233:LEU:O	2:C:1233:LEU:HD12	2.18	0.44
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.82	0.44
3:D:572:THR:HG22	3:D:594:GLN:OE1	2.18	0.44
3:D:888:CYS:SG	3:D:890:THR:HB	2.58	0.44
1:F:163:GLU:HG3	1:F:170:ARG:NH1	2.18	0.44
1:F:158:ARG:HE	1:F:172:LEU:HD13	1.82	0.44
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.46	0.44
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.53	0.44
2:H:557:ARG:HH12	2:H:611:GLU:CD	2.21	0.44
3:I:124:ILE:HG13	3:I:189:LEU:HD11	1.99	0.44
3:I:12:THR:C	3:I:13:LYS:HD2	2.39	0.44
3:I:41:PRO:HB3	3:I:270:ARG:HG3	1.99	0.44
3:I:873:GLU:OE2	3:I:877:VAL:HB	2.18	0.44
5:X:469:GLN:O	5:X:473:GLU:HB2	2.18	0.44
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.26	0.44
1:A:178:SER:HA	1:A:179:PRO:HD3	1.75	0.44
1:B:22:THR:HG22	1:B:208:ASN:O	2.18	0.44
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.33	0.44
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.99	0.44
2:C:1081:PRO:O	2:C:1085:MET:HG3	2.17	0.44
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.30	0.44
2:C:297:VAL:HB	2:C:317:LEU:HD21	2.00	0.44
2:C:345:PRO:O	2:C:349:GLU:HG2	2.18	0.44
2:C:697:LYS:NZ	2:C:791:LEU:HD11	2.32	0.44
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.43	0.44
3:D:490:ILE:HG23	3:D:500:ILE:CD1	2.48	0.44
3:D:515:ARG:NH2	3:D:717:VAL:HG12	2.32	0.44
3:D:766:GLY:C	3:D:767:LEU:HD22	2.37	0.44
3:D:801:VAL:O	3:D:805:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:842:ARG:HD2	3:D:882:VAL:HG21	1.99	0.44
1:F:11:PRO:HD2	1:G:227:GLN:HA	1.99	0.44
2:H:828:PHE:HB2	2:H:1060:ILE:HD13	2.00	0.44
2:H:106:GLU:CG	2:H:109:ALA:H	2.31	0.44
2:H:632:ASP:O	2:H:633:LEU:HD23	2.18	0.44
2:H:850:ILE:HG23	2:H:885:GLY:O	2.17	0.44
2:H:890:LYS:NZ	2:H:890:LYS:HB3	2.32	0.44
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.99	0.44
3:I:30:ILE:HD13	3:I:33:TRP:CZ3	2.53	0.44
3:I:388:ARG:NH2	3:I:414:GLU:OE2	2.51	0.44
3:I:801:VAL:O	3:I:805:GLN:HG2	2.17	0.44
5:X:254:GLU:O	5:X:258:GLN:HG3	2.18	0.44
5:X:532:LEU:O	5:X:536:THR:HG23	2.18	0.44
5:Y:123:ILE:O	5:Y:127:ILE:HG12	2.18	0.44
1:B:180:VAL:HG11	1:B:183:ILE:HG12	2.00	0.43
1:B:190:ALA:N	1:B:198:LEU:O	2.37	0.43
2:C:19:PRO:HA	2:C:1157:GLN:HE21	1.83	0.43
2:C:1247:SER:O	2:C:1248:THR:HG23	2.18	0.43
2:C:24:VAL:HA	2:C:25:PRO:HD3	1.86	0.43
2:C:384:LEU:O	2:C:388:LEU:HG	2.17	0.43
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.51	0.43
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.53	0.43
2:H:562:GLU:HG2	2:H:574:SER:HB3	1.98	0.43
2:H:73:TYR:O	2:H:74:ARG:HB2	2.17	0.43
3:I:63:GLY:O	3:I:98:ARG:NH2	2.51	0.43
3:I:832:LYS:HZ2	3:I:832:LYS:HB2	1.83	0.43
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.48	0.43
5:Y:451:ARG:O	5:Y:452:ILE:HG13	2.18	0.43
5:Y:477:GLU:OE1	5:Y:477:GLU:N	2.46	0.43
1:A:33:ARG:HG2	1:A:199:ASP:OD2	2.18	0.43
1:B:46:ILE:HG23	1:B:50:SER:HB2	2.00	0.43
2:C:1185:PRO:HB2	2:C:1186:VAL:H	1.69	0.43
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.49	0.43
2:C:515:MET:HE2	2:C:523:GLU:CG	2.48	0.43
2:C:678:ARG:HG3	2:C:1106:ARG:HB3	2.00	0.43
3:D:62:PHE:O	3:D:101:ARG:HG3	2.18	0.43
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.48	0.43
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	2.00	0.43
1:F:31:LEU:HB2	1:F:199:ASP:O	2.17	0.43
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.53	0.43
3:I:1257:VAL:HA	3:I:1260:MET:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:222:LYS:HZ2	3:I:1276:GLU:HB2	1.82	0.43
3:I:1307:LEU:HD23	3:I:1307:LEU:H	1.82	0.43
3:I:843:VAL:HG21	3:I:897:HIS:HA	2.00	0.43
5:X:299:LYS:O	5:X:303:ILE:HG12	2.18	0.43
5:X:465:ARG:O	5:X:468:ARG:HG2	2.17	0.43
5:Y:240:ARG:HD3	5:Y:244:THR:CB	2.47	0.43
2:C:1166:ASP:C	2:C:1168:GLU:H	2.22	0.43
2:C:11:ILE:HD13	2:C:697:LYS:HE3	1.99	0.43
2:C:170:VAL:O	2:C:171:LEU:HB2	2.18	0.43
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.44	0.43
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.50	0.43
1:G:110:VAL:HG21	1:G:140:ILE:HD11	2.01	0.43
2:H:1067:ALA:HB3	2:H:1235:LEU:HD11	2.00	0.43
2:H:216:THR:O	2:H:220:ILE:HG13	2.18	0.43
2:H:73:TYR:N	2:H:73:TYR:CD2	2.86	0.43
3:I:508:LEU:HD23	3:I:508:LEU:O	2.19	0.43
3:I:52:GLU:OE1	5:Y:451:ARG:HD2	2.17	0.43
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.26	0.43
3:I:905:ARG:NH2	4:J:10:VAL:HG11	2.30	0.43
5:X:105:MET:O	5:X:385:ARG:NH1	2.50	0.43
5:X:456:MET:O	5:X:460:ILE:HG13	2.18	0.43
3:D:137:ARG:CZ	5:X:95:THR:HG23	2.48	0.43
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	1.99	0.43
1:A:179:PRO:O	1:A:207:THR:OG1	2.25	0.43
1:A:246:LYS:N	1:A:246:LYS:HD3	2.33	0.43
2:C:1002:LEU:HG	2:C:1007:LYS:HG2	1.99	0.43
2:C:1158:LYS:O	2:C:1158:LYS:HD2	2.19	0.43
2:C:161:LYS:HB3	2:C:161:LYS:NZ	2.34	0.43
2:C:219:GLN:O	2:C:223:LEU:HG	2.17	0.43
2:C:590:PRO:O	2:C:659:GLN:NE2	2.50	0.43
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.18	0.43
3:D:136:GLU:HA	3:D:139:LEU:HD12	2.00	0.43
3:D:390:LEU:HD12	3:D:390:LEU:N	2.32	0.43
3:D:681:LYS:HB2	3:D:681:LYS:HZ2	1.84	0.43
1:F:77:ASP:O	1:F:81:ILE:HG13	2.18	0.43
2:H:177:ILE:N	2:H:177:ILE:HD12	2.33	0.43
2:H:944:ARG:HD3	2:H:944:ARG:O	2.17	0.43
3:I:239:LEU:HD12	3:I:239:LEU:O	2.19	0.43
3:I:363:LEU:HA	3:I:450:HIS:ND1	2.33	0.43
3:I:527:LEU:HD13	3:I:531:LYS:CB	2.48	0.43
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:533:LEU:N	2:C:533:LEU:HD23	2.31	0.43
3:D:1159:ILE:HD12	3:D:1186:TYR:CE2	2.53	0.43
3:D:1162:ILE:HG12	3:D:1203:ARG:HG2	2.00	0.43
3:D:215:LYS:O	3:D:219:LYS:HG3	2.19	0.43
3:D:500:ILE:H	3:D:500:ILE:CD1	2.31	0.43
3:D:66:LYS:HB3	3:D:66:LYS:NZ	2.33	0.43
3:D:79:LYS:HE3	5:X:568:ASN:C	2.38	0.43
3:D:886:VAL:HG13	3:D:1230:THR:HG21	2.00	0.43
1:G:183:ILE:HD11	1:G:205:MET:HE2	2.00	0.43
2:H:657:THR:OG1	2:H:1187:PHE:HB2	2.18	0.43
2:H:866:ASP:HA	2:H:872:TYR:OH	2.17	0.43
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	2.00	0.43
3:I:179:LYS:N	3:I:179:LYS:HD3	2.33	0.43
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.51	0.43
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.18	0.43
2:C:363:LEU:HD13	2:C:382:GLU:HG2	2.00	0.43
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.83	0.43
1:G:227:GLN:O	1:G:228:LEU:HD23	2.19	0.43
1:F:150:ARG:HD2	1:G:8:PHE:CZ	2.54	0.43
2:H:106:GLU:CB	2:H:107:ARG:HA	2.49	0.43
2:H:1163:THR:HG22	2:H:1164:PHE:H	1.84	0.43
2:H:748:ILE:HD12	2:H:748:ILE:C	2.39	0.43
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.89	0.43
3:I:1284:ARG:HA	3:I:1287:ILE:CD1	2.49	0.43
1:G:191:ARG:NH2	3:I:441:LEU:O	2.52	0.43
3:I:532:GLU:OE2	3:I:574:VAL:HG13	2.19	0.43
3:I:611:ILE:HG22	3:I:865:HIS:CE1	2.54	0.43
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.76	0.43
3:I:796:LEU:HG	3:I:800:LEU:HD23	2.01	0.43
2:C:1086:PRO:HG2	2:C:1094:VAL:HG21	2.01	0.43
2:C:51:ALA:HB3	2:C:465:ARG:HH11	1.83	0.43
2:C:500:ALA:O	2:C:504:GLU:HB2	2.18	0.43
2:C:611:GLU:HG2	2:C:616:ILE:HD11	2.00	0.43
