



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:07 AM GMT

PDB ID : 2VZ8
Title : CRYSTAL STRUCTURE OF MAMMALIAN FATTY ACID SYNTHASE
Authors : Maier, T.; Leibundgut, M.; Ban, N.
Deposited on : 2008-07-31
Resolution : 3.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

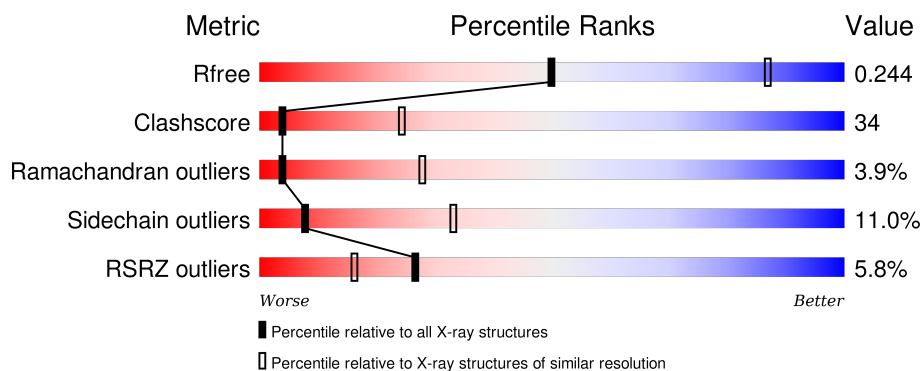
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2512	<div> <div>4%</div> <div>35%</div> <div>36%</div> <div>6%</div> <div>22%</div> </div>
1	B	2512	<div> <div>6%</div> <div>36%</div> <div>37%</div> <div>6%</div> <div>20%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30281 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1962	Total	C	N	O	S	0	0	0
			14977	9466	2630	2803	78			
1	B	2004	Total	C	N	O	S	0	0	0
			15304	9671	2684	2869	80			

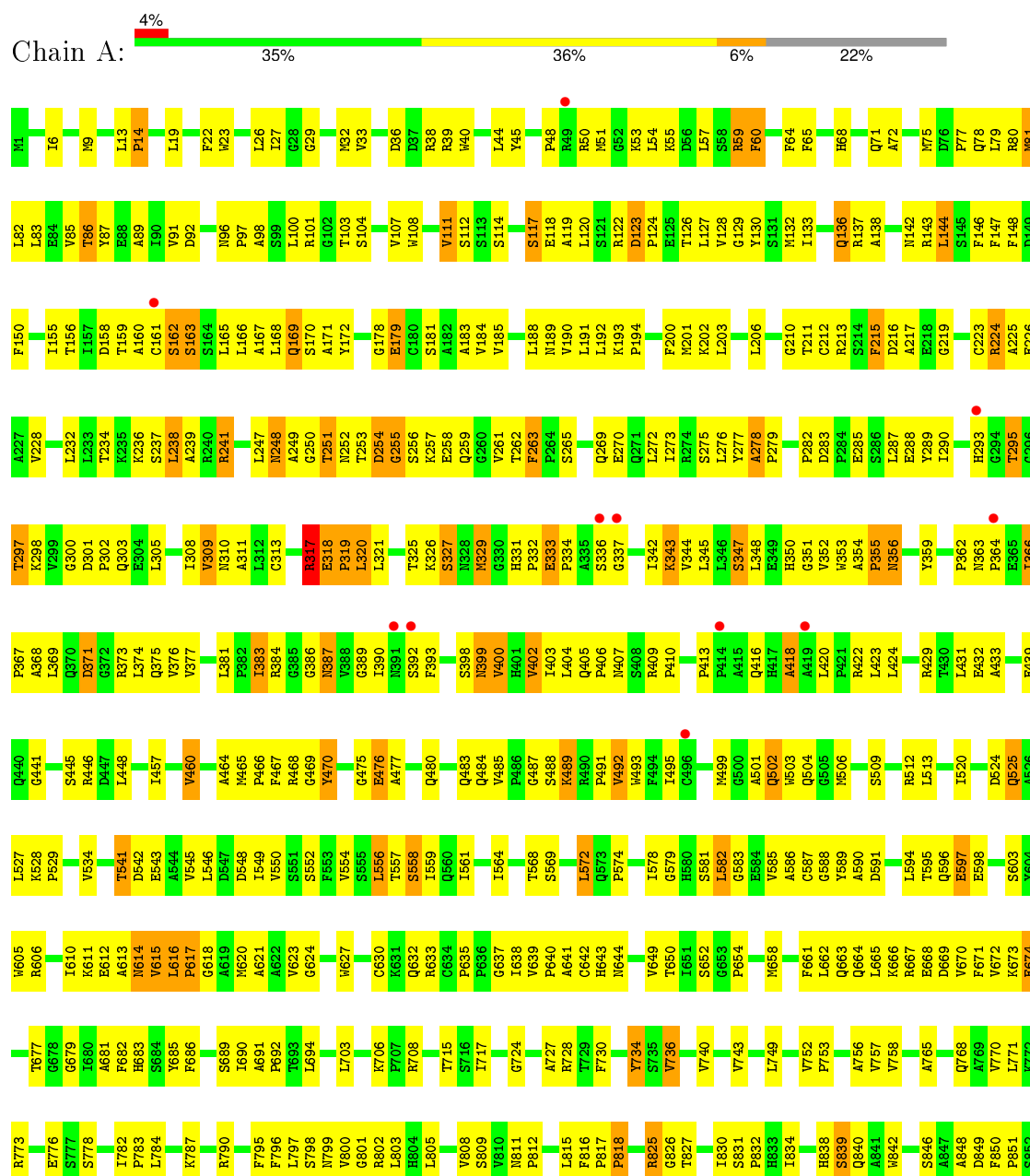
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	834	ILE	UNK	CONFLICT SEE REMARK 9	UNP A5YV76
B	834	ILE	UNK	CONFLICT SEE REMARK 9	UNP A5YV76

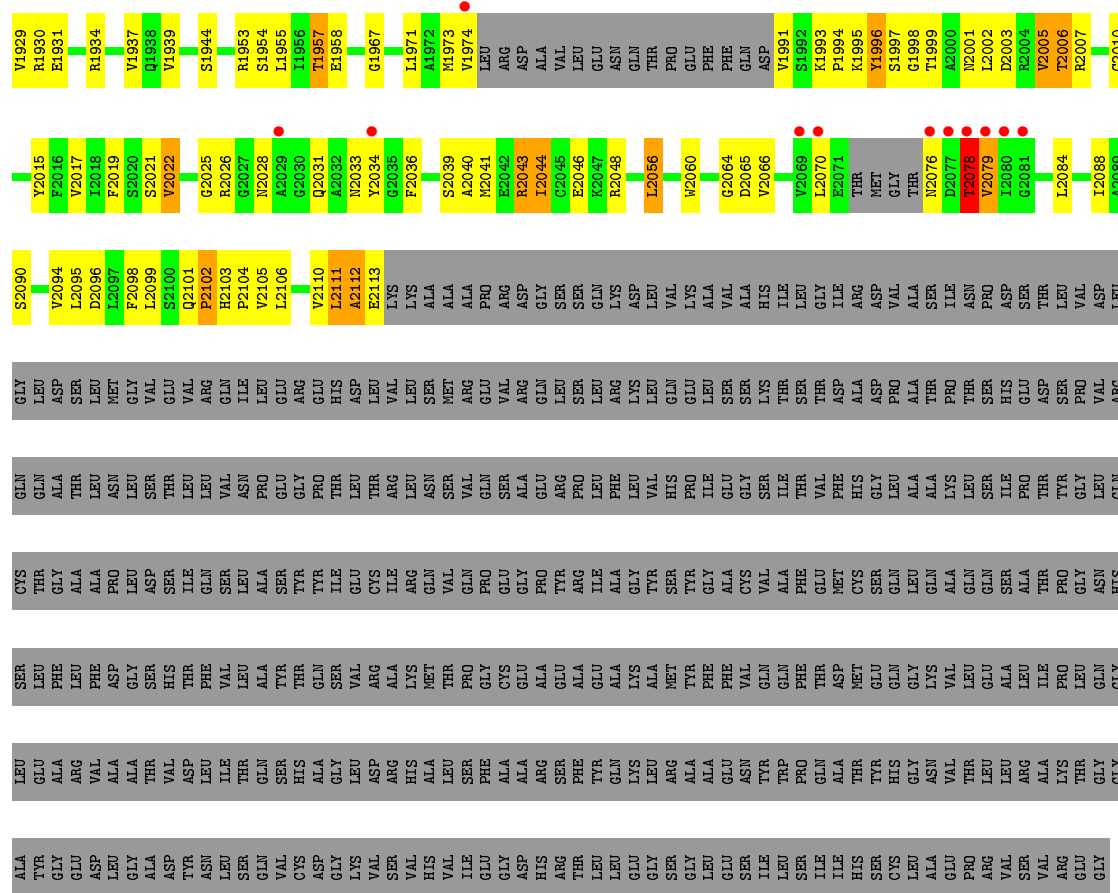
3 Residue-property plots

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

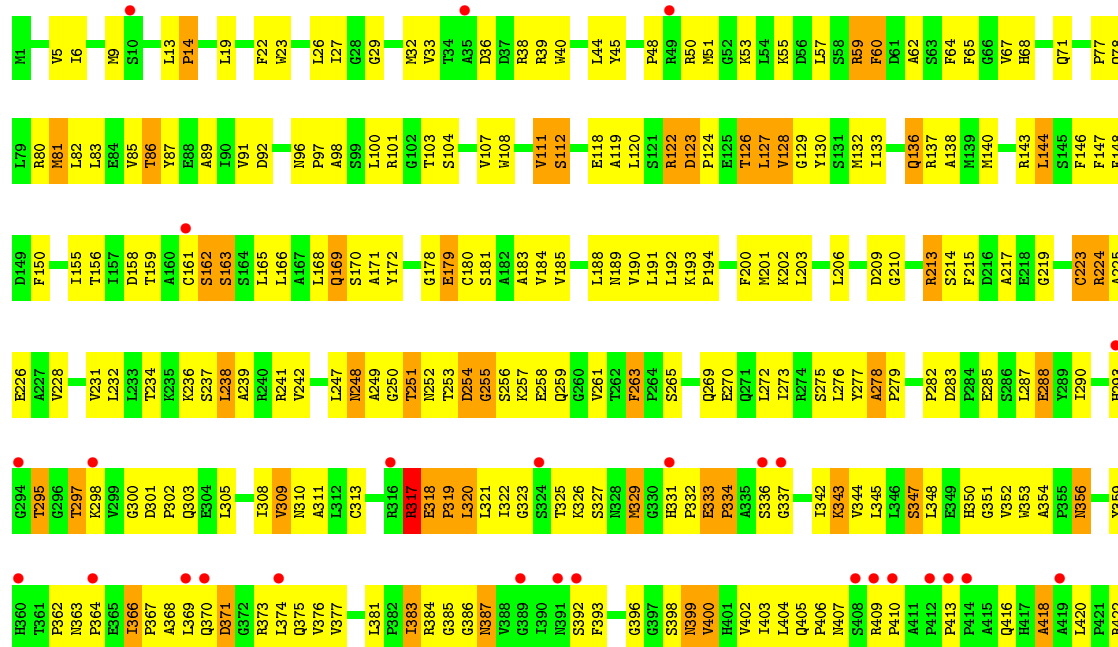
• Molecule 1: FATTY ACID SYNTHASE



V1853	L1769	L1689	V1617	S1542	L1477	L1416	GLY	L1292	A1223	VAL	G1098	Q1023	S941	G853
I1864	G1770	L1889	P1618	S1543	L1480	S1417	HIS	H1293	P1224	VAL	S1101	Q1024	S944	S884
Q1855	D1773	C1693	A1619	I1544	T1481	V1418	PRO	V1294	A1225	PRO	S1102	N1025	F944	S855
R1857	L1774	C1694	E1620	R1545	P1483	E1419	LEU	Q1296	K1227	GLY	V1103	D1026	E945	C856
E1858	L1622	V1695	G1621	S1549	A1483	D1420	GLY	G1297	A1228	ASP	A1104	S1030	S947	S857
E1859	N1777	V1696	A1623	H1552	P1484	T1421	MET	Q1298	G1229	GLY	P1105	S1031	D848	S858
E1860	H1778	T1697	E1624	H1553	E1485	S1422	VAL	N1299	V1230	ALA	A1106	F1031	S949	V861
Q1861	A1779	S1625	V1624	Y1553	M1486	F1423	GLY	W1299	D1231	GLN	R1107	L1032	Y862	V862
P1862	L1780	A1554	P1626	A1554	H1487	R1424	PHE	P1300	D1231	ALA	P1108	D1033	I954	K863
P1863	G1781	L1555	P1626	P1488	V1425	R1424	LEU	A1302	A1233	PRO	Q1109	A1034	L953	V866
A1864	G1782	P1556	S1489	P1488	V1426	D1427	THR	N1303	L1234	ARG	E1110	M1035	V869	S870
P1865	A1783	A1557	S1490	S1489	D1428	S1428	SER	P1304	E1235	GLY	H1111	L1036	V869	P871
	V1784	S1558	S1491	S1491	L1429	L1429	PRO	A1305	N1236	ALA	L1112	H1037	V869	S870
P1869	F1785	C1589	E1492	E1492	K1430	K1430	GLY	P1306	M1237	PRO	F1113	M1038	W962	P871
P1870	L1786	Q1560	L1493	L1493	D1431	D1431	GLN	GLY	A1238	GLN	P1114	S1039	E963	P871
I1871	K1787	L1493	L1493	L1493	I1432	I1432	GLY	SER	P1239	GLN	L1115	I1040	S964	Y874
L1873	V1789	L1497	L1497	L1497	L1433	L1433	GLY	LEU	P1240	SER	L1116	P1043	D966	Y874
T1874	F1720	L1563	L1563	L1563	A1434	A1434	ARG	GLY	K1241	LEU	F1117	P1043	D967	V876
	A1721	C1564	C1564	C1564	D1435	D1435	HIS	LYS	M1242	ARG	K1118	Y1049	H877	H877
S1877	N1722	Y1567	D1500	D1500	D1435	D1435	LEU	A1312	K1243	LEU	F1119	Y1049	P970	R883
K1878	S1723	Y1568	L1501	L1501	S1437	S1437	LEU	D1313	V1245	LEU	T1122	L1050	P970	R883
T1879	R1724	T1569	V1502	V1502	S1438	S1438	SER	L1314	V1245	LEU	P1123	P1051	D971	R883
F1880	D1725	S1570	M1503	M1503	R1439	R1439	GLN	L1315	V1245	LEU	H1124	R1052	T972	P887
L1795	T1726	L1571	V1505	V1505	P1440	P1440	GLY	L1316	L1248	ALA	F1125	R1053	P887	P887
L1796	E1644	L1571	Y1506	Y1506	V1441	V1441	THR	G1317	A1249	ALA	E1126	F1054	G888	G888
	S1647	H1572	H1572	H1572	W1442	W1442	THR	F1317	G1250	CYS	L1133	R1068	V976	G889
P1882	P1648	F1573	F1573	F1573	M1443	M1443	GLY	N1318	G1250	GLN	T1134	K1066	D977	T889
P1883	P1649	R1574	R1574	R1574	M1444	M1444	ASP	A1320	G1252	LEU	A1135	Q1067	P976	G890
K1885	T1639	D1575	G1509	G1509	M1444	M1444	GLY	L1319	Q1253	LEU	LEU	K1067	P977	P977
K1886	W1640	V1576	V1510	V1510	V1446	V1446	PRO	A1320	Q1253	GLN	GLN	Y1069	P978	P978
E1802	E1644	V1576	V1511	V1511	V1446	V1446	ALA	ALA	L1254	LEU	L1130	L1068	L894	L894
G1803	S1647	H1572	H1512	H1512	G1447	G1447	THR	THR	Y1255	ASN	H1133	T1070	T895	T895
	G1581	A1513	A1513	A1513	C1448	C1448	LEU	LEU	S1256	GLY	T1134	T1070	W896	W896
P1889	K1582	F1514	F1514	F1514	S1449	S1449	GLY	GLY	R1257	ASN	LEU	T1070	S981	S981
L1890	S1584	H1516	H1516	H1516	L1389	L1389	PRO	PRO	P1259	GLN	GLN	T1070	T982	T982
	P1585	F1517	F1517	F1517	S1451	S1451	ALA	ALA	L1261	LEU	LEU	T1070	E984	E984
					G1452	G1452	VAL	VAL	L1262	GLY	CYS	T1070	F985	F985
					V1453	V1453	VAL	VAL	L1262	LEU	GLY	T1070	S988	S988
					V1454	V1454	VAL	VAL	L1262	LEU	GLY	T1070	Q989	Q989
					V1455	V1455	VAL	VAL	L1262	LEU	GLY	T1070	Y993	Y993
					V1457	V1457	ASN	ASN	V1267	VAL	ARG	A1077	D995	D995