2:C:622:ASN:OD1	2:C:623:LEU:N	2.51	0.43
2:C:617:ALA:HB2	2:C:650:VAL:HG21	2.01	0.43
2:C:811:ASN:HA	2:C:815:SER:HB2	2.00	0.43
3:D:355:ILE:HA	3:D:447:ILE:HG23	1.99	0.43
3:D:619:ILE:HD13	7:D:1503:O2:H2	1.83	0.43
3:D:620:PHE:O	3:D:624:ILE:HG23	2.19	0.43
1:F:11:PRO:HA	1:F:30:PRO:O	2.19	0.43
1:G:227:GLN:O	1:G:229:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:VAL:HG12	1:G:173:VAL:HG11	2.01	0.43
2:H:555:TYR:OH	2:H:637:ARG:NH2	2.52	0.43
2:H:582:ASN:HB3	2:H:586:PHE:C	2.39	0.43
2:H:816:ILE:HD13	2:H:1074:GLY:CA	2.43	0.43
2:H:988:LYS:HB3	2:H:988:LYS:NZ	2.33	0.43
2:H:993:PRO:HB2	2:H:994:ARG:H	1.60	0.43
3:I:1287:ILE:O	3:I:1291:GLU:HG2	2.19	0.43
3:I:37:GLU:HB2	3:I:104:HIS:HE1	1.83	0.43
5:X:141:ILE:HG13	5:X:256:PHE:CD1	2.53	0.43
5:X:343:LYS:O	5:X:346:GLN:HB3	2.18	0.43
5:X:469:GLN:O	5:X:473:GLU:N	2.47	0.43
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.18	0.43
2:C:826:ASP:HA	2:C:829:THR:HG23	1.99	0.43
3:D:1167:LYS:HB3	3:D:1170:LYS:HD2	2.00	0.43
3:D:259:ARG:HH21	5:X:504:PRO:CB	2.26	0.43
3:D:573:THR:HG22	3:D:576:ARG:CD	2.48	0.43
2:H:1185:PRO:HB2	2:H:1186:VAL:H	1.66	0.43
2:H:1209:GLN:O	2:H:1210:ILE:HG13	2.19	0.43
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.34	0.43
2:H:333:ILE:N	2:H:333:ILE:HD12	2.34	0.43
2:H:622:ASN:OD1	2:H:623:LEU:N	2.52	0.43
1:F:66:HIS:HB3	2:H:874:GLY:HA2	2.00	0.43
3:I:885:VAL:O	3:I:1258:ARG:HD3	2.19	0.43
3:I:159:ILE:N	3:I:159:ILE:HD12	2.33	0.43
3:I:276:ASN:O	3:I:280:LYS:HG3	2.19	0.43
3:I:733:SER:O	3:I:737:ILE:HG12	2.19	0.43
1:A:152:TYR:CE2	2:C:824:GLN:HA	2.53	0.43
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.19	0.43
2:C:17:LYS:N	2:C:17:LYS:HD2	2.34	0.43
3:D:1257:VAL:HA	3:D:1260:MET:CB	2.47	0.43
2:C:1287:LEU:HD23	3:D:1357:ILE:CD1	2.48	0.43
3:D:393:THR:H	3:D:396:ALA:HB3	1.83	0.43
3:D:591:ILE:HA	3:D:594:GLN:HB2	2.01	0.43
3:D:491:LEU:HB2	3:D:904:ALA:HA	2.00	0.43
1:F:219:ARG:O	1:F:223:ILE:HG13	2.18	0.43
1:G:110:VAL:HB	1:G:131:CYS:HB2	1.99	0.43
2:H:842:ASP:HB2	2:H:1046:VAL:HG11	2.01	0.43
2:H:768:MET:O	2:H:785:ASP:N	2.50	0.43
2:H:894:GLN:O	2:H:895:LEU:HB2	2.18	0.43
2:H:999:GLU:HG2	2:H:1000:LEU:N	2.34	0.43
5:X:283:GLN:O	5:X:287:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HA	1:A:30:PRO:O	2.18	0.43
1:A:257:VAL:HG13	1:A:276:HIS:O	2.19	0.43
1:B:213:PRO:HA	1:B:216:ALA:HB3	2.00	0.43
2:C:1209:GLN:O	2:C:1210:ILE:HG13	2.19	0.43
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.34	0.43
2:C:453:ILE:HG22	2:C:585:GLY:O	2.19	0.43
3:D:112:ALA:HA	3:D:238:ILE:HG22	2.00	0.43
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.24	0.43
3:D:416:ILE:O	3:D:416:ILE:HD12	2.19	0.43
3:D:901:ARG:HB3	3:D:908:ILE:HA	2.01	0.43
1:F:28:LEU:HD13	1:G:231:PHE:HE2	1.82	0.43
2:H:971:LEU:HG	2:H:1018:TYR:HD1	1.84	0.43
2:H:1276:TRP:CE2	3:I:801:VAL:HG11	2.54	0.43
2:H:896:THR:HG22	2:H:898:GLU:OE1	2.18	0.43
2:H:935:THR:HA	2:H:1048:LYS:HB3	2.00	0.43
3:I:120:LEU:HB3	3:I:121:PRO:HD3	1.97	0.43
3:I:1287:ILE:O	3:I:1290:ARG:HG2	2.18	0.43
3:I:1307:LEU:HD23	3:I:1307:LEU:N	2.34	0.43
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.49	0.43
3:I:431:ARG:HH21	3:I:493:PRO:HG3	1.83	0.43
3:I:655:SER:O	3:I:658:GLU:HG2	2.19	0.43
3:I:809:VAL:CG1	3:I:913:GLU:H	2.32	0.43
2:C:1329:GLU:O	2:C:1332:SER:HB3	2.19	0.42
2:C:515:MET:HA	2:C:526:HIS:CE1	2.54	0.42
2:C:794:LEU:HD21	2:C:796:LEU:CG	2.46	0.42
3:D:1284:ARG:HA	3:D:1287:ILE:CD1	2.49	0.42
3:D:377:PHE:O	3:D:381:ILE:HG13	2.18	0.42
3:D:508:LEU:HD22	3:D:508:LEU:O	2.18	0.42
3:D:660:GLU:O	3:D:664:ILE:HG12	2.19	0.42
3:D:704:GLU:O	3:D:705:THR:OG1	2.27	0.42
2:H:1314:GLN:HG2	2:H:1315:MET:H	1.83	0.42
2:H:130:MET:CG	2:H:134:GLY:HA2	2.48	0.42
2:H:170:VAL:O	2:H:171:LEU:HB2	2.19	0.42
3:I:149:GLY:HA2	3:I:156:ARG:HG2	2.01	0.42
3:I:252:LEU:N	3:I:252:LEU:HD23	2.33	0.42
5:X:250:LEU:O	5:X:254:GLU:HG2	2.18	0.42
5:Y:460:ILE:HG12	5:Y:497:VAL:HG13	2.01	0.42
1:A:22:THR:HB	1:A:207:THR:O	2.18	0.42
2:C:1252:SER:HB3	2:C:1259:LEU:HD23	2.01	0.42
2:C:49:LEU:HG	2:C:461:GLU:HB2	2.00	0.42
2:C:542:ARG:HG2	2:C:543:ALA:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:556:GLY:O	2:C:579:ALA:HB2	2.18	0.42
2:C:966:ILE:HG23	2:C:967:LEU:HD12	2.01	0.42
2:C:994:ARG:N	2:C:994:ARG:HD3	2.34	0.42
3:D:506:VAL:HG23	3:D:628:GLY:HA3	2.00	0.42
3:D:800:LEU:O	3:D:803:VAL:HG12	2.18	0.42
1:F:167:PRO:HG2	1:F:170:ARG:HG3	2.00	0.42
1:G:222:THR:O	1:G:226:GLU:HG2	2.19	0.42
2:H:347:ILE:HD11	2:H:433:ILE:HD11	2.01	0.42
2:H:518:ASN:OD1	2:H:1236:ASN:ND2	2.52	0.42
2:H:557:ARG:NH2	2:H:607:SER:O	2.51	0.42
1:F:134:THR:HG21	2:H:727:VAL:O	2.18	0.42
2:H:896:THR:CG2	2:H:897:PRO:HD2	2.49	0.42
2:H:972:PHE:HA	2:H:975:ILE:HG22	2.01	0.42
3:I:124:ILE:HA	3:I:237:MET:HE2	2.00	0.42
3:I:595:ALA:HB1	3:I:596:LEU:HD23	2.01	0.42
1:A:152:TYR:CE1	1:A:154:PRO:HD3	2.53	0.42
1:A:227:GLN:NE2	1:B:11:PRO:HD3	2.32	0.42
1:A:250:ASP:HB3	1:A:253:LEU:HD13	2.00	0.42
1:B:19:VAL:HG12	1:B:19:VAL:O	2.20	0.42
2:C:1293:VAL:HG21	2:C:1304:MET:CB	2.49	0.42
2:C:333:ILE:N	2:C:333:ILE:HD12	2.33	0.42
2:C:645:PHE:CD1	2:C:650:VAL:HB	2.54	0.42
3:D:1221:LEU:HB2	3:D:1229:VAL:HG21	2.01	0.42
3:D:1229:VAL:O	3:D:1233:ILE:HG13	2.19	0.42
3:D:362:ARG:NH1	7:D:1503:O2:H7	2.32	0.42
3:D:288:PRO:O	3:D:292:VAL:HG12	2.19	0.42
3:D:527:LEU:HB2	3:D:535:ARG:CZ	2.50	0.42
3:D:584:PRO:HD3	3:D:620:PHE:CD1	2.54	0.42
3:D:746:LEU:HB3	3:D:754:ILE:CG2	2.49	0.42
3:D:843:VAL:HA	3:D:861:ASN:HA	2.01	0.42
3:D:789:LYS:HD2	3:D:932:MET:SD	2.59	0.42
3:D:614:LEU:HD12	4:E:5:THR:HG21	2.01	0.42
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.49	0.42
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.83	0.42
2:H:812:PHE:N	2:H:815:SER:HB2	2.34	0.42
2:H:941:LYS:O	2:H:941:LYS:HD2	2.19	0.42
3:I:1173:ARG:CZ	3:I:1176:VAL:HG21	2.50	0.42
3:I:128:LEU:HD13	3:I:189:LEU:HD23	2.01	0.42
3:I:661:VAL:O	3:I:665:GLN:HG3	2.19	0.42
3:I:704:GLU:HB3	3:I:705:THR:H	1.72	0.42
3:I:805:GLN:HE21	3:I:805:GLN:HB2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:448:ARG:HH11	5:X:452:ILE:HD12	1.85	0.42
1:A:152:TYR:CD1	1:A:154:PRO:HD3	2.54	0.42
2:C:51:ALA:C	2:C:53:PHE:H	2.22	0.42
2:C:68:LEU:HA	2:C:68:LEU:HD12	1.90	0.42
2:C:890:LYS:NZ	2:C:890:LYS:HB3	2.33	0.42
3:D:201:LEU:HD12	3:D:205:LEU:HD11	2.02	0.42
3:D:114:ILE:CG2	3:D:308:ASP:HB3	2.50	0.42
3:D:355:ILE:HG12	3:D:464:ASP:O	2.19	0.42
3:D:58:CYS:SG	3:D:61:ILE:HG13	2.58	0.42
3:D:909:ILE:HG13	3:D:909:ILE:H	1.56	0.42
2:H:699:LEU:HD13	2:H:1181:PRO:HB3	2.01	0.42
2:H:1225:VAL:HG12	3:I:636:GLY:O	2.19	0.42
2:H:96:LEU:HB2	2:H:127:ILE:CD1	2.49	0.42
2:H:302:ILE:HA	2:H:309:LEU:HA	2.01	0.42
2:H:59:ILE:HG12	2:H:65:ASN:O	2.20	0.42
2:H:81:ASP:OD1	2:H:83:GLN:HG2	2.19	0.42
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	2.02	0.42
3:I:1282:TYR:HA	3:I:1285:VAL:CG2	2.49	0.42
3:I:403:ARG:O	3:I:405:GLU:N	2.53	0.42
3:I:58:CYS:SG	3:I:61:ILE:HG13	2.60	0.42
3:I:678:ARG:O	3:I:682:VAL:HG13	2.20	0.42
5:Y:469:GLN:O	5:Y:473:GLU:HB2	2.19	0.42
1:A:311:GLY:O	5:X:599:ARG:NE	2.52	0.42
2:C:1029:LEU:O	2:C:1032:LYS:HG3	2.18	0.42
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.55	0.42
2:C:184:LEU:HD13	2:C:389:PHE:CZ	2.54	0.42
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.30	0.42
3:D:252:LEU:HG	3:D:252:LEU:O	2.20	0.42
3:D:425:ARG:CZ	3:D:459:ALA:HA	2.49	0.42
2:H:94:ALA:O	2:H:126:GLU:HG2	2.19	0.42
2:H:27:LEU:O	2:H:528:ARG:NH1	2.49	0.42
2:H:896:THR:O	2:H:899:GLU:N	2.48	0.42
3:I:313:GLY:O	3:I:314:ARG:HB2	2.20	0.42
3:I:370:LYS:HG3	3:I:371:LYS:H	1.84	0.42
2:H:1285:TYR:CG	3:I:475:GLU:HG3	2.54	0.42
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	2.02	0.42
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	2.00	0.42
5:Y:532:LEU:O	5:Y:536:THR:HG23	2.19	0.42
1:B:153:VAL:O	1:B:175:ALA:N	2.52	0.42
2:C:342:ASP:O	2:C:437:ASN:ND2	2.52	0.42
2:C:68:LEU:HD22	2:C:475:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:487:LEU:H	2:C:487:LEU:HD12	1.84	0.42
2:C:748:ILE:HD12	2:C:748:ILE:C	2.39	0.42
3:D:159:ILE:N	3:D:159:ILE:HD12	2.34	0.42
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.19	0.42
3:D:558:ASP:OD1	3:D:559:ALA:N	2.52	0.42
3:D:77:ARG:CG	3:D:78:LEU:H	2.31	0.42
2:H:1166:ASP:C	2:H:1168:GLU:H	2.23	0.42
2:H:1314:GLN:HG3	4:J:28:ARG:HH12	1.83	0.42
2:H:22:LEU:HD13	2:H:23:ASP:O	2.19	0.42
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.52	0.42
3:I:1324:SER:CB	3:I:1348:LYS:HD3	2.48	0.42
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.54	0.42
3:I:607:THR:O	3:I:611:ILE:HG12	2.19	0.42
3:I:796:LEU:O	3:I:800:LEU:HD23	2.19	0.42
5:X:139:GLU:HA	5:X:142:THR:CG2	2.48	0.42
5:Y:278:ASP:O	5:Y:282:THR:OG1	2.24	0.42
2:C:104:ILE:HD11	2:C:115:LYS:HB2	2.02	0.42
2:C:1270:PHE:CE1	2:C:1290:MET:HG2	2.55	0.42
2:C:836:LEU:HB3	2:C:918:LEU:HD21	2.02	0.42
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.55	0.42
3:D:490:ILE:HG23	3:D:500:ILE:HD11	2.01	0.42
1:G:191:ARG:HH12	3:I:443:GLU:HG2	1.84	0.42
2:H:17:LYS:HD2	2:H:17:LYS:N	2.35	0.42
2:H:431:LYS:O	2:H:435:ILE:HG13	2.19	0.42
2:H:553:THR:O	2:H:557:ARG:HD3	2.19	0.42
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.50	0.42
3:I:1297:LYS:NZ	3:I:1297:LYS:CA	2.82	0.42
3:I:147:ILE:HG13	3:I:149:GLY:H	1.84	0.42
3:I:270:ARG:HE	5:Y:449:THR:HG22	1.85	0.42
2:H:1268:GLN:O	3:I:346:ARG:HA	2.20	0.42
3:I:397:ALA:O	3:I:401:VAL:HG13	2.20	0.42
3:I:534:GLU:O	3:I:538:ARG:HB2	2.20	0.42
3:I:66:LYS:HB3	3:I:66:LYS:NZ	2.34	0.42
3:I:491:LEU:HB2	3:I:904:ALA:HA	2.01	0.42
3:I:474:LEU:HB3	4:J:28:ARG:HH21	1.85	0.42
5:X:439:ILE:O	5:X:443:ILE:HG13	2.19	0.42
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.67	0.42
2:C:348:SER:O	2:C:352:ARG:HG3	2.20	0.42
2:C:632:ASP:O	2:C:633:LEU:HD23	2.20	0.42
2:C:99:LYS:HZ3	2:C:99:LYS:HB3	1.83	0.42
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:382:TYR:CE1	3:D:401:VAL:HG21	2.55	0.42
3:D:50:LYS:HG2	3:D:51:PRO:CD	2.48	0.42
3:D:619:ILE:O	3:D:623:GLN:HG2	2.19	0.42
2:H:1073:LYS:HD3	3:I:462:ASP:CB	2.21	0.42
2:H:1146:GLN:CD	2:H:1160:ASP:HB2	2.40	0.42
2:H:560:PRO:HA	3:I:780:ARG:NH2	2.34	0.42
2:H:766:ASN:H	2:H:787:PRO:HG3	1.85	0.42
3:I:105:ILE:HG13	3:I:244:VAL:CG2	2.50	0.42
5:X:316:PHE:CZ	5:X:334:SER:HA	2.55	0.42
5:Y:119:ILE:CD1	5:Y:122:ARG:HH21	2.33	0.42
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.20	0.42
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.20	0.42
2:C:768:MET:O	2:C:785:ASP:N	2.48	0.42
3:D:154:LEU:HD22	3:D:176:PHE:HE1	1.83	0.42
3:D:466:MET:HE2	3:D:466:MET:HB3	1.88	0.42
2:C:1315:MET:HE2	3:D:473:THR:OG1	2.20	0.42
3:D:583:VAL:HG13	3:D:584:PRO:HD2	2.01	0.42
3:D:843:VAL:HG21	3:D:897:HIS:HA	2.02	0.42
1:G:52:PRO:HG3	1:G:150:ARG:HH12	1.84	0.42
2:H:80:PHE:O	2:H:84:GLU:HB3	2.19	0.42
3:I:1148:ARG:HB2	3:I:1148:ARG:NH2	2.35	0.42
3:I:1343:GLU:HA	3:I:1344:LEU:CB	2.35	0.42
3:I:269:TYR:HA	3:I:272:VAL:HG12	2.02	0.42
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.19	0.42
5:X:24:TYR:O	5:X:26:GLU:N	2.52	0.42
5:X:373:ARG:HG3	5:X:377:LYS:HE3	2.00	0.42
5:X:448:ARG:HD3	5:X:450:ILE:HG13	2.01	0.42
5:X:608:ARG:HB3	5:X:608:ARG:NH1	2.35	0.42
5:Y:262:VAL:HG12	5:Y:264:LYS:H	1.84	0.42
1:A:45:ARG:HG2	2:C:1083:GLU:OE1	2.20	0.42
2:C:80:PHE:HB3	2:C:85:CYS:SG	2.59	0.42
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.54	0.42
3:D:574:VAL:O	3:D:578:ILE:HG22	2.20	0.42
3:D:901:ARG:CB	3:D:908:ILE:HA	2.50	0.42
1:F:234:LEU:HD12	1:F:234:LEU:N	2.35	0.42
1:G:227:GLN:C	1:G:229:GLU:H	2.23	0.42
2:H:1161:LEU:HD21	2:H:1172:LEU:HD11	2.02	0.42
2:H:1252:SER:HB3	2:H:1259:LEU:CD2	2.50	0.42
2:H:92:TYR:CD1	2:H:129:LEU:HB2	2.55	0.42
2:H:549:ASP:OD1	2:H:550:VAL:N	2.53	0.42
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:262:VAL:HG12	5:X:264:LYS:H	1.85	0.42
5:X:477:GLU:H	5:X:477:GLU:CD	2.23	0.42
5:X:52:GLY:O	5:X:53:ILE:HB	2.20	0.42
1:B:22:THR:HB	1:B:207:THR:O	2.19	0.41
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.79	0.41
2:C:56:VAL:HB	2:C:57:PHE:H	1.51	0.41
2:C:988:LYS:NZ	2:C:988:LYS:HB3	2.34	0.41
2:C:72:SER:O	2:C:98:VAL:HG23	2.20	0.41
3:D:1180:VAL:HG22	3:D:1185:PRO:HA	2.02	0.41
3:D:141:PHE:HD2	3:D:141:PHE:HA	1.71	0.41
3:D:18:ASP:HA	3:D:1369:ARG:HH22	1.84	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.85	0.41
2:H:1158:LYS:HD2	2:H:1158:LYS:O	2.20	0.41
2:H:122:VAL:HG22	2:H:123:TYR:N	2.34	0.41
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.19	0.41
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.87	0.41
2:H:303:ASP:HB2	2:H:310:ILE:CD1	2.46	0.41
2:H:469:VAL:O	2:H:472:GLU:HB3	2.20	0.41
2:H:481:LEU:C	2:H:481:LEU:HD13	2.40	0.41
2:H:54:ARG:N	2:H:55:SER:C	2.74	0.41
2:H:699:LEU:HD12	2:H:1121:ALA:HB1	2.01	0.41
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	2.02	0.41
3:I:131:PRO:CG	3:I:135:ILE:HD13	2.46	0.41
3:I:326:SER:O	3:I:330:MET:HG3	2.19	0.41
3:I:33:TRP:HB3	3:I:102:MET:HG3	2.02	0.41
3:I:532:GLU:OE1	3:I:578:ILE:HB	2.20	0.41
3:I:746:LEU:HD22	3:I:746:LEU:H	1.85	0.41
5:Y:363:ARG:HE	5:Y:363:ARG:HA	1.84	0.41
1:B:228:LEU:HD12	1:B:228:LEU:C	2.41	0.41
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.85	0.41
3:D:591:ILE:HD12	3:D:592:VAL:HG13	2.02	0.41
1:F:167:PRO:HD2	1:F:170:ARG:NE	2.35	0.41
2:H:103:VAL:HG22	2:H:104:ILE:N	2.34	0.41
2:H:1323:PHE:O	2:H:1327:LEU:HG	2.20	0.41
2:H:170:VAL:HG23	2:H:171:LEU:N	2.31	0.41
2:H:985:GLU:HG2	2:H:989:LEU:HD13	2.01	0.41
2:H:992:LEU:HD23	2:H:996:ARG:CG	2.50	0.41
3:I:1292:LEU:HD12	3:I:1292:LEU:N	2.36	0.41
2:H:1335:ILE:CD1	3:I:22:ILE:HD11	2.49	0.41
3:I:290:ILE:O	3:I:293:ARG:HG3	2.20	0.41
3:I:298:MET:CE	5:Y:402:LEU:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:382:TYR:HE1	3:I:401:VAL:CG2	2.33	0.41
3:I:500:ILE:H	3:I:500:ILE:CD1	2.33	0.41
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.35	0.41
3:I:73:GLY:O	3:I:76:LYS:HE3	2.19	0.41
3:I:843:VAL:HG11	3:I:897:HIS:HB3	2.02	0.41