							GLY	GLY	D1269	LEU	GLY	A1077	L998	L998
							GLY	GLY		LEU	GLY	A1077	Y1001	Y1001
							GLY	GLY		LEU	GLY	A1077	D1002	D1002
							GLY	GLY		LEU	GLY	A1077	Y1003	Y1003
							GLY	GLY		LEU	GLY	A1077	L925	L925
							GLY	GLY		LEU	GLY	A1077	T930	T930
							GLY	GLY		LEU	GLY	A1077	V931	V931
							GLY	GLY		LEU	GLY	A1077	F914	F914
							GLY	GLY		LEU	GLY	A1077	E915	E915
							GLY	GLY		LEU	GLY	A1077	D916	D916
							GLY	GLY		LEU	GLY	A1077	Y917	Y917
							GLY	GLY		LEU	GLY	A1077	L925	L925
							GLY	GLY		LEU	GLY	A1077	T930	T930
							GLY	GLY		LEU	GLY	A1077	V931	V931
							GLY	GLY		LEU	GLY	A1077	F1007	F1007
							GLY	GLY		LEU	GLY	A1077	Q1008	Q1008
							GLY	GLY		LEU	GLY	A1077	L1009	L1009
							GLY	GLY		LEU	GLY	A1077	E934	E934
							GLY	GLY		LEU	GLY	A1077	V935	V935
							GLY	GLY		LEU	GLY	A1077	R936	R936
							GLY	GLY		LEU	GLY	A1077	L937	L937
							GLY	GLY		LEU	GLY	A1077	L938	L938
							GLY	GLY		LEU	GLY	A1077	E939	E939
							GLY	GLY		LEU	GLY	A1077	D1014	D1014
							GLY	GLY		LEU	GLY	A1077	L1015	L1015
							GLY	GLY		LEU	GLY	A1077	F1016	F1016
							GLY	GLY		LEU	GLY	A1077	E1016	E1016



• Molecule 1: FATTY ACID SYNTHASE



G1466	G1467	R1468	T1469	R1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	T1480	P1481	P1482	P1483	P1484	P1485	P1486	P1487	P1488	S1491	L1492	L1493	L1501	M1502	M1503	M1504	M1505	M1506	M1507	G1512	A1513	F1514	R1515	H1516	F1517	P1518	L1519	E1520	R1523	P1524	E1525	K1526	Q1527	T1528	T1529	A1530	F1532	R1533	L1536	S1537	P1538	R1538																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
L1423	L1424	R1429	T1430	L1431	E1432	A1433	Q1504	G1505	M1506	D1591	E1592	F1593	G1594	H1595	I1596	J1597	K1598	L1599	M1600	N1601	O1602	P1603	Q1604	R1605	S1606	T1607	U1608	V1609	W1610	X1611	Y1612	Z1613	A1614	B1615	C1616	D1617	E1618	F1619	G1620	H1621	I1622	J1623	K1624	L1625	M1626	N1627	O1628	P1629	Q1630	R1631	S1632	T1633	U1634	V1635	W1636	X1637	Y1638	Z1639																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
E1668	D1669	F1670	G1671	H1672	I1673	J1674	K1675	L1676	M1677	N1678	O1679	P1680	Q1681	R1682	S1683	T1684	U1685	V1686	W1687	X1688	Y1689	Z1690	A1691	B1692	C1693	D1694	E1695	F1696	G1697	H1698	I1699	J1700	K1701	L1702	M1703	N1704	O1705	P1706	Q1707	R1708	S1709	T1710	U1711	V1712	W1713	X1714	Y1715	Z1716	A1717	B1718	C1719	D1720	E1721	F1722	G1723	H1724	I1725	J1726	K1727	L1728	M1729	N1730	O1731	P1732	Q1733	R1734	S1735	T1736	U1737	V1738	W1739	X1740	Y1741	Z1742	A1743	B1744	C1745	D1746	E1747																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
S1839	Q1840	P1845	L1846	A1847	F1848	G1849	H1850	I1851	J1852	K1853	L1854	M1855	N1856	O1857	P1858	Q1859	R1860	S1861	T1862	U1863	V1864	W1865	X1866	Y1867	Z1868	A1869	B1870	C1871	D1872	E1873	F1874	G1875	H1876	I1877	J1878	K1879	L1880	M1881	N1882	O1883	P1884	Q1885	R1886	S1887	T1888	U1889	V1890	W1891	X1892	Y1893	Z1894	A1895	B1896	C1897	D1898	E1899	F1900	G1901	H1902	I1903	J1904	K1905	L1906	M1907	N1908	O1909	P1910	Q1911	R1912	S1913	T1914	U1915	V1916	W1917	X1918	Y1919	Z1920	A1921	B1922	C1923	D1924	E1925	F1926	G1927	H1928	I1929	J1930	K1931	L1932	M1933	N1934	O1935	P1936	Q1937	R1938	S1939	T1940	U1941	V1942	W1943	X1944	Y1945	Z1946	A1947	B1948	C1949	D1950	E1951	F1952	G1953	H1954	I1955	J1956	K1957	L1958	M1959	N1960	O1961	P1962	Q1963	R1964	S1965	T1966	U1967	V1968	W1969	X1970	Y1971	Z1972	A1973	B1974	C1975	D1976	E1977	F1978	G1979	H1980	I1981	J1982	K1983	L1984	M1985	N1986	O1987	P1988	Q1989	R1990	S1991	T1992	U1993	V1994	W1995	X1996	Y1997	Z1998	A1999	B2000	C2001	D2002	E2003	F2004	G2005	H2006	I2007	J2008	K2009	L2010	M2011	N2012	O2013	P2014	Q2015	R2016	S2017	T2018	U2019	V2020	W2021	X2022	Y2023	Z2024	A2025	B2026	C2027	D2028	E2029	F2030	G2031	H2032	I2033	J2034	K2035	L2036	M2037	N2038	O2039	P2040	Q2041	R2042	S2043	T2044	U2045	V2046	W2047	X2048	Y2049	Z2050	A2051	B2052	C2053	D2054	E2055	F2056	G2057	H2058	I2059	J2060	K2061	L2062	M2063	N2064	O2065	P2066	Q2067	R2068	S2069	T2070	U2071	V2072	W2073	X2074	Y2075	Z2076	A2077	B2078	C2079	D2080	E2081	F2082	G2083	H2084	I2085	J2086	K2087	L2088	M2089	N2090	O2091	P2092	Q2093	R2094	S2095	T2096	U2097	V2098	W2099	X2100	Y2101	Z2102	A2103	B2104	C2105	D2106	E2107	F2108	G2109	H2110	I2111	J2112	K2113	L2114	M2115	N2116	O2117	P2118	Q2119	R2120	S2121	T2122	U2123	V2124	W2125	X2126	Y2127	Z2128	A2129	B2130	C2131	D2132	E2133	F2134	G2135	H2136	I2137	J2138	K2139	L2140	M2141	N2142	O2143	P2144	Q2145	R2146	S2147	T2148	U2149	V2150	W2151	X2152	Y2153	Z2154	A2155	B2156	C2157	