5:Y:133:SER:OG	5:Y:365:MET:HB2	2.20	0.41
1:B:207:THR:OG1	1:B:208:ASN:N	2.54	0.41
1:B:31:LEU:HB2	1:B:199:ASP:O	2.19	0.41
2:C:1142:ARG:O	2:C:1146:GLN:HB2	2.20	0.41
2:C:1283:ALA:HB1	2:C:1286:THR:HB	2.02	0.41
2:C:1333:LEU:HB2	2:C:1335:ILE:HG22	2.03	0.41
2:C:135:THR:OG1	2:C:142:GLU:HG3	2.20	0.41
2:C:230:PHE:HB2	2:C:333:ILE:HB	2.01	0.41
2:C:82:VAL:HG13	2:C:83:GLN:N	2.36	0.41
2:C:81:ASP:OD1	2:C:83:GLN:HG2	2.21	0.41
2:C:943:LYS:O	2:C:947:GLU:HG2	2.20	0.41
3:D:1284:ARG:HA	3:D:1287:ILE:CG1	2.47	0.41
2:H:263:VAL:HA	2:H:267:ARG:HH21	1.86	0.41
2:H:513:GLN:NE2	2:H:513:GLN:HA	2.24	0.41
2:H:896:THR:HG23	2:H:897:PRO:HD2	2.02	0.41
2:H:964:LEU:HD12	2:H:1025:PHE:CG	2.55	0.41
3:I:120:LEU:HD12	3:I:120:LEU:N	2.35	0.41
3:I:141:PHE:O	3:I:297:ARG:HD3	2.21	0.41
5:Y:316:PHE:CZ	5:Y:334:SER:HA	2.55	0.41
1:A:22:THR:O	1:A:207:THR:N	2.50	0.41
1:A:45:ARG:NH1	2:C:1084:ASP:HB3	2.36	0.41
2:C:170:VAL:HG23	2:C:171:LEU:N	2.28	0.41
2:C:27:LEU:O	2:C:528:ARG:NH1	2.52	0.41
2:C:697:LYS:HE2	2:C:697:LYS:HB2	1.89	0.41
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.21	0.41
3:D:369:PRO:HB2	3:D:372:MET:HB2	2.01	0.41
2:C:812:PHE:CE1	3:D:451:PRO:HB2	2.55	0.41
1:B:86:LYS:NZ	3:D:526:VAL:O	2.48	0.41
3:D:805:GLN:HB2	3:D:805:GLN:HE21	1.72	0.41
1:F:222:THR:O	1:F:226:GLU:HG3	2.20	0.41
2:H:1199:LEU:HD13	2:H:1206:THR:HA	2.02	0.41
2:H:1239:VAL:HG12	2:H:1240:ASP:N	2.34	0.41
2:H:142:GLU:O	2:H:143:ARG:HB2	2.21	0.41
2:H:619:ALA:HA	2:H:653:MET:CE	2.51	0.41
2:H:518:ASN:ND2	2:H:761:GLN:HG2	2.35	0.41
2:H:843:THR:HB	2:H:845:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:219:LYS:O	3:I:223:LEU:HG	2.20	0.41
1:A:166:ARG:HG3	1:A:166:ARG:O	2.21	0.41
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.85	0.41
1:B:47:LEU:HD13	1:B:205:MET:HE2	2.03	0.41
2:C:317:LEU:HD13	2:C:322:LEU:HD21	2.01	0.41
2:C:546:GLU:O	2:C:548:ARG:N	2.48	0.41
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.55	0.41
3:D:1149:ARG:HA	3:D:1150:PRO:HD3	1.90	0.41
3:D:363:LEU:HA	3:D:450:HIS:ND1	2.36	0.41
3:D:678:ARG:HD2	3:D:678:ARG:C	2.41	0.41
1:F:190:ALA:N	1:F:198:LEU:O	2.48	0.41
1:F:46:ILE:O	1:F:50:SER:HB2	2.20	0.41
3:I:1193:TRP:CD1	3:I:1194:ARG:HD2	2.55	0.41
3:I:135:ILE:O	3:I:139:LEU:HD12	2.20	0.41
3:I:217:LEU:O	3:I:221:ILE:HG23	2.21	0.41
3:I:279:LEU:HD23	3:I:295:GLU:HB3	2.02	0.41
3:I:303:VAL:O	3:I:307:LEU:HG	2.20	0.41
3:I:479:GLU:O	3:I:483:LEU:HB2	2.21	0.41
5:X:133:SER:OG	5:X:365:MET:HB2	2.21	0.41
5:Y:528:LEU:O	5:Y:528:LEU:HD12	2.20	0.41
2:C:1087:TYR:CE2	2:C:1215:GLY:HA2	2.50	0.41
1:A:45:ARG:HH12	2:C:1216:ARG:HA	1.86	0.41
2:C:397:LEU:O	2:C:398:SER:OG	2.33	0.41
3:D:128:LEU:HA	3:D:192:MET:CE	2.49	0.41
3:D:214:ARG:HA	3:D:217:LEU:HD12	2.02	0.41
3:D:269:TYR:CG	3:D:306:LEU:HD11	2.54	0.41
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.56	0.41
3:D:649:LYS:O	3:D:653:ILE:HG12	2.21	0.41
4:E:16:ARG:O	4:E:19:LEU:HB3	2.20	0.41
2:H:1165:SER:O	2:H:1168:GLU:HB3	2.21	0.41
3:I:1229:VAL:O	3:I:1233:ILE:HG13	2.20	0.41
3:I:130:MET:HA	3:I:131:PRO:HD3	1.96	0.41
5:X:45:ILE:HD12	5:X:45:ILE:C	2.40	0.41
5:Y:343:LYS:O	5:Y:346:GLN:HB3	2.19	0.41
5:Y:582:VAL:CB	5:Y:586:ARG:HG2	2.50	0.41
3:I:392:THR:HG22	5:Y:606:VAL:HG11	2.01	0.41
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.98	0.41
2:C:99:LYS:HA	2:C:121:GLU:HA	2.02	0.41
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.84	0.41
2:C:869:GLY:C	2:C:870:ILE:HD12	2.41	0.41
2:C:901:LEU:HD13	5:X:559:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:382:TYR:CE1	3:D:398:LYS:HA	2.55	0.41
3:D:45:ASN:OD1	3:D:46:TYR:N	2.54	0.41
3:D:532:GLU:OE1	3:D:578:ILE:HB	2.21	0.41
3:D:555:TYR:HD1	3:D:589:TYR:HE2	1.69	0.41
1:F:89:ALA:HB3	1:F:124:VAL:HB	2.03	0.41
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	2.03	0.41
2:H:680:LEU:O	2:H:680:LEU:HD23	2.21	0.41
2:H:843:THR:HB	2:H:845:LEU:CD2	2.51	0.41
3:I:1322:ALA:O	3:I:1326:GLN:HG3	2.21	0.41
3:I:382:TYR:CE1	3:I:398:LYS:HA	2.56	0.41
3:I:473:THR:HB	3:I:476:ALA:CB	2.49	0.41
3:I:494:ALA:HA	3:I:1252:HIS:CE1	2.53	0.41
5:X:363:ARG:HE	5:X:363:ARG:HA	1.85	0.41
5:Y:453:PRO:CD	5:Y:456:MET:HB2	2.42	0.41
5:Y:476:ARG:HB2	5:Y:477:GLU:OE1	2.20	0.41
2:C:820:GLU:HB2	2:C:1081:PRO:HA	2.02	0.41
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	2.03	0.41
2:C:177:ILE:HG13	2:C:183:TRP:CZ3	2.56	0.41
2:C:429:MET:O	2:C:433:ILE:HG13	2.20	0.41
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.20	0.41
2:C:975:ILE:O	2:C:978:VAL:HG12	2.21	0.41
3:D:1149:ARG:H	3:D:1149:ARG:CD	2.23	0.41
3:D:27:PRO:HD3	3:D:236:TRP:CE3	2.56	0.41
3:D:53:ARG:HA	3:D:53:ARG:HD2	1.96	0.41
3:D:609:TYR:HA	3:D:617:THR:OG1	2.21	0.41
3:D:746:LEU:H	3:D:746:LEU:HD22	1.85	0.41
1:G:76:GLU:OE2	1:G:131:CYS:HA	2.20	0.41
2:H:103:VAL:HG22	2:H:104:ILE:H	1.86	0.41
2:H:1285:TYR:HA	2:H:1288:GLN:HB3	2.02	0.41
2:H:811:ASN:HA	2:H:815:SER:HB2	2.03	0.41
2:H:977:ALA:O	2:H:980:VAL:HG12	2.20	0.41
3:I:422:LEU:O	3:I:422:LEU:HD12	2.20	0.41
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.20	0.41
3:I:873:GLU:H	3:I:873:GLU:HG3	1.64	0.41
5:X:261:LEU:HD12	5:X:261:LEU:N	2.36	0.41
5:X:270:VAL:HA	5:X:273:MET:HE3	2.01	0.41
5:X:35:ILE:HG13	5:X:36:VAL:N	2.21	0.41
5:Y:112:THR:HG22	5:Y:113:ARG:N	2.30	0.41
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	2.01	0.41
5:Y:261:LEU:N	5:Y:261:LEU:HD12	2.36	0.41
5:Y:105:MET:SD	5:Y:388:ILE:HD12	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HG3	2:C:694:ARG:NH1	2.35	0.41
2:C:103:VAL:HG22	2:C:104:ILE:N	2.36	0.41
2:C:688:GLN:O	2:C:1236:ASN:N	2.54	0.41
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.03	0.41
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.56	0.41
2:C:752:ASN:C	2:C:753:LEU:HG	2.40	0.41
2:C:82:VAL:O	2:C:86:GLN:HG3	2.20	0.41
3:D:1161:GLY:HA2	3:D:1181:ASP:HB2	2.01	0.41
3:D:128:LEU:HD12	3:D:192:MET:CE	2.35	0.41
2:H:374:GLU:HA	2:H:375:PRO:HD3	1.93	0.41
2:H:690:VAL:HA	2:H:691:PRO:HD3	1.91	0.41
3:I:1173:ARG:CA	3:I:1174:ARG:CB	2.86	0.41
3:I:155:GLU:H	3:I:155:GLU:CD	2.24	0.41
3:I:552:ILE:HD13	3:I:570:LYS:HB2	2.03	0.41
2:C:122:VAL:CG2	5:X:472:GLN:HE21	2.34	0.41
5:Y:456:MET:O	5:Y:460:ILE:HG13	2.20	0.41
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.55	0.41
2:C:442:VAL:HG12	2:C:443:ASP:N	2.36	0.41
2:C:773:LEU:C	2:C:773:LEU:HD22	2.41	0.41
3:D:155:GLU:CD	3:D:158:GLN:HB2	2.41	0.41
3:D:647:PRO:HG3	3:D:697:MET:HA	2.03	0.41
2:H:1138:VAL:O	2:H:1139:ALA:HB3	2.20	0.41
2:H:127:ILE:HA	2:H:128:PRO:HD3	1.89	0.41
2:H:1287:LEU:O	2:H:1291:LEU:HB2	2.21	0.41
2:H:618:GLN:HG2	2:H:637:ARG:NH2	2.36	0.41
3:I:116:PHE:HB3	3:I:237:MET:HE3	2.03	0.41
3:I:526:VAL:HG12	3:I:549:LYS:O	2.20	0.41
3:I:746:LEU:HD22	3:I:746:LEU:N	2.36	0.41
5:X:262:VAL:HG13	5:X:263:PRO:CD	2.48	0.41
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.20	0.41
5:Y:374:ARG:O	5:Y:378:GLU:HG3	2.21	0.41
1:B:176:CYS:C	1:B:178:SER:N	2.74	0.41
2:C:1272:GLU:O	2:C:1275:VAL:HG22	2.21	0.41
2:C:1287:LEU:O	2:C:1291:LEU:HB2	2.21	0.41
2:C:516:ASP:OD1	2:C:518:ASN:ND2	2.54	0.41
2:C:661:VAL:HG23	2:C:662:SER:O	2.22	0.41
2:C:84:GLU:HG3	2:C:88:ARG:HD3	2.03	0.41
2:C:892:GLU:C	2:C:894:GLN:H	2.24	0.41
2:C:931:VAL:HG21	2:C:944:ARG:CZ	2.52	0.41
3:D:1292:LEU:HD12	3:D:1292:LEU:N	2.35	0.41
3:D:1266:ILE:HG22	3:D:1302:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:361:LEU:HD22	3:D:361:LEU:N	2.36	0.41
3:D:409:TRP:O	3:D:412:LEU:HB3	2.21	0.41
2:C:1243:MET:SD	3:D:445:LYS:HB3	2.61	0.41
3:D:681:LYS:HD3	3:D:682:VAL:N	2.36	0.41
4:E:15:ASN:HD21	4:E:18:ASP:CB	2.32	0.41
1:G:110:VAL:HG11	1:G:140:ILE:HD11	2.02	0.41
2:H:1142:ARG:O	2:H:1146:GLN:HB2	2.20	0.41
2:H:698:PRO:HB3	2:H:1231:TYR:CE1	2.56	0.41
2:H:31:GLN:HG3	2:H:130:MET:HE1	2.03	0.41
2:H:691:PRO:HA	2:H:788:SER:OG	2.21	0.41
2:H:812:PHE:H	2:H:815:SER:HB2	1.86	0.41
2:H:97:ARG:HA	2:H:122:VAL:O	2.20	0.41
3:I:128:LEU:HD12	3:I:192:MET:HE1	2.02	0.41
3:I:527:LEU:HB3	3:I:528:THR:H	1.72	0.41
3:I:856:ILE:HD12	3:I:857:LEU:H	1.86	0.41
3:I:903:LEU:HD11	3:I:909:ILE:CG2	2.45	0.41
4:J:39:VAL:CG1	4:J:40:PRO:HD2	2.50	0.41
5:Y:492:ASP:HA	5:Y:495:ARG:HG3	2.01	0.41
1:B:16:ILE:HG12	1:B:26:VAL:HG22	2.02	0.40
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.86	0.40
2:C:1165:SER:O	2:C:1168:GLU:HB3	2.21	0.40
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.56	0.40
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.02	0.40
2:C:73:TYR:HA	2:C:98:VAL:HA	2.02	0.40
2:C:854:ILE:HB	2:C:857:VAL:HG11	2.03	0.40
3:D:1274:PHE:CD2	3:D:1275:LEU:HG	2.50	0.40
3:D:217:LEU:O	3:D:221:ILE:HG23	2.20	0.40
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.21	0.40
1:F:59:VAL:HG21	1:F:85:LEU:HD13	2.03	0.40
2:H:130:MET:HG3	2:H:134:GLY:HA2	2.03	0.40
2:H:740:GLU:CD	2:H:740:GLU:H	2.24	0.40
2:H:892:GLU:C	2:H:894:GLN:H	2.24	0.40
3:I:545:HIS:HB2	3:I:546:ALA:CA	2.51	0.40
5:Y:448:ARG:HD3	5:Y:450:ILE:HG13	2.02	0.40
5:Y:591:GLU:O	5:Y:595:LEU:HG	2.21	0.40
1:A:102:LEU:HD12	1:A:115:ILE:HG12	2.03	0.40
1:A:323:PRO:HA	1:A:324:ALA:HA	1.77	0.40
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.31	0.40
1:A:67:GLU:HA	1:A:78:ILE:HG21	2.03	0.40
2:C:1163:THR:HG22	2:C:1164:PHE:H	1.86	0.40
2:C:1269:ARG:HD2	3:D:344:GLY:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:538:LEU:HD12	2:C:538:LEU:H	1.86	0.40
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.40
2:C:618:GLN:HG2	2:C:637:ARG:HH22	1.86	0.40
2:C:848:GLU:HG2	2:C:888:THR:HA	2.02	0.40
3:D:1282:TYR:HA	3:D:1285:VAL:CG2	2.52	0.40
3:D:707:ILE:HG22	3:D:708:ASN:H	1.86	0.40
3:D:697:MET:SD	3:D:741:ALA:HB3	2.62	0.40
3:D:836:ARG:HA	3:D:836:ARG:HD2	1.88	0.40
3:D:857:LEU:HB2	3:D:860:ARG:HB2	2.03	0.40
2:H:219:GLN:O	2:H:223:LEU:HG	2.21	0.40
2:H:817:LEU:HB3	2:H:1097:VAL:HG13	2.03	0.40
2:H:821:ARG:HB2	2:H:1082:ILE:HD13	2.04	0.40
2:H:844:LYS:HB2	2:H:844:LYS:HZ3	1.86	0.40
2:H:870:ILE:HD12	2:H:870:ILE:N	2.36	0.40
3:I:385:LEU:HD23	3:I:411:ILE:HG13	2.03	0.40
3:I:519:ASN:HD21	3:I:707:ILE:CG2	2.33	0.40
5:X:253:SER:O	5:X:257:LYS:HG3	2.21	0.40
5:X:551:LEU:HD22	5:X:597:LYS:HD2	2.02	0.40
5:Y:558:VAL:O	5:Y:562:ARG:HB2	2.21	0.40
1:A:313:SER:OG	1:A:314:LEU:N	2.53	0.40
2:C:1004:ASP:N	2:C:1004:ASP:OD1	2.55	0.40
2:C:106:GLU:HB3	2:C:107:ARG:CA	2.51	0.40
2:C:1259:LEU:HD12	2:C:1259:LEU:C	2.40	0.40
2:C:18:ARG:HG3	2:C:19:PRO:HD2	2.03	0.40
2:C:517:GLN:HG3	2:C:759:SER:OG	2.21	0.40
3:D:1158:GLU:HA	3:D:1223:LEU:CD2	2.50	0.40
3:D:1256:ILE:O	3:D:1260:MET:HB2	2.22	0.40
3:D:1341:ARG:HD3	3:D:1343:GLU:CD	2.42	0.40
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.49	0.40
2:H:1087:TYR:CE2	2:H:1215:GLY:HA2	2.55	0.40
2:H:1214:ASP:HB3	2:H:1218:GLY:H	1.86	0.40
3:I:1243:LEU:O	3:I:1243:LEU:HD23	2.22	0.40
3:I:510:LEU:HD12	3:I:601:ILE:HD11	2.03	0.40
3:I:545:HIS:HA	3:I:546:ALA:HA	1.80	0.40
5:X:283:GLN:CD	5:X:343:LYS:HD2	2.41	0.40
3:D:395:LYS:NZ	5:X:607:LEU:O	2.50	0.40
5:Y:292:VAL:HG13	5:Y:297:MET:O	2.21	0.40
1:B:27:THR:HG22	1:B:202:VAL:HG22	2.03	0.40
1:B:61:ILE:HB	1:B:64:VAL:HB	2.03	0.40
2:C:115:LYS:O	2:C:116:ASP:HB2	2.21	0.40
2:C:409:LEU:HD11	2:C:428:VAL:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:505:PHE:HA	2:C:509:SER:HB3	2.04	0.40
3:D:147:ILE:HD12	3:D:178:ALA:HB2	2.03	0.40
3:D:205:LEU:HB3	3:D:217:LEU:HD22	2.04	0.40
3:D:588:PRO:O	3:D:589:TYR:HB2	2.21	0.40
3:D:679:TYR:O	3:D:683:ILE:HG13	2.21	0.40
3:D:746:LEU:N	3:D:746:LEU:HD22	2.36	0.40
3:D:483:LEU:HD11	4:E:20:VAL:HG21	2.03	0.40
2:H:1212:LEU:HD12	2:H:1225:VAL:HG21	2.03	0.40
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.85	0.40
2:H:623:LEU:HD12	2:H:623:LEU:N	2.36	0.40
3:I:310:GLY:HA2	3:I:314:ARG:HG2	2.04	0.40
3:I:325:LYS:NZ	3:I:325:LYS:HB3	2.36	0.40
3:I:529:GLY:HA3	3:I:530:PRO:HD3	1.91	0.40
3:I:591:ILE:CD1	3:I:592:VAL:HG13	2.52	0.40
5:X:410:ILE:O	5:X:414:LYS:HG3	2.22	0.40
5:X:469:GLN:HE21	5:X:473:GLU:HG3	1.87	0.40
5:X:559:LEU:HD23	5:X:559:LEU:HA	1.90	0.40
1:A:50:SER:HA	1:A:150:ARG:HD2	2.02	0.40
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.56	0.40
2:C:1195:ILE:O	2:C:1199:LEU:HG	2.22	0.40
2:C:178:PRO:HA	2:C:397:LEU:CD2	2.46	0.40
2:C:465:ARG:O	2:C:469:VAL:HG23	2.21	0.40
2:C:59:ILE:HG12	2:C:65:ASN:O	2.20	0.40
2:C:936:ARG:HB3	2:C:939:VAL:HG21	2.04	0.40
3:D:1138:LEU:N	3:D:1139:PRO:CD	2.84	0.40
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.86	0.40
3:D:412:LEU:HA	3:D:415:VAL:HG22	2.04	0.40
3:D:355:ILE:HG21	3:D:466:MET:SD	2.61	0.40
3:D:678:ARG:O	3:D:682:VAL:HG13	2.21	0.40
3:D:709:ARG:O	3:D:712:GLN:N	2.53	0.40
3:D:84:ILE:HG13	3:D:84:ILE:H	1.76	0.40
2:H:1108:ASN:O	2:H:1108:ASN:ND2	2.52	0.40
2:H:1329:GLU:O	2:H:1332:SER:HB3	2.21	0.40
3:I:1278:GLU:HG3	3:I:1279:GLN:N	2.37	0.40
3:I:609:TYR:HE2	3:I:614:LEU:HD13	1.86	0.40
2:H:894:GLN:NE2	3:I:77:ARG:HD3	2.32	0.40
3:I:887:SER:O	3:I:888:CYS:HB3	2.21	0.40
3:I:915:ILE:O	3:I:918:ILE:HG23	2.22	0.40
3:I:417:ARG:NH1	4:J:43:ASN:O	2.55	0.40
5:X:374:ARG:HH21	5:X:377:LYS:HD2	1.87	0.40
5:X:400:GLN:HE21	5:X:403:ASP:CG	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:530:LEU:H	5:X:530:LEU:HD12	1.86	0.40
5:X:558:VAL:O	5:X:562:ARG:HB2	2.22	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	321/329 (98%)	266 (83%)	40 (12%)	15 (5%)	2	24
1	B	217/329 (66%)	187 (86%)	22 (10%)	8 (4%)	3	28
1	F	227/329 (69%)	193 (85%)	28 (12%)	6 (3%)	5	35
1	G	213/329 (65%)	186 (87%)	22 (10%)	5 (2%)	6	37
2	C	1333/1342 (99%)	1073 (80%)	208 (16%)	52 (4%)	3	27
2	H	1333/1342 (99%)	1078 (81%)	206 (16%)	49 (4%)	3	28
3	D	1154/1407 (82%)	926 (80%)	182 (16%)	46 (4%)	3	26
3	I	1154/1407 (82%)	925 (80%)	184 (16%)	45 (4%)	3	27
4	E	88/91 (97%)	77 (88%)	6 (7%)	5 (6%)	1	21
4	J	74/91 (81%)	64 (86%)	6 (8%)	4 (5%)	2	22
5	X	511/613 (83%)	450 (88%)	46 (9%)	15 (3%)	4	33
5	Y	454/613 (74%)	409 (90%)	34 (8%)	11 (2%)	6	36
All	All	7079/8222 (86%)	5834 (82%)	984 (14%)	261 (4%)	3	28