D2158	E2159	F2160	G2161	H2162	I2163	J2164	K2165	L2166	M2167	N2168	O2169	P2170	Q2171	R2172	S2173	T2174	U2175	V2176	W2177	X2178	Y2179	Z2180	A2181	B2182	C2183	D2184	E2185	F2186	G2187	H2188	I2189	J2190	K2191	L2192	M2193	N2194	O2195	P2196	Q2197	R2198	S2199	T2200	U2201	V2202	W2203	X2204	Y2205	Z2206	A2207	B2208	C2209	D2210	E2211	F2212	G2213	H2214	I2215	J2216	K2217	L2218	M2219	N2220	O2221	P2222	Q2223	R2224	S2225	T2226	U2227	V2228	W2229	X2230	Y2231	Z2232	A2233	B2234	C2235	D2236	E2237	F2238	G2239	H2240	I2241	J2242	K2243	L2244	M2245	N2246	O2247	P2248	Q2249	R2250	S2251	T2252	U2253	V2254	W2255	X2256	Y2257	Z2258	A2259	B2260	C2261	D2262	E2263	F2264	G2265	H2266	I2267	J2268	K2269	L2270	M2271	N2272	O2273	P2274	Q2275	R2276	S2277	T2278	U2279	V2280	W2281	X2282	Y2283	Z2284	A2285	B2286	C2287	D2288	E2289	F2290	G2291	H2292	I2293	J2294	K2295	L2296	M2297	N2298	O2299	P2300	Q2301	R2302	S2303	T2304	U2305	V2306	W2307	X2308	Y2309	Z2310	A2311	B2312	C2313	D2314	E2315	F2316	G2317	H2318	I2319	J2320	K2321	L2322	M2323	N2324	O2325	P2326	Q2327	R2328	S2329	T2330	U2331	V2332	W2333	X2334	Y2335	Z2336	A2337	B2338	C2339	D2340	E2341	F2342	G2343	H2344	I2345	J2346	K2347	L2348	M2349	N2350	O2351	P2352	Q2353	R2354	S2355	T2356	U2357	V2358	W2359	X2360	Y2361	Z2362	A2363	B2364	C2365	D2366	E2367	F2368	G2369	H2370	I2371	J2372	K2373	L2374	M2375	N2376	O2377	P2378	Q2379	R2380	S2381	T2382	U2383	V2384	W2385	X2386	Y2387	Z2388	A2389	B2390	C2391	D2392	E2393	F2394	G2395	H2396	I2397	J2398	K2399	L2400	M2401	N2402	O2403	P2404	Q2405	R2406	S2407	T2408	U2409	V2410	W2411	X2412	Y2413	Z2414	A2415	B2416	C2417	D2418	E2419	F2420	G2421	H2422	I2423	J2424	K2425	L2426	M2427	N2428	O2429	P2430	Q2431	R2432	S2433	T2434	U2435	V2436	W2437	X2438	Y2439	Z2440	A2441	B2442	C2443	D2444	E2445	F2446	G2447	H2448	I2449	J2450	K2451	L2452	M2453	N2454	O2455	P2456	Q2457	R2458	S2459	T2460	U2461	V2462	W2463	X2464	Y2465	Z2466	A2467	B2468	C2469	D2470	E2471	F2472	G2473	H2474	I2475	J2476	K2477	L2478	M2479	N2480	O2481	P2482	Q2483	R2484	S2485	T2486	U2487	V2488	W2489	X2490	Y2491	Z2492	A2493	B2494	C2495	D2496	E2497	F2498	G2499	H2500	I2501	J2502	K2503	L2504	M2505	N2506	O2507	P2508	Q2509	R2510	S2511	T2512	U2513	V2514	W2515	X2516	Y2517	Z2518	A2519	B2520	C2521	D2522	E2523	F2524	G2525	H2526	I2527	J2528	K2529	L2530	M2531	N2532	O2533	P2534	Q2535	R2536	S2537	T2538	U2539	V2540	W2541	X2542	Y2543	Z2544	A2545	B2546	C2547	D2548	E2549	F2550	G2551	H2552	I2553	J2554	K2555	L2556	M2557	N2558	O2559	P2560	Q2561	R2562	S2563	T2564	U2565	V2566	W2567	X2568	Y2569	Z2570	A2571	B2572	C2573	D2574	E2575	F2576	G2577	H2578	I2579	J2580	K2581	L2582	M2583	N2584	O2585	P2586	Q2587	R2588	S2589	T2590	U2591	V2592	W2593	X2594	Y2595	Z2596	A2597	B2598	C2599	D2600	E2601	F2602	G2603	H2604	I2605	J2606	K2607	L2608	M2609	N2610	O2611	P2612	Q2613	R2614	S2615	T2616	U2617	V2618	W2619	X2620	Y2621	Z2622	A2623	B2624	C2625	D2626	E2627	F2628	G2629	H2630	I2631	J2632	K2633	L2634	M2635	N2636	O2637	P2638	Q2639	R2640	S2641	T2642	U2643	V2644	W2645	X2646	Y2647	Z2648	A2649	B2650	C2651	D2652	E2653	F2654	G2655	H2656	I2657	J2658	K2659	L2660	M2661	N2662	O2663	P2664	Q2665	R2666	S2667	T2668	U2669	V2670	W2671	X2672	Y2673	Z2674	A2675	B2676	C2677	D2678	E2679	F2680	G2681	H2682	I2683	J2684	K2685	L2686	M2687	N2688	O2689	P2690	Q2691	R2692	S2693	T2694	U2695	V2696	W2697	X2698	Y2699	Z2700	A2701	B2702	C2703	D2704	E2705	F2706	G2707	H2708	I2709	J2710	K2711	L2712	M2713	N2714	O2715	P2716	Q2717	R2718	S2719	T2720	U2721	V2722	W2723	X2724	Y2725	Z2726	A2727	B2728	C2729	D2730	E2731	F2732	G2733	H2734	I2735	J2736	K2737	L2738	M2739	N2740	O2741	P2742	Q2743	R2744	S2745	T2746	U2747	V2748	W2749	X2750	Y2751	Z2752	A2753	B2754	C2755	D2756	E2757	F2758	G2759	H2760	I2761	J2762	K2763	L2764	M2765	N2766	O2767	P2768	Q2769	R2770	S2771	T2772	U2773	V2774	W2775	X2776	Y2777	Z2778	A2779	B2780	C2781	D2782	E2783	F2784	G2785	H2786	I2787	J2788	K2789	L2790	M2791	N2792	O2793	P2794	Q2795	R2796	S2797	T2798	U2799	V2800	W2801	X2802	Y2803	Z2804	A2805	B2806	C2807	D2808	E2809	F2810	G2811	H2812	I2813	J2814	K2815	L2816	M2817	N2818	O2819	P2820	Q2821	R2822	S2823	T2824	U2825	V2826	W2827	X2828	Y2829	Z2830	A2831	B2832	C2833	D2834	E2835	F2836	G2837	H2838	I2839	J2840	K2841	L2842	M2843	N2844	O2845	P2846	Q2847	R2848	S2849	T2850	U2851	V2852	W2853	X2854	Y2855	Z2856	A2857	B2858	C2859	D2860	E2861	F2862	G2863	H2864	I2865	J2866	K2867	L2868	M2869	N2870	O2871	P2872	Q2873	R2874	S2875	T2876	U2877	V2878	W2879	X2880	Y2881	Z2882	A2883	B2884	C2885	D2886	E2887	F2888	G2889	H2890	I2891	J2892	K2893	L2894	M2895	N2896	O2897	P2898	Q2899	R2900	S2901	T2902	U2903	V2904	W2905	X2906	Y2907	Z2908	A2909	B2910	C2911	D2912	E2913	F2914	G2915	H2916	I2917	J2918	K2919	L2920	M2921	N2922	O2923	P2924	Q2925	R2926	S2927	T2928	U2929	V2930	W2931	X2932	Y2933	Z2934	A2935	B2936	C2937	D2938	E2939	F2940	G2941	H2942	I2943	J2944	K2945	L2946	M2947	N2948	O2949	P2950	Q2951	R2952	S2953	T2954	U2955	V2956	W2957	X2958	Y2959	Z2960	A2961	B2962	C2963	D2964	E2965	F2966	G2967	H2968	I2969	J2970	K2971	L2972	M2973	N2974	O2975	P2976	Q2977	R2978	S2979	T2980	U2981	V2982	W2983	X2984	Y2985	Z2986</