All (261) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	B	20	SER

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Mol	Chain	Res	Type
1	B	52	PRO
2	C	21	VAL
2	C	39	ILE
2	C	43	PRO
2	C	110	PRO
2	C	114	VAL
2	C	170	VAL
2	C	661	VAL
2	C	669	PRO
2	C	686	GLN
2	C	748	ILE
2	C	993	PRO
2	C	1185	PRO
2	C	1186	VAL
2	C	1341	ASP
3	D	120	LEU
3	D	311	ARG
3	D	390	LEU
3	D	404	GLU
3	D	406	ALA
3	D	708	ASN
3	D	710	ASP
3	D	847	ASP
3	D	1268	ASN
3	D	1339	GLY
3	D	1344	LEU
5	X	241	SER
5	X	490	PRO
1	F	52	PRO
1	G	52	PRO
1	G	177	TYR
2	H	21	VAL
2	H	39	ILE
2	H	79	VAL
2	H	110	PRO
2	H	114	VAL
2	H	661	VAL
2	H	669	PRO
2	H	748	ILE
2	H	993	PRO
2	H	1185	PRO
2	H	1341	ASP

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Mol	Chain	Res	Type
3	I	120	LEU
3	I	390	LEU
3	I	404	GLU
3	I	710	ASP
3	I	847	ASP
3	I	1339	GLY
5	Y	241	SER
1	A	52	PRO
1	A	160	HIS
1	A	187	VAL
1	A	193	GLU
1	B	19	VAL
1	B	177	TYR
2	C	56	VAL
2	C	78	PRO
2	C	79	VAL
2	C	753	LEU
2	C	1236	ASN
2	C	1239	VAL
2	C	1240	ASP
3	D	89	GLY
3	D	155	GLU
3	D	316	ILE
3	D	542	ALA
3	D	595	ALA
3	D	721	SER
3	D	887	SER
3	D	901	ARG
3	D	913	GLU
3	D	914	ALA
4	E	6	VAL
4	E	35	LYS
5	X	20	GLY
2	H	56	VAL
2	H	78	PRO
2	H	170	VAL
2	H	298	ALA
2	H	535	PRO
2	H	753	LEU
2	H	1186	VAL
2	H	1239	VAL
2	H	1240	ASP

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Mol	Chain	Res	Type
2	H	1256	GLN
3	I	89	GLY
3	I	155	GLU
3	I	345	LYS
3	I	406	ALA
3	I	540	GLY
3	I	542	ALA
3	I	707	ILE
3	I	708	ASN
3	I	731	ARG
3	I	851	PRO
3	I	901	ARG
3	I	913	GLU
3	I	914	ALA
3	I	1268	ASN
3	I	1344	LEU
4	J	6	VAL
4	J	35	LYS
5	Y	490	PRO
5	Y	564	GLY
1	A	14	VAL
1	B	235	ARG
2	C	44	GLU
2	C	53	PHE
2	C	143	ARG
2	C	437	ASN
2	C	699	LEU
2	C	740	GLU
2	C	812	PHE
2	C	1107	MET
2	C	1256	GLN
3	D	559	ALA
3	D	703	THR
3	D	707	ILE
3	D	731	ARG
3	D	848	VAL
3	D	851	PRO
3	D	902	ASP
5	X	23	THR
5	X	308	GLY
5	X	514	ASP
5	X	581	ASP

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Mol	Chain	Res	Type
1	F	160	HIS
1	F	188	GLU
1	G	188	GLU
1	G	228	LEU
2	H	13	LYS
2	H	44	GLU
2	H	53	PHE
2	H	437	ASN
2	H	740	GLU
2	H	812	PHE
2	H	1107	MET
2	H	1236	ASN
3	I	53	ARG
3	I	132	LEU
3	I	559	ALA
3	I	595	ALA
3	I	703	THR
3	I	721	SER
3	I	887	SER
3	I	1195	GLN
5	Y	108	VAL
5	Y	308	GLY
5	Y	491	GLU
5	Y	581	ASP
1	A	166	ARG
1	A	188	GLU
1	A	194	GLN
1	B	188	GLU
2	C	298	ALA
2	C	1080	ASN
2	C	1139	ALA
3	D	53	ARG
3	D	132	LEU
3	D	598	LYS
3	D	728	SER
3	D	855	ASP
3	D	888	CYS
3	D	1195	GLN
3	D	1363	TYR
4	E	5	THR
5	X	50	ASP
5	X	108	VAL

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Mol	Chain	Res	Type
5	X	504	PRO
1	F	153	VAL
1	F	166	ARG
2	H	43	PRO
2	H	143	ARG
2	H	699	LEU
2	H	739	ASP
2	H	895	LEU
2	H	1003	THR
2	H	1080	ASN
2	H	1093	PRO
2	H	1270	PHE
3	I	598	LYS
3	I	728	SER
3	I	848	VAL
3	I	855	ASP
3	I	888	CYS
5	Y	504	PRO
5	Y	514	ASP
1	A	93	GLN
1	A	163	GLU
1	A	195	ARG
2	C	13	LYS
2	C	487	LEU
2	C	543	ALA
2	C	746	ALA
2	C	895	LEU
2	C	1093	PRO
2	C	1237	HIS
2	C	1238	LEU
2	C	1270	PHE
3	D	62	PHE
3	D	210	SER
3	D	540	GLY
3	D	1167	LYS
5	X	25	ALA
5	X	491	GLU
5	X	564	GLY
5	X	600	HIS
1	F	33	ARG
2	H	488	MET
2	H	746	ALA

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Mol	Chain	Res	Type
2	H	1045	GLY
2	H	1237	HIS
3	I	62	PHE
3	I	210	SER
3	I	902	ASP
4	J	5	THR
5	Y	600	HIS
1	A	153	VAL
1	B	49	SER
1	B	228	LEU
2	C	59	ILE
2	C	69	GLN
2	C	739	ASP
2	C	1003	THR
2	C	1315	MET
3	D	417	ARG
3	D	742	GLY
3	D	1173	ARG
4	E	15	ASN
4	E	59	ILE
1	G	49	SER
2	H	1139	ALA
2	H	1238	LEU
3	I	108	ALA
3	I	443	GLU
3	I	712	GLN
3	I	742	GLY
3	I	1167	LYS
4	J	59	ILE
1	A	232	VAL
2	C	104	ILE
2	H	59	ILE
2	H	104	ILE
2	C	1045	GLY
3	I	850	LYS
1	A	322	PRO
2	C	373	GLY
3	D	850	LYS
2	H	373	GLY
5	X	35	ILE
3	I	316	ILE
5	Y	97	PRO

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Mol	Chain	Res	Type
2	C	117	ILE
3	D	471	PRO
3	D	1184	ASP
3	I	471	PRO
2	H	489	PRO
2	H	1181	PRO
2	C	1181	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	281/286 (98%)	273 (97%)	8 (3%)	43	65
1	B	189/286 (66%)	186 (98%)	3 (2%)	62	79
1	F	197/286 (69%)	194 (98%)	3 (2%)	65	80
1	G	185/286 (65%)	182 (98%)	3 (2%)	62	79
2	C	1150/1157 (99%)	1094 (95%)	56 (5%)	25	52
2	H	1150/1157 (99%)	1097 (95%)	53 (5%)	27	54
3	D	971/1168 (83%)	921 (95%)	50 (5%)	24	51
3	I	971/1168 (83%)	918 (94%)	53 (6%)	21	49
4	E	74/75 (99%)	72 (97%)	2 (3%)	44	66
4	J	65/75 (87%)	65 (100%)	0	100	100
5	X	460/540 (85%)	447 (97%)	13 (3%)	43	65
5	Y	407/540 (75%)	392 (96%)	15 (4%)	34	59
All	All	6100/7024 (87%)	5841 (96%)	259 (4%)	30	55

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	79	LEU
1	A	117	HIS

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Mol	Chain	Res	Type
1	A	158	ARG
1	A	243	LYS
1	A	246	LYS
1	A	262	LEU
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	182	ARG
2	C	9	LYS
2	C	15	PHE
2	C	18	ARG
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN
2	C	56	VAL
2	C	70	TYR
2	C	80	PHE
2	C	88	ARG
2	C	121	GLU
2	C	127	ILE
2	C	150	HIS
2	C	163	LYS
2	C	479	LEU
2	C	487	LEU
2	C	514	PHE
2	C	603	ILE
2	C	645	PHE
2	C	661	VAL
2	C	690	VAL
2	C	693	LEU
2	C	773	LEU
2	C	800	MET
2	C	807	TRP
2	C	817	LEU
2	C	845	LEU
2	C	908	GLU
2	C	941	LYS
2	C	944	ARG
2	C	953	LEU
2	C	955	GLN
2	C	964	LEU
2	C	975	ILE

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Mol	Chain	Res	Type
2	C	994	ARG
2	C	1002	LEU
2	C	1010	GLN
2	C	1017	GLN
2	C	1032	LYS
2	C	1042	LEU
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1209	GLN
2	C	1211	ARG
2	C	1233	LEU
2	C	1241	ASP
2	C	1259	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1288	GLN
2	C	1291	LEU
2	C	1326	LEU
2	C	1339	LEU
2	C	1341	ASP
3	D	13	LYS
3	D	20	ILE
3	D	31	ARG
3	D	50	LYS
3	D	92	VAL
3	D	104	HIS
3	D	114	ILE
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	141	PHE
3	D	151	MET
3	D	169	LEU
3	D	179	LYS
3	D	188	LEU
3	D	235	GLU
3	D	239	LEU
3	D	250	ARG
3	D	309	ASN
3	D	430	HIS

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Mol	Chain	Res	Type
3	D	500	ILE
3	D	505	ASP
3	D	508	LEU
3	D	527	LEU
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	614	LEU
3	D	668	PHE
3	D	678	ARG
3	D	681	LYS
3	D	709	ARG
3	D	713	GLU
3	D	771	GLN
3	D	795	TYR
3	D	805	GLN
3	D	816	THR
3	D	832	LYS
3	D	867	GLN
3	D	873	GLU
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG
3	D	1134	ILE
3	D	1148	ARG
3	D	1149	ARG
3	D	1188	GLU
3	D	1247	LYS
3	D	1306	LEU
4	E	8	ASP
4	E	15	ASN
5	X	21	TYR
5	X	28	ASN
5	X	99	ARG
5	X	136	GLU
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	452	ILE
5	X	476	ARG
5	X	495	ARG

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Mol	Chain	Res	Type
5	X	545	HIS
5	X	562	ARG
5	X	607	LEU
1	F	158	ARG
1	F	160	HIS
1	F	163	GLU
1	G	37	HIS
1	G	218	ARG
1	G	228	LEU
2	H	9	LYS
2	H	15	PHE
2	H	18	ARG
2	H	37	LYS
2	H	42	ASP
2	H	46	GLN
2	H	56	VAL
2	H	70	TYR
2	H	73	TYR
2	H	80	PHE
2	H	88	ARG
2	H	99	LYS
2	H	127	ILE
2	H	150	HIS
2	H	163	LYS
2	H	311	CYS
2	H	464	PHE
2	H	479	LEU
2	H	488	MET
2	H	513	GLN
2	H	514	PHE
2	H	645	PHE
2	H	661	VAL
2	H	690	VAL
2	H	711	ASP
2	H	773	LEU
2	H	800	MET
2	H	807	TRP
2	H	817	LEU
2	H	845	LEU
2	H	941	LYS
2	H	944	ARG
2	H	955	GLN

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Mol	Chain	Res	Type
2	H	964	LEU
2	H	971	LEU
2	H	975	ILE
2	H	994	ARG
2	H	1002	LEU
2	H	1005	GLU
2	H	1010	GLN
2	H	1017	GLN
2	H	1032	LYS
2	H	1042	LEU
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1211	ARG
2	H	1233	LEU
2	H	1264	GLN
2	H	1288	GLN
2	H	1291	LEU
2	H	1341	ASP
3	I	31	ARG
3	I	50	LYS
3	I	92	VAL
3	I	104	HIS
3	I	114	ILE
3	I	133	ARG
3	I	139	LEU
3	I	140	TYR
3	I	141	PHE
3	I	151	MET
3	I	169	LEU
3	I	179	LYS
3	I	188	LEU
3	I	235	GLU
3	I	239	LEU
3	I	248	ASP
3	I	250	ARG
3	I	309	ASN
3	I	316	ILE
3	I	325	LYS
3	I	416	ILE
3	I	430	HIS

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Mol	Chain	Res	Type
3	I	475	GLU
3	I	500	ILE
3	I	505	ASP
3	I	527	LEU
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	571	ASP
3	I	594	GLN
3	I	668	PHE
3	I	678	ARG
3	I	681	LYS
3	I	709	ARG
3	I	771	GLN
3	I	795	TYR
3	I	805	GLN
3	I	816	THR
3	I	832	LYS
3	I	867	GLN
3	I	873	GLU
3	I	911	LYS
3	I	918	ILE
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1149	ARG
3	I	1247	LYS
3	I	1297	LYS
3	I	1306	LEU
3	I	1369	ARG
5	Y	136	GLU
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS
5	Y	379	MET
5	Y	384	LEU
5	Y	452	ILE
5	Y	457	ILE
5	Y	476	ARG
5	Y	495	ARG
5	Y	545	HIS

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Mol	Chain	Res	Type
5	Y	562	ARG
5	Y	565	ILE
5	Y	589	GLN
5	Y	607	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	227	GLN
1	A	239	GLN
1	B	66	HIS
1	B	84	ASN
2	C	41	GLN
2	C	69	GLN
2	C	238	GLN
2	C	273	HIS
2	C	314	ASN
2	C	462	ASN
2	C	510	GLN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	554	HIS
2	C	673	HIS
2	C	799	ASN
2	C	955	GLN
2	C	1010	GLN
2	C	1108	ASN
2	C	1111	GLN
2	C	1134	GLN
2	C	1146	GLN
2	C	1175	ASN
2	C	1264	GLN
2	C	1288	GLN
3	D	94	GLN
3	D	419	HIS
3	D	477	GLN
3	D	488	ASN
3	D	504	GLN
3	D	519	ASN
3	D	623	GLN

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Mol	Chain	Res	Type
3	D	875	ASN
3	D	907	HIS
3	D	1197	ASN
3	D	1268	ASN
3	D	1350	ASN
4	E	31	GLN
5	X	30	HIS
5	X	54	GLN
5	X	258	GLN
5	X	301	ASN
5	X	400	GLN
5	X	406	GLN
5	X	437	GLN
5	X	446	GLN
5	X	461	ASN
5	X	469	GLN
1	G	37	HIS
1	G	41	ASN
1	G	66	HIS
2	H	46	GLN
2	H	69	GLN
2	H	238	GLN
2	H	462	ASN
2	H	510	GLN
2	H	513	GLN
2	H	517	GLN
2	H	673	HIS
2	H	799	ASN
2	H	894	GLN
2	H	955	GLN
2	H	1010	GLN
2	H	1017	GLN
2	H	1108	ASN
2	H	1111	GLN
2	H	1134	GLN
2	H	1175	ASN
2	H	1220	GLN
2	H	1264	GLN
2	H	1288	GLN
3	I	94	GLN
3	I	274	ASN
3	I	300	GLN

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Mol	Chain	Res	Type
3	I	419	HIS
3	I	477	GLN
3	I	504	GLN
3	I	519	ASN
3	I	1227	HIS
3	I	1350	ASN
4	J	15	ASN
4	J	31	GLN
5	Y	301	ASN
5	Y	342	GLN
5	Y	400	GLN
5	Y	437	GLN
5	Y	461	ASN
5	Y	469	GLN
5	Y	589	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	0O2	D	1503	-	32,42,42	2.20	11 (34%)	45,68,68	1.97	12 (26%)

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
7	0O2	D	1503	-	-	7/29/49/49	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1503	0O2	O6-C6	4.80	1.36	1.24
7	D	1503	0O2	C2-N2	4.59	1.43	1.33
7	D	1503	0O2	O2'-C2'	-4.42	1.32	1.43
7	D	1503	0O2	C2'-C1'	-4.35	1.47	1.53
7	D	1503	0O2	C6-C5	-3.62	1.35	1.41
7	D	1503	0O2	C8-N7	3.60	1.41	1.34
7	D	1503	0O2	O4'-C4'	-2.61	1.39	1.45
7	D	1503	0O2	C2'-C3'	-2.60	1.47	1.52
7	D	1503	0O2	O4'-C1'	-2.40	1.37	1.41
7	D	1503	0O2	PC-O3'	-2.29	1.54	1.60
7	D	1503	0O2	O5'-C5'	-2.02	1.37	1.44

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1503	0O2	PA-O3A-PB	-5.74	113.14	132.83
7	D	1503	0O2	PC-O3C-PD	-5.41	114.28	132.83
7	D	1503	0O2	O3G-PG-O3B	3.47	116.28	104.64
7	D	1503	0O2	N3-C2-N1	-3.34	122.77	127.22
7	D	1503	0O2	C2-N3-C4	3.11	118.91	115.36
7	D	1503	0O2	O3'-C3'-C2'	2.72	121.55	111.68
7	D	1503	0O2	O4'-C4'-C3'	2.42	110.06	104.87
7	D	1503	0O2	O3C-PC-O3'	2.42	107.36	102.48
7	D	1503	0O2	PB-O3B-PG	-2.42	124.52	132.83
7	D	1503	0O2	PC-O3'-C3'	2.19	127.36	119.41
7	D	1503	0O2	C1'-N9-C4	2.15	130.43	126.64
7	D	1503	0O2	O2G-PG-O3B	2.03	111.46	104.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