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.32Å 244.70Å 135.25Å 90.00° 101.65° 90.00°	Depositor
Resolution (Å)	29.50 – 3.22 29.50 – 3.22	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.50-3.22) 97.6 (29.50-3.22)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.259 0.202 , 0.244	Depositor DCC
R_{free} test set	4841 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 73.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 96482 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30281	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.45	1/15302 (0.0%)	0.63	0/20792
1	B	0.41	0/15634	0.60	1/21243 (0.0%)
All	All	0.43	1/30936 (0.0%)	0.61	1/42035 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1759	CYS	CB-SG	-5.79	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1694	ARG	NE-CZ-NH1	6.90	123.75	120.30

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	14977	0	14938	1049	0
1	B	15304	0	15266	1083	0
All	All	30281	0	30204	2085	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 34.

All (2085) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1694:ARG:HH11	1:B:1694:ARG:HG3	1.17	1.10
1:B:1303:ASN:H	1:B:1304:PRO:HD3	1.25	1.02
1:A:1473:LEU:HD21	1:A:1503:MET:HG2	1.36	1.02
1:A:165:LEU:HD23	1:A:400:VAL:HG22	1.37	1.02
1:B:1456:MET:HG2	1:B:2036:PHE:HB2	1.41	1.01
1:A:1736:THR:HG23	1:A:1739:LYS:H	1.26	1.00
1:B:1003:TYR:CZ	1:B:1037:HIS:HE1	1.79	1.00
1:A:1539:GLY:HA2	1:A:1580:THR:O	1.62	0.99
1:A:642:CYS:HB2	1:A:650:THR:HB	1.42	0.98
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.42	0.98
1:B:1338:LEU:HD13	1:B:1406:GLN:HE21	1.27	0.98
1:A:118:GLU:HG3	1:B:118:GLU:HG3	1.43	0.98
1:B:1387:LEU:HD22	1:B:1404:CYS:HB3	1.43	0.98
1:B:1651:VAL:HG13	1:B:1680:VAL:HA	1.45	0.97
1:B:1348:THR:HG22	1:B:1349:LEU:H	1.27	0.97
1:A:1003:TYR:CZ	1:A:1037:HIS:HE1	1.83	0.97
1:A:368:ALA:H	1:A:371:ASP:HB3	1.31	0.96
1:B:1418:VAL:HG13	1:B:1425:TRP:CZ2	1.99	0.96
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.44	0.96
1:B:165:LEU:HD23	1:B:400:VAL:HG22	1.43	0.96
1:B:1457:VAL:HG21	1:B:1473:LEU:HD22	1.47	0.95
1:B:368:ALA:H	1:B:371:ASP:HB3	1.31	0.95
1:B:1473:LEU:HD21	1:B:1503:MET:HG2	1.49	0.95
1:B:1299:TRP:HZ3	1:B:1301:PRO:HA	1.29	0.95
1:B:1335:ALA:HA	1:B:1406:GLN:HE22	1.30	0.94
1:B:1330:ALA:O	1:B:1334:MET:HG2	1.67	0.93
1:B:616:LEU:HB2	1:B:686:PHE:HE2	1.30	0.93
1:B:1565:SER:HB2	1:B:1857:ARG:NH2	1.84	0.93
1:B:1312:ALA:HB2	1:B:1337:THR:HG22	1.48	0.91
1:B:1736:THR:HG23	1:B:1739:LYS:H	1.33	0.91
1:A:1115:ILE:HD11	1:A:2111:LEU:HG	1.51	0.91
1:A:1457:VAL:HG21	1:A:1473:LEU:HD22	1.51	0.90
1:A:1418:VAL:HG13	1:A:1425:TRP:CZ2	2.06	0.90
1:B:1662:ARG:HH11	1:B:1662:ARG:CG	1.82	0.90
1:B:662:LEU:HD22	1:B:672:VAL:HG11	1.54	0.89
1:B:1446:VAL:HA	1:B:1476:ASN:ND2	1.87	0.89
1:B:50:ARG:HD3	1:B:210:GLY:O	1.74	0.88
1:A:82:LEU:O	1:A:86:THR:HG23	1.74	0.88
1:B:1446:VAL:HA	1:B:1476:ASN:HD21	1.37	0.88
1:A:1644:GLU:HB3	1:A:1825:PRO:HB3	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:VAL:HG22	1:A:977:ASP:H	1.38	0.88
1:B:384:ARG:HH11	1:B:384:ARG:HG3	1.38	0.88
1:A:1662:ARG:HH11	1:A:1662:ARG:CG	1.87	0.88
1:B:616:LEU:HB2	1:B:686:PHE:CE2	2.09	0.87
1:B:82:LEU:O	1:B:86:THR:HG23	1.75	0.87
1:B:1299:TRP:CZ3	1:B:1301:PRO:HA	2.09	0.87
1:A:1348:THR:HG22	1:A:1349:LEU:H	1.37	0.87
1:A:384:ARG:HH11	1:A:384:ARG:HG3	1.39	0.87
1:A:1545:ARG:HH11	1:A:1545:ARG:HG3	1.39	0.86
1:A:1477:LEU:HD11	1:A:2043:ARG:HD2	1.56	0.86
1:A:1662:ARG:HG3	1:A:1662:ARG:HH11	1.40	0.86
1:A:50:ARG:HD3	1:A:210:GLY:O	1.75	0.86
1:B:64:PHE:HB2	1:B:429:ARG:HH21	1.40	0.86
1:A:861:VAL:HG22	1:A:934:GLU:HB3	1.58	0.85
1:B:643:HIS:HA	1:B:649:VAL:HG22	1.59	0.84
1:B:1530:HIS:HB2	1:B:1552:HIS:HB2	1.60	0.84
1:B:1312:ALA:CB	1:B:1337:THR:HG22	2.08	0.83
1:A:96:ASN:HD21	1:A:98:ALA:HB3	1.41	0.83
1:A:64:PHE:HB2	1:A:429:ARG:HH21	1.41	0.83
1:B:112:SER:CB	1:B:334:PRO:HG3	2.09	0.83
1:A:112:SER:HB2	1:A:334:PRO:HG3	1.59	0.83
1:A:944:PHE:CD2	1:A:959:VAL:HG22	2.14	0.83
1:B:1082:VAL:HG22	1:B:1089:VAL:HG22	1.61	0.83
1:A:1245:VAL:HG13	1:A:1273:THR:HB	1.57	0.83
1:A:616:LEU:HD23	1:A:617:PRO:HD2	1.58	0.83
1:A:1082:VAL:HG22	1:A:1089:VAL:HG22	1.60	0.83
1:A:1289:LEU:HD22	1:A:1294:VAL:HB	1.60	0.83
1:A:319:PRO:HD2	1:A:373:ARG:O	1.78	0.83
1:A:1528:THR:HG22	1:A:1530:HIS:H	1.43	0.83
1:A:112:SER:CB	1:A:334:PRO:HG3	2.07	0.83
1:B:96:ASN:HD21	1:B:98:ALA:HB3	1.42	0.82
1:A:663:GLN:O	1:A:667:ARG:HD2	1.79	0.82
1:A:468:ARG:HD3	1:A:485:VAL:HG21	1.59	0.82
1:A:123:ASP:HB3	1:A:126:THR:HB	1.62	0.82
1:B:1732:VAL:O	1:B:1736:THR:HB	1.78	0.82
1:B:319:PRO:HD2	1:B:373:ARG:O	1.79	0.82
1:B:944:PHE:CD2	1:B:959:VAL:HG22	2.15	0.82
1:B:982:THR:HG23	1:B:983:ALA:H	1.45	0.82
1:B:1416:LEU:HD21	1:B:1425:TRP:HB2	1.59	0.82
1:B:112:SER:HB2	1:B:334:PRO:HG3	1.60	0.81
1:A:1285:ALA:HB1	1:A:1289:LEU:HG	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:ASP:HB3	1:A:1257:ARG:CZ	2.09	0.81
1:A:1341:GLY:HA2	1:A:1406:GLN:O	1.80	0.81
1:A:278:ALA:HB3	1:A:279:PRO:HD3	1.63	0.81
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.09	0.81
1:B:980:ASP:HB2	1:B:982:THR:HG22	1.63	0.81
1:A:1616:MET:HE3	1:A:1650:ILE:HA	1.62	0.81
1:B:861:VAL:HG22	1:B:934:GLU:HB3	1.63	0.81
1:B:1662:ARG:HH11	1:B:1662:ARG:HG3	1.44	0.80
1:B:278:ALA:HB3	1:B:279:PRO:HD3	1.61	0.80
1:B:1456:MET:CG	1:B:2036:PHE:HB2	2.11	0.80
1:B:1003:TYR:CZ	1:B:1037:HIS:CE1	2.67	0.80
1:B:1222:ASP:HB3	1:B:1257:ARG:CZ	2.11	0.80
1:A:368:ALA:N	1:A:371:ASP:HB3	1.96	0.80
1:B:14:PRO:HG2	1:B:329:MET:HG3	1.64	0.79
1:A:416:GLN:O	1:A:420:LEU:HB2	1.82	0.79
1:A:215:PHE:CD2	1:A:305:LEU:HD11	2.18	0.79
1:B:1285:ALA:HB1	1:B:1289:LEU:HG	1.64	0.79
1:B:1303:ASN:N	1:B:1304:PRO:HD3	1.96	0.79
1:B:416:GLN:O	1:B:420:LEU:HB2	1.81	0.79
1:B:368:ALA:N	1:B:371:ASP:HB3	1.98	0.79
1:A:1735:HIS:CD2	1:A:1735:HIS:H	2.00	0.79
1:B:1545:ARG:HD2	1:B:1876:LEU:HD11	1.63	0.79
1:A:642:CYS:HB2	1:A:650:THR:CB	2.12	0.78
1:B:1245:VAL:HG13	1:B:1273:THR:HB	1.64	0.78
1:A:1003:TYR:CZ	1:A:1037:HIS:CE1	2.70	0.78
1:B:333:GLU:HB2	1:B:334:PRO:CD	2.12	0.78
1:A:118:GLU:HG3	1:B:118:GLU:CG	2.14	0.78
1:A:1034:ALA:HA	1:A:1037:HIS:CD2	2.19	0.78
1:A:856:CYS:SG	1:B:856:CYS:HB2	2.23	0.78
1:A:14:PRO:HG2	1:A:329:MET:HG3	1.64	0.78
1:A:1466:GLY:HA2	1:A:1469:ILE:HG13	1.65	0.78
1:B:1034:ALA:HA	1:B:1037:HIS:CD2	2.19	0.78
1:A:118:GLU:CG	1:B:118:GLU:HG3	2.13	0.78
1:B:1888:VAL:HG22	1:B:1913:VAL:HB	1.66	0.77
1:B:1407:GLN:CG	1:B:1409:PRO:HD2	2.14	0.77
1:A:1732:VAL:O	1:A:1736:THR:HB	1.82	0.77
1:A:903:LEU:HD22	1:A:905:GLN:NE2	1.99	0.77
1:B:1338:LEU:HD21	1:B:1341:GLY:HA2	1.64	0.77
1:A:1003:TYR:CE2	1:A:1037:HIS:HE1	2.02	0.77
1:A:1736:THR:CG2	1:A:1740:GLY:H	1.98	0.77
1:B:1641:THR:HG23	1:B:1644:GLU:OE1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1736:THR:CG2	1:B:1740:GLY:H	1.98	0.76
1:A:1890:THR:HA	1:A:1915:THR:HB	1.66	0.76
1:B:1538:ARG:HH22	1:B:1585:PRO:HG2	1.50	0.76
1:B:254:ASP:HB3	1:B:257:LYS:HE2	1.67	0.76
1:B:297:THR:HB	1:B:300:GLY:H	1.51	0.76
1:A:627:TRP:HB2	1:A:643:HIS:CD2	2.21	0.76
1:B:1407:GLN:HG3	1:B:1409:PRO:HD2	1.66	0.76
1:B:1259:PRO:HB2	1:B:1292:LEU:HD22	1.68	0.76
1:B:1890:THR:HA	1:B:1915:THR:HB	1.66	0.76
1:B:1735:HIS:CD2	1:B:1735:HIS:H	2.02	0.76
1:B:642:CYS:HB2	1:B:650:THR:HB	1.66	0.76
1:A:278:ALA:CB	1:A:279:PRO:HD3	2.16	0.76
1:B:278:ALA:CB	1:B:279:PRO:HD3	2.16	0.76
1:B:903:LEU:HD22	1:B:905:GLN:NE2	2.01	0.76
1:B:1003:TYR:CE2	1:B:1037:HIS:HE1	2.03	0.76
1:B:1289:LEU:HD22	1:B:1294:VAL:HB	1.69	0.75
1:B:506:MET:HE3	1:B:559:ILE:HD12	1.68	0.75
1:A:502:GLN:HG3	1:A:556:LEU:HD11	1.67	0.75
1:B:1674:HIS:CD2	1:B:1698:THR:HG21	2.22	0.75
1:B:1541:LEU:HD22	1:B:1544:ILE:HD11	1.68	0.75
1:B:1477:LEU:HD11	1:B:2043:ARG:HD2	1.68	0.75
1:A:200:PHE:HB3	1:A:206:LEU:HG	1.67	0.75
1:B:1533:VAL:CG1	1:B:1622:LEU:HB3	2.17	0.75
1:A:297:THR:HB	1:A:300:GLY:H	1.52	0.75
1:A:217:ALA:HB2	1:A:364:PRO:HD3	1.69	0.74
1:A:1222:ASP:HB3	1:A:1257:ARG:NH1	2.03	0.74
1:B:1618:PRO:HD3	1:B:1629:LEU:HD11	1.68	0.74
1:A:938:LEU:HB3	1:B:945:GLU:OE1	1.86	0.74
1:A:1130:LEU:HD11	1:A:1221:LEU:HD13	1.69	0.74
1:B:1418:VAL:HG13	1:B:1425:TRP:CE2	2.22	0.74
1:A:36:ASP:HB3	1:A:38:ARG:HG3	1.69	0.74
1:A:1387:LEU:HD22	1:A:1404:CYS:HB3	1.70	0.73
1:A:1736:THR:HG23	1:A:1739:LYS:N	2.01	0.73
1:B:622:ALA:HA	1:B:650:THR:HA	1.69	0.73
1:B:1227:LYS:HB2	1:B:1261:LEU:HD22	1.69	0.73
1:A:581:SER:HB2	1:A:683:HIS:NE2	2.03	0.73
1:A:1445:ALA:O	1:A:1476:ASN:ND2	2.20	0.73
1:A:1818:ILE:HA	1:A:1823:VAL:HG13	1.68	0.73
1:B:44:LEU:HG	1:B:45:TYR:CE1	2.24	0.73
1:A:1227:LYS:HB2	1:A:1261:LEU:HD22	1.71	0.73
1:B:1694:ARG:HH11	1:B:1694:ARG:CG	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1612:ARG:O	1:A:1636:VAL:HG12	1.89	0.73
1:B:1533:VAL:HG12	1:B:1622:LEU:HB3	1.70	0.73
1:A:1953:ARG:HG2	1:A:2005:VAL:HG13	1.70	0.73
1:B:682:PHE:HB3	1:B:683:HIS:CD2	2.24	0.73
1:B:1338:LEU:HD13	1:B:1406:GLN:NE2	2.03	0.73
1:B:1818:ILE:HA	1:B:1823:VAL:HG13	1.71	0.73
1:A:333:GLU:CB	1:A:334:PRO:HD3	2.17	0.72
1:B:1439:ARG:HB3	1:B:1440:PRO:HD3	1.71	0.72
1:B:1327:PRO:O	1:B:1381:LEU:HD21	1.90	0.72
1:A:1859:GLU:HG2	1:A:1860:GLU:N	2.04	0.72
1:B:123:ASP:O	1:B:127:LEU:HB3	1.89	0.72
1:B:1345:LEU:HD12	1:B:1402:PHE:O	1.89	0.72
1:A:1678:GLY:O	1:A:1682:GLN:HG3	1.89	0.72
1:A:1824:GLN:HG3	1:A:1825:PRO:HD2	1.70	0.72
1:A:82:LEU:HD22	1:A:188:LEU:HD11	1.72	0.72
1:B:82:LEU:HD22	1:B:188:LEU:HD11	1.71	0.72
1:A:1234:LEU:HD22	1:A:1262:LEU:HD22	1.72	0.72
1:B:265:SER:O	1:B:269:GLN:HG3	1.90	0.72
1:A:1299:TRP:HE1	1:A:1306:PRO:HD2	1.53	0.72
1:A:137:ARG:HD2	1:B:137:ARG:NH1	2.05	0.72
1:B:668:GLU:O	1:B:669:ASP:HB2	1.90	0.71
1:B:1408:THR:N	1:B:1409:PRO:HD3	2.05	0.71
1:B:1222:ASP:HB3	1:B:1257:ARG:NH1	2.04	0.71
1:B:1953:ARG:HG2	1:B:2005:VAL:HG13	1.70	0.71
1:A:633:ARG:NH2	1:A:668:GLU:OE1	2.23	0.71
1:A:1419:GLU:CD	1:A:1447:GLY:HA3	2.10	0.71
1:B:36:ASP:HB3	1:B:38:ARG:HG3	1.72	0.71
1:A:1418:VAL:HG13	1:A:1425:TRP:CE2	2.25	0.71
1:B:502:GLN:HG3	1:B:556:LEU:HD11	1.70	0.71
1:A:2105:VAL:O	1:A:2106:LEU:HD23	1.91	0.71
1:B:1926:ALA:O	1:B:1930:ARG:HB2	1.90	0.71
1:A:1472:VAL:HG12	1:A:1473:LEU:H	1.56	0.71
1:A:1569:THR:HG21	1:A:1622:LEU:HA	1.72	0.71
1:A:1576:VAL:HG21	1:A:1843:MET:HG2	1.71	0.71
1:A:1535:VAL:HG12	1:A:1537:SER:H	1.55	0.71
1:A:87:TYR:CE2	1:A:97:PRO:HG2	2.26	0.71
1:A:1888:VAL:HG22	1:A:1913:VAL:HB	1.70	0.70
1:B:627:TRP:HB2	1:B:643:HIS:CE1	2.27	0.70
1:A:44:LEU:HG	1:A:45:TYR:CE1	2.26	0.70
1:B:23:TRP:HA	1:B:26:LEU:HD12	1.73	0.70
1:B:1234:LEU:HD22	1:B:1262:LEU:HD22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:ASP:O	1:B:711:ARG:HG2	1.91	0.70
1:A:1669:GLU:O	1:A:1693:CYS:HB3	1.91	0.70
1:B:1670:SER:O	1:B:1742:ASP:HB2	1.91	0.70
1:A:944:PHE:HD2	1:A:959:VAL:HG22	1.55	0.70
1:B:136:GLN:HE21	1:B:136:GLN:C	1.95	0.70
1:B:1254:LEU:HD21	1:B:1318:ASN:HB2	1.72	0.70
1:B:1477:LEU:CD1	1:B:2043:ARG:HD2	2.21	0.70
1:A:1887:TYR:HD2	1:A:1967:GLY:HA3	1.57	0.70
1:B:1975:LEU:HD22	1:B:1977:ASP:OD2	1.91	0.70
1:A:254:ASP:HB3	1:A:257:LYS:HE2	1.72	0.70
1:A:1991:VAL:O	1:A:1994:PRO:HD2	1.91	0.70
1:B:641:ALA:HB1	1:B:683:HIS:HB2	1.74	0.70
1:A:77:PRO:O	1:A:81:MET:HG2	1.91	0.69
1:B:944:PHE:HD2	1:B:959:VAL:HG22	1.55	0.69
1:B:1335:ALA:HA	1:B:1406:GLN:NE2	2.07	0.69
1:A:1735:HIS:HD2	1:A:1735:HIS:H	1.40	0.69
1:B:1671:VAL:HG23	1:B:1743:LEU:HB2	1.73	0.69
1:B:1338:LEU:CD1	1:B:1406:GLN:HE21	2.05	0.69
1:B:1651:VAL:CG1	1:B:1680:VAL:HA	2.19	0.69
1:B:87:TYR:O	1:B:91:VAL:HG22	1.92	0.69
1:A:610:ILE:HG12	1:A:690:ILE:HG21	1.74	0.69
1:A:917:VAL:HG13	1:A:1054:PHE:HB2	1.74	0.69
1:B:1887:TYR:HD2	1:B:1967:GLY:HA3	1.56	0.69
1:B:1736:THR:HG23	1:B:1739:LYS:N	2.07	0.69
1:A:2015:TYR:CD2	1:A:2099:LEU:HD22	2.28	0.69
1:B:1288:LYS:O	1:B:1291:GLN:HG2	1.92	0.69
1:B:1382:PHE:HB3	1:B:1387:LEU:HB2	1.73	0.69
1:A:136:GLN:C	1:A:136:GLN:HE21	1.96	0.69
1:B:87:TYR:CE2	1:B:97:PRO:HG2	2.28	0.68
1:A:504:GLN:HA	1:A:541:THR:HG21	1.75	0.68
1:B:1653:THR:HG22	1:B:1810:VAL:HG12	1.73	0.68
1:B:1303:ASN:O	1:B:1333:ASN:HB2	1.93	0.68
1:A:111:VAL:CG2	1:A:188:LEU:HB2	2.23	0.68
1:A:1477:LEU:CD1	1:A:2043:ARG:HD2	2.22	0.68
1:B:627:TRP:HB2	1:B:643:HIS:ND1	2.08	0.68
1:B:917:VAL:HG13	1:B:1054:PHE:HB2	1.75	0.68
1:A:252:ASN:ND2	1:A:272:LEU:HB2	2.07	0.68
1:A:23:TRP:HA	1:A:26:LEU:HD12	1.75	0.68
1:A:2070:LEU:HD21	1:A:2076:ASN:N	2.08	0.68
1:A:1348:THR:HG21	1:A:1378:TRP:CZ2	2.29	0.68
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:MET:HE3	1:A:559:ILE:HD12	1.74	0.68
1:A:1126:GLU:HB3	1:A:1129:CYS:SG	2.34	0.68
1:A:1254:LEU:HD13	1:A:1316:VAL:HG12	1.75	0.68
1:A:1489:SER:H	1:A:1493:LEU:HD22	1.58	0.68
1:B:1460:LEU:HD13	1:B:2032:ALA:CB	2.23	0.68
1:B:1227:LYS:HE3	1:B:1231:ASP:OD2	1.94	0.68
1:A:1606:ARG:HH21	1:A:1860:GLU:HG3	1.59	0.68
1:A:1416:LEU:HD21	1:A:1425:TRP:HB2	1.76	0.67
1:B:1576:VAL:HG21	1:B:1843:MET:HG2	1.76	0.67
1:B:1477:LEU:O	1:B:1507:ARG:HG2	1.94	0.67
1:B:1035:MET:HE3	1:B:1089:VAL:HG12	1.77	0.67
1:A:1735:HIS:N	1:A:1735:HIS:CD2	2.61	0.67
1:B:1139:GLU:CD	1:B:1218:SER:HB2	2.14	0.67
1:A:1651:VAL:HG12	1:A:1680:VAL:HA	1.77	0.67
1:B:2015:TYR:CD2	1:B:2099:LEU:HD22	2.30	0.67
1:B:635:PRO:HD2	1:B:638:ILE:HB	1.77	0.67
1:B:111:VAL:CG2	1:B:188:LEU:HB2	2.25	0.67
1:B:1814:LEU:O	1:B:1818:ILE:HG13	1.94	0.67
1:A:460:VAL:HG21	1:A:465:MET:HG3	1.76	0.67
1:B:1430:LYS:HE3	1:B:1981:GLU:HA	1.75	0.67
1:B:1341:GLY:HA3	1:B:1407:GLN:HA	1.76	0.67
1:A:614:ASN:O	1:A:615:VAL:O	2.13	0.67
1:B:1954:SER:O	1:B:1958:GLU:HG3	1.95	0.67
1:B:1279:PRO:HG3	1:B:1298:GLN:NE2	2.10	0.67
1:B:288:GLU:OE1	1:B:383:ILE:HG13	1.95	0.67
1:B:643:HIS:CD2	1:B:746:GLN:HB3	2.30	0.67
1:B:1735:HIS:N	1:B:1735:HIS:CD2	2.62	0.67
1:B:1666:GLN:O	1:B:1669:GLU:HB2	1.95	0.67
1:A:277:TYR:CE2	1:A:287:LEU:HD11	2.30	0.67
1:A:1226:LEU:HD23	1:A:1401:LEU:HD21	1.77	0.67
1:A:581:SER:HB2	1:A:683:HIS:CE1	2.30	0.67
1:B:1126:GLU:HB3	1:B:1129:CYS:SG	2.35	0.67
1:B:1433:LEU:HD21	1:B:1465:GLY:HA3	1.77	0.67
1:B:1991:VAL:O	1:B:1994:PRO:HD2	1.95	0.67
1:B:1824:GLN:HG3	1:B:1825:PRO:HD2	1.76	0.67
1:B:1538:ARG:HH22	1:B:1585:PRO:CG	2.08	0.66
1:A:1285:ALA:O	1:A:1289:LEU:N	2.27	0.66
1:A:1618:PRO:HD3	1:A:1629:LEU:HD11	1.77	0.66
1:A:1814:LEU:O	1:A:1818:ILE:HG13	1.95	0.66
1:A:2098:PHE:CE2	1:A:2106:LEU:HB2	2.30	0.66
1:B:252:ASN:ND2	1:B:272:LEU:HB2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:ALA:O	1:B:1037:HIS:HB2	1.95	0.66
1:A:976:VAL:O	1:A:978:PRO:HD3	1.94	0.66
1:A:265:SER:O	1:A:269:GLN:HG3	1.95	0.66
1:B:98:ALA:HA	1:B:101:ARG:HG3	1.78	0.66
1:B:1671:VAL:CG2	1:B:1743:LEU:HB2	2.25	0.66
1:A:1564:CYS:CB	1:A:1628:LEU:HD21	2.25	0.66
1:B:1694:ARG:NH1	1:B:1694:ARG:HG3	1.95	0.66
1:A:1644:GLU:HB3	1:A:1825:PRO:CB	2.24	0.66
1:A:503:TRP:CD1	1:A:787:LYS:HB2	2.31	0.66
1:B:1395:SER:HB3	1:B:1399:SER:O	1.95	0.66
1:B:1673:ILE:O	1:B:1697:THR:HA	1.95	0.66
1:A:1470:ARG:O	1:A:1472:VAL:HG23	1.96	0.66
1:B:680:ILE:HG12	1:B:681:ALA:N	2.11	0.66
1:B:620:MET:SD	1:B:682:PHE:HB2	2.35	0.66
1:A:1411:ASP:HB2	1:A:1440:PRO:HD3	1.76	0.66
1:B:1244:VAL:HB	1:B:1272:TYR:HD1	1.61	0.66
1:B:1244:VAL:HG13	1:B:1314:LEU:HD23	1.77	0.66
1:A:1857:ARG:HH11	1:A:1869:PRO:HB3	1.61	0.66
1:B:123:ASP:CB	1:B:126:THR:HB	2.25	0.66
1:A:254:ASP:CB	1:A:257:LYS:HE2	2.26	0.66
1:A:1252:GLY:HA3	1:A:1318:ASN:HB3	1.77	0.66
1:A:168:LEU:HB2	1:A:185:VAL:HG11	1.77	0.66
1:A:87:TYR:O	1:A:91:VAL:HG22	1.96	0.65
1:B:59:ARG:HG3	1:B:838:HIS:HB3	1.78	0.65
1:B:982:THR:C	1:B:984:GLU:H	2.00	0.65
1:A:1974:VAL:HG22	1:A:1994:PRO:HG2	1.77	0.65
1:A:1653:THR:HG22	1:A:1796:LEU:HD21	1.78	0.65
1:B:2003:ASP:O	1:B:2007:ARG:HG3	1.95	0.65
1:B:1095:LEU:C	1:B:1095:LEU:HD12	2.17	0.65
1:B:496:CYS:O	1:B:583:GLY:HA3	1.96	0.65
1:B:645:SER:HB3	1:B:770:VAL:HG13	1.77	0.65
1:A:2003:ASP:O	1:A:2007:ARG:HG3	1.96	0.65
1:B:1247:VAL:HG11	1:B:1301:PRO:HG3	1.76	0.65
1:A:1035:MET:HE3	1:A:1089:VAL:HG12	1.78	0.65
1:A:1439:ARG:HB3	1:A:1440:PRO:HD3	1.79	0.65
1:A:502:GLN:HB2	1:A:546:LEU:HD22	1.78	0.65
1:A:1268:MET:HA	1:A:1268:MET:HE2	1.79	0.65
1:B:2070:LEU:HD21	1:B:2076:ASN:N	2.11	0.65
1:B:1486:MET:O	1:B:1488:PRO:HD3	1.97	0.65
1:B:1282:LEU:HD21	1:B:1296:GLN:HB2	1.78	0.65
1:A:1244:VAL:HG13	1:A:1314:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:THR:HG21	1:A:1032:LEU:HB2	1.78	0.65
1:B:1220:LEU:HB3	1:B:1257:ARG:HH22	1.61	0.65
1:B:1279:PRO:HG3	1:B:1298:GLN:HE22	1.61	0.65
1:A:399:ASN:H	1:A:399:ASN:HD22	1.43	0.65
1:B:1528:THR:HG22	1:B:1530:HIS:H	1.61	0.65
1:B:1736:THR:HG23	1:B:1740:GLY:H	1.61	0.65
1:B:1569:THR:HG21	1:B:1622:LEU:HA	1.79	0.65
1:A:1628:LEU:HD13	1:A:1633:THR:HG21	1.79	0.65
1:B:615:VAL:HG22	1:B:686:PHE:HD2	1.63	0.64
1:B:2105:VAL:O	1:B:2106:LEU:HD23	1.97	0.64
1:A:2102:PRO:HD2	1:A:2103:HIS:HD2	1.63	0.64
1:B:1532:PHE:HD2	1:B:1549:SER:HA	1.61	0.64
1:A:1838:ALA:HA	1:A:1841:ARG:HG3	1.77	0.64
1:B:1408:THR:N	1:B:1409:PRO:CD	2.61	0.64
1:B:64:PHE:HB2	1:B:429:ARG:NH2	2.11	0.64
1:A:302:PRO:HA	1:A:366:ILE:HG21	1.79	0.64
1:A:44:LEU:HG	1:A:45:TYR:CD1	2.32	0.64
1:B:1433:LEU:HD11	1:B:1465:GLY:O	1.97	0.64
1:B:1466:GLY:HA2	1:B:1469:ILE:HG13	1.77	0.64
1:A:325:THR:OG1	1:A:343:LYS:HG2	1.97	0.64
1:A:1395:SER:HB3	1:A:1399:SER:O	1.97	0.64
1:B:217:ALA:HB2	1:B:364:PRO:HD3	1.79	0.64
1:A:1001:TYR:HB3	1:A:1003:TYR:CE1	2.32	0.64
1:B:1472:VAL:HG12	1:B:1473:LEU:H	1.62	0.64
1:A:1227:LYS:HE3	1:A:1231:ASP:OD2	1.98	0.64
1:B:660:GLU:HG2	1:B:663:GLN:NE2	2.12	0.64
1:B:736:VAL:O	1:B:740:VAL:HG23	1.98	0.64
1:B:64:PHE:CE2	1:B:464:ALA:HB1	2.32	0.64
1:B:2102:PRO:HD2	1:B:2103:HIS:HD2	1.62	0.64
1:A:1594:THR:OG1	1:A:1596:ASP:HB2	1.98	0.64
1:A:1532:PHE:CE1	1:A:1597:CYS:HB3	2.32	0.64
1:B:1348:THR:HG22	1:B:1349:LEU:N	2.06	0.64
1:A:1220:LEU:HB3	1:A:1257:ARG:HH22	1.63	0.64
1:B:1449:SER:O	1:B:1477:LEU:HD22	1.98	0.64
1:A:1859:GLU:HG2	1:A:1860:GLU:H	1.59	0.64
1:A:2002:LEU:O	1:A:2006:THR:HB	1.97	0.64
1:B:168:LEU:HB2	1:B:185:VAL:HG11	1.78	0.64
1:A:59:ARG:HG3	1:A:838:HIS:HB3	1.79	0.64
1:A:137:ARG:NH1	1:B:137:ARG:HD2	2.12	0.64
1:B:1285:ALA:O	1:B:1289:LEU:N	2.29	0.64
1:B:127:LEU:HG	1:B:127:LEU:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:LEU:HB3	1:B:810:VAL:HB	1.78	0.64
1:B:302:PRO:HA	1:B:366:ILE:HG21	1.80	0.64
1:A:1564:CYS:SG	1:A:1628:LEU:HD21	2.38	0.64
1:B:2002:LEU:O	1:B:2006:THR:HB	1.97	0.64
1:B:319:PRO:HB2	1:B:320:LEU:HD23	1.79	0.64
1:B:2098:PHE:CE2	1:B:2106:LEU:HB2	2.33	0.64
1:A:132:MET:HE1	1:B:200:PHE:CE2	2.33	0.64
1:B:1836:VAL:HG13	1:B:1854:ILE:CD1	2.28	0.63
1:A:1411:ASP:O	1:A:1413:PRO:HD3	1.98	0.63
1:B:1991:VAL:HG21	1:B:2033:ASN:ND2	2.13	0.63
1:A:1926:ALA:O	1:A:1930:ARG:HB2	1.98	0.63
1:A:1442:TRP:CZ2	1:A:1497:LEU:HD23	2.32	0.63
1:A:112:SER:HB3	1:A:334:PRO:HG3	1.79	0.63
1:B:44:LEU:HG	1:B:45:TYR:CD1	2.33	0.63
1:A:984:GLU:O	1:A:985:PHE:HB2	1.96	0.63
1:A:736:VAL:O	1:A:740:VAL:HG23	1.99	0.63
1:A:1746:ASN:HD21	1:A:1753:LEU:HD12	1.62	0.63
1:B:1303:ASN:N	1:B:1304:PRO:CD	2.61	0.63
1:B:351:GLY:C	1:B:383:ILE:HG22	2.19	0.63
1:B:159:THR:HB	1:B:162:SER:OG	1.99	0.63
1:B:1735:HIS:HD2	1:B:1735:HIS:H	1.43	0.63
1:B:1475:SER:HB3	1:B:1505:VAL:HG13	1.81	0.63
1:B:9:MET:HE3	1:B:345:LEU:HD12	1.80	0.63
1:A:501:ALA:HB3	1:A:556:LEU:HD21	1.80	0.63
1:B:1139:GLU:OE2	1:B:1218:SER:HB2	1.99	0.63
1:A:1954:SER:O	1:A:1958:GLU:HG3	1.97	0.63
1:A:1472:VAL:HG12	1:A:1473:LEU:N	2.13	0.63
1:B:1460:LEU:HD13	1:B:2032:ALA:HB2	1.81	0.63
1:B:254:ASP:CB	1:B:257:LYS:HE2	2.28	0.63
1:B:853:GLY:O	1:B:854:SER:HB3	1.97	0.63
1:B:1268:MET:HA	1:B:1268:MET:HE2	1.79	0.62
1:B:460:VAL:HG21	1:B:465:MET:HG3	1.79	0.62
1:A:1486:MET:HE1	1:A:1506:TYR:HB3	1.81	0.62
1:A:1616:MET:HB3	1:A:1800:PHE:CZ	2.33	0.62
1:A:1302:ALA:O	1:A:1303:ASN:HB2	1.97	0.62
1:B:2006:THR:HG21	1:B:2048:ARG:HH22	1.62	0.62
1:A:1545:ARG:HG3	1:A:1545:ARG:NH1	2.12	0.62
1:B:251:THR:HB	1:B:399:ASN:O	2.00	0.62
1:A:641:ALA:HB1	1:A:683:HIS:HB2	1.81	0.62
1:A:399:ASN:N	1:A:399:ASN:ND2	2.46	0.62
1:B:1433:LEU:HD13	1:B:1469:ILE:HD11	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1857:ARG:NH1	1:B:1871:ILE:HD11	2.15	0.62
1:B:643:HIS:HD2	1:B:746:GLN:HB3	1.65	0.62
1:A:581:SER:O	1:A:583:GLY:N	2.33	0.62
1:B:200:PHE:HB3	1:B:206:LEU:HG	1.81	0.62
1:B:325:THR:OG1	1:B:343:LYS:HG2	1.99	0.62
1:B:1857:ARG:CZ	1:B:1871:ILE:HD11	2.30	0.62
1:A:1484:PRO:O	1:A:1485:GLU:HB2	2.00	0.62
1:B:399:ASN:HD22	1:B:399:ASN:H	1.47	0.62
1:B:1917:ARG:HH12	1:B:1974:VAL:HG12	1.63	0.62
1:A:1762:GLN:HG2	1:A:1787:LYS:O	1.99	0.62
1:B:77:PRO:O	1:B:81:MET:HG2	1.99	0.62
1:A:1734:ARG:O	1:A:1736:THR:N	2.32	0.62
1:A:319:PRO:HB2	1:A:320:LEU:HD23	1.82	0.62
1:A:542:ASP:O	1:A:545:VAL:HG12	1.99	0.62
1:B:752:VAL:HG11	1:B:775:LEU:HD21	1.81	0.62
1:A:159:THR:HB	1:A:162:SER:OG	1.99	0.62
1:A:542:ASP:H	1:A:545:VAL:HG12	1.63	0.62
1:B:9:MET:HE1	1:B:345:LEU:HB2	1.82	0.62
1:A:1009:LEU:HD13	1:A:1023:GLN:O	2.00	0.62
1:A:1429:LEU:HD11	1:A:1443:LEU:HD11	1.80	0.62
1:B:1454:VAL:HG13	1:B:1503:MET:HE1	1.80	0.62
1:A:251:THR:HB	1:A:399:ASN:O	2.00	0.62
1:B:570:LEU:HD13	1:B:800:VAL:HG13	1.82	0.62
1:A:1836:VAL:HG13	1:A:1854:ILE:CD1	2.29	0.62
1:B:420:LEU:HD11	1:B:512:ARG:HB3	1.82	0.62
1:B:972:THR:HG22	1:B:1081:VAL:CG2	2.29	0.62
1:B:1335:ALA:CA	1:B:1406:GLN:HE22	2.09	0.62
1:B:1001:TYR:HB3	1:B:1003:TYR:CE1	2.35	0.62
1:B:1139:GLU:OE2	1:B:1216:LEU:HD12	1.99	0.62
1:A:353:TRP:NE1	1:A:383:ILE:HB	2.14	0.62
1:A:817:PRO:O	1:A:818:PRO:O	2.18	0.62
1:A:874:TYR:HB2	1:A:1006:PHE:CD2	2.34	0.62
1:A:23:TRP:CE2	1:A:350:HIS:CD2	2.88	0.61
1:B:112:SER:HB3	1:B:334:PRO:HG3	1.82	0.61
1:A:976:VAL:HG13	1:A:977:ASP:N	2.14	0.61
1:A:123:ASP:HB3	1:A:126:THR:CB	2.28	0.61
1:A:808:VAL:HG12	1:A:809:SER:N	2.15	0.61
1:B:1580:THR:HG22	1:B:1581:GLY:N	2.14	0.61
1:A:317:ARG:O	1:A:319:PRO:HD3	1.99	0.61
1:A:1095:LEU:HD12	1:A:1095:LEU:C	2.20	0.61
1:A:1420:ASP:O	1:A:1425:TRP:CH2	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:HIS:CE1	1:B:333:GLU:HA	2.35	0.61
1:B:277:TYR:CE2	1:B:287:LEU:HD11	2.34	0.61
1:B:103:THR:HG22	1:B:104:SER:N	2.15	0.61
1:A:384:ARG:HH11	1:A:384:ARG:CG	2.13	0.61
1:B:1974:VAL:HG22	1:B:1994:PRO:HG2	1.81	0.61
1:A:1765:ARG:HG3	1:A:1790:THR:HG23	1.83	0.61
1:A:1124:HIS:CD2	1:A:1512:GLY:HA2	2.35	0.61
1:B:1768:GLU:HA	1:B:1768:GLU:OE1	2.00	0.61
1:A:1454:VAL:HG13	1:A:1503:MET:HE1	1.82	0.61
1:A:331:HIS:CE1	1:A:333:GLU:HA	2.35	0.61
1:B:889:THR:HG21	1:B:1032:LEU:HB2	1.80	0.61
1:B:347:SER:HB2	1:B:352:VAL:O	2.00	0.61
1:A:368:ALA:CA	1:A:371:ASP:HB3	2.31	0.61
1:A:1466:GLY:HA2	1:A:1469:ILE:CG1	2.29	0.61
1:B:1838:ALA:HA	1:B:1841:ARG:HG3	1.80	0.61
1:B:248:ASN:ND2	1:B:249:ALA:H	1.98	0.61
1:B:1647:SER:HA	1:B:1851:LYS:HG3	1.81	0.61
1:B:416:GLN