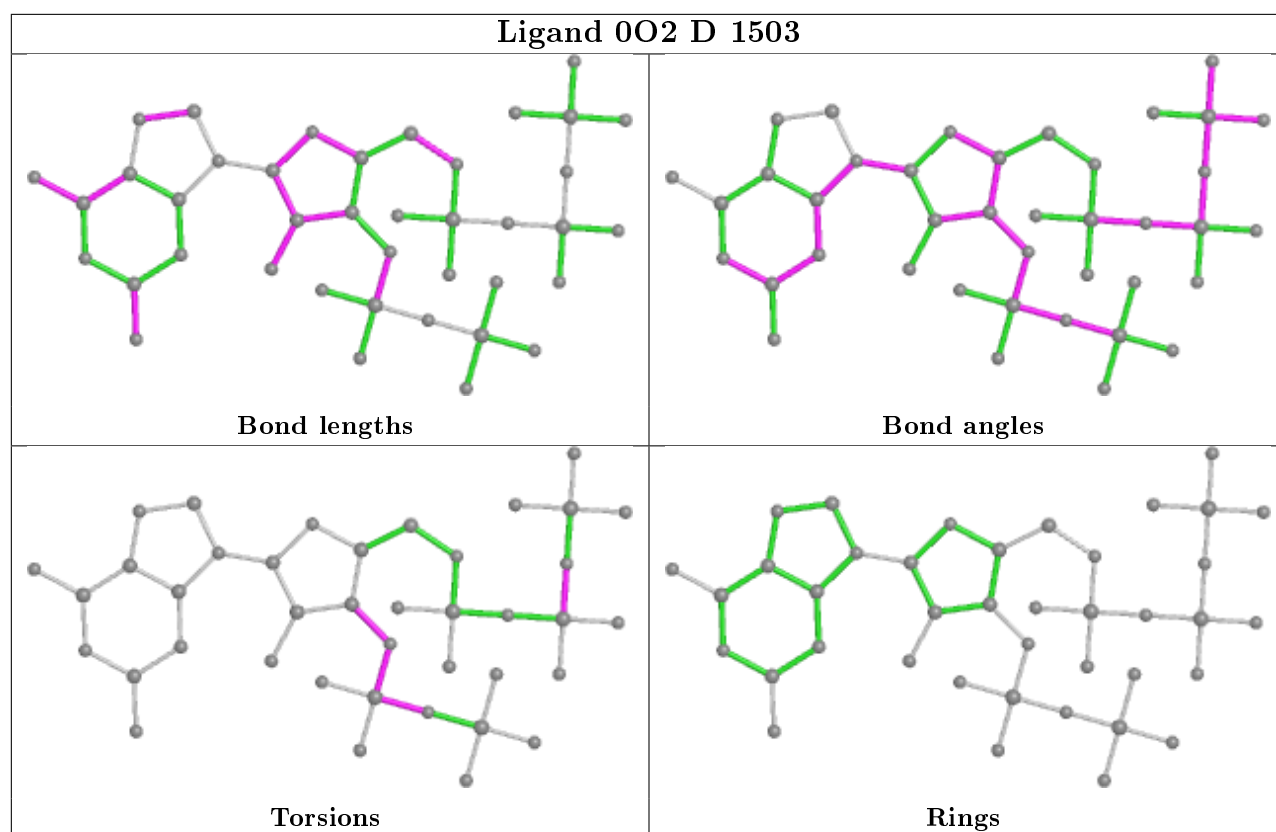
Mol	Chain	Res	Type	Atoms
7	D	1503	0O2	C3'-O3'-PC-O1C
7	D	1503	0O2	C2'-C3'-O3'-PC
7	D	1503	0O2	C3'-O3'-PC-O3C
7	D	1503	0O2	C3'-O3'-PC-O2C
7	D	1503	0O2	PD-O3C-PC-O2C
7	D	1503	0O2	C4'-C3'-O3'-PC
7	D	1503	0O2	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1503	0O2	9	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/329 (98%)	-0.19	4 (1%) 79 70	0, 55, 172, 230	0
1	B	221/329 (67%)	-0.04	7 (3%) 47 37	0, 86, 193, 260	0
1	F	229/329 (69%)	-0.01	13 (5%) 23 20	2, 123, 212, 293	0
1	G	217/329 (65%)	0.04	4 (1%) 68 59	5, 113, 204, 271	0
2	C	1335/1342 (99%)	-0.29	20 (1%) 73 64	0, 38, 168, 304	0
2	H	1335/1342 (99%)	-0.13	39 (2%) 51 41	0, 78, 206, 346	0
3	D	1160/1407 (82%)	-0.21	16 (1%) 75 65	0, 28, 152, 297	0
3	I	1160/1407 (82%)	-0.10	40 (3%) 45 36	0, 54, 183, 316	0
4	E	90/91 (98%)	-0.22	0 100 100	0, 33, 116, 167	0
4	J	76/91 (83%)	0.08	1 (1%) 77 68	12, 83, 181, 230	0
5	X	517/613 (84%)	-0.11	20 (3%) 39 31	0, 98, 238, 341	0
5	Y	458/613 (74%)	-0.09	16 (3%) 44 35	1, 100, 216, 296	0
All	All	7121/8222 (86%)	-0.15	180 (2%) 57 47	0, 63, 198, 346	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	10	ALA	9.3
2	H	982	GLY	9.3
3	I	521	LYS	8.7
2	H	981	ALA	8.0
2	H	983	GLY	7.7
3	I	9	LYS	7.0
3	I	1376	GLY	6.2
3	I	208	THR	5.6
1	F	162	GLU	5.1
5	Y	309	ASN	5.0
3	I	1294	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
5	Y	311	THR	4.6
1	F	193	GLU	4.5
3	I	12	THR	4.5
2	H	1009	ASN	4.5
3	I	207	GLU	4.4
3	D	1171	GLY	4.3
2	H	1020	GLU	4.3
2	C	251	ALA	4.2
2	H	1008	GLN	4.2
1	F	148	ARG	4.2
3	D	1133	ASP	4.1
5	X	35	ILE	4.1
5	X	34	ASP	4.0
3	I	1295	ASN	4.0
3	I	11	GLN	3.9
5	Y	239	GLY	3.9
3	I	13	LYS	3.9
2	C	252	SER	3.8
2	C	266	GLY	3.8
1	A	196	THR	3.8
1	F	195	ARG	3.8
3	D	1170	LYS	3.7
3	I	1375	ALA	3.7
5	X	328	GLU	3.5
3	I	1167	LYS	3.5
5	Y	305	LEU	3.4
2	C	1166	ASP	3.4
2	H	172	TYR	3.4
3	D	1199	PHE	3.4
5	X	240	ARG	3.4
2	H	1019	ASP	3.3
3	I	1203	ARG	3.3
2	C	165	HIS	3.3
2	H	305	SER	3.2
2	H	987	GLU	3.2
2	H	113	THR	3.2
2	H	376	PRO	3.2
5	X	16	GLY	3.1
5	Y	478	PRO	3.1
2	C	282	VAL	3.1
2	H	988	LYS	3.0
2	C	272	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
3	I	212	THR	3.0
1	F	194	GLN	3.0
3	I	1133	ASP	3.0
2	C	265	LYS	3.0
3	I	676	GLY	3.0
5	Y	315	TRP	3.0
1	F	161	SER	3.0
1	F	164	ASP	2.9
2	H	1012	GLU	2.9
1	A	191	ARG	2.9
3	I	1161	GLY	2.9
2	C	306	THR	2.8
1	B	169	GLY	2.8
2	H	60	GLN	2.8
3	D	1168	GLU	2.8
5	Y	212	ILE	2.8
1	B	75	GLN	2.8
3	I	667	GLN	2.8
2	C	311	CYS	2.8
2	H	375	PRO	2.8
1	F	192	VAL	2.7
3	I	855	ASP	2.7
2	C	305	SER	2.7
2	H	332	ARG	2.7
5	X	36	VAL	2.7
1	G	96	ASP	2.7
2	H	1000	LEU	2.7
5	X	423	ARG	2.7
3	I	175	GLU	2.7
1	B	73	GLY	2.7
2	C	310	ILE	2.7
2	H	980	VAL	2.7
5	X	64	ASP	2.7
2	H	115	LYS	2.7
5	X	20	GLY	2.6
3	D	81	ARG	2.6
5	Y	240	ARG	2.6
5	X	420	GLU	2.6
5	X	339	ARG	2.6
2	C	250	THR	2.6
2	H	1001	GLY	2.6
5	Y	307	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	74	VAL	2.6
3	I	677	GLU	2.6
2	C	233	ARG	2.5
3	I	709	ARG	2.5
1	B	147	GLN	2.5
2	H	1316	GLU	2.5
2	H	1003	THR	2.5
5	Y	310	GLU	2.5
1	F	163	GLU	2.5
3	I	1172	LYS	2.5
2	H	996	ARG	2.5
3	I	708	ASN	2.5
5	X	318	ALA	2.5
5	Y	304	THR	2.5
2	C	267	ARG	2.5
1	G	18	GLN	2.5
2	H	742	TYR	2.5
5	X	239	GLY	2.5
2	C	238	GLN	2.5
3	D	834	PRO	2.5
1	F	196	THR	2.4
5	X	56	MET	2.4
3	D	1376	GLY	2.4
2	H	169	LYS	2.4
3	D	1172	LYS	2.4
2	H	105	TYR	2.4
1	B	136	GLU	2.4
5	X	153	ALA	2.4
5	Y	308	GLY	2.4
3	I	675	ALA	2.4
2	H	979	LEU	2.4
2	H	999	GLU	2.4
3	I	564	VAL	2.4
1	F	113	ALA	2.3
3	I	876	SER	2.3
3	I	1213	GLY	2.3
3	I	151	MET	2.3
3	D	1134	ILE	2.3
3	I	1204	VAL	2.3
5	Y	154	GLU	2.3
3	D	212	THR	2.3
3	I	209	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	163	LYS	2.3
2	H	986	ALA	2.3
5	Y	578	LYS	2.3
3	I	205	LEU	2.3
1	G	148	ARG	2.3
5	Y	321	ALA	2.3
1	A	4	SER	2.3
2	H	990	ASP	2.3
5	X	57	GLU	2.2
2	C	258	ASN	2.2
3	I	174	ASP	2.2
2	H	1002	LEU	2.2
3	I	14	THR	2.2
2	H	781	ASP	2.2
4	J	35	LYS	2.2
3	D	211	GLU	2.2
2	H	984	VAL	2.2
1	F	95	LYS	2.2
2	C	375	PRO	2.2
3	I	1170	LYS	2.1
5	X	305	LEU	2.1
2	H	1134	GLN	2.1
2	H	1006	GLU	2.1
1	A	190	ALA	2.1
1	G	147	GLN	2.1
2	C	1002	LEU	2.1
3	I	520	ALA	2.1
2	H	1258	PRO	2.1
3	D	80	HIS	2.1
3	I	834	PRO	2.1
3	I	1160	SER	2.1
2	H	912	ASP	2.1
5	X	315	TRP	2.1
1	B	105	SER	2.1
1	F	33	ARG	2.0
3	D	89	GLY	2.0
3	D	831	VAL	2.0
5	X	336	GLU	2.0
2	C	1001	GLY	2.0
5	X	335	GLU	2.0
3	D	333	GLY	2.0
3	I	91	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
5	Y	423	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

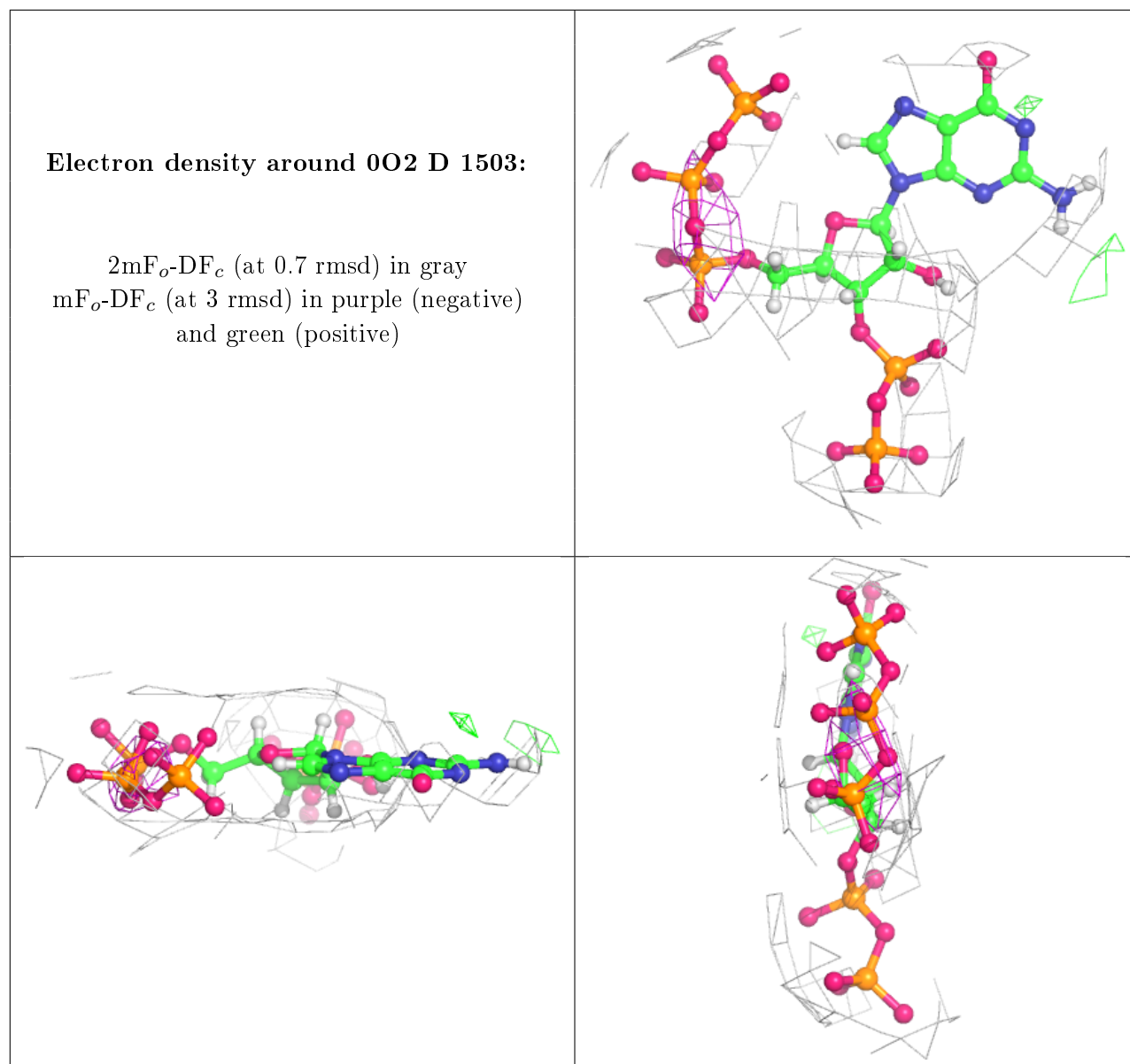
There are no carbohydrates in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	0O2	D	1503	40/40	0.90	0.17	20,20,20,20	0
6	ZN	I	1501	1/1	0.97	0.04	60,60,60,60	0
6	ZN	D	1502	1/1	0.97	0.18	8,8,8,8	0
6	ZN	D	1501	1/1	0.98	0.06	54,54,54,54	0
6	ZN	I	1502	1/1	0.99	0.17	49,49,49,49	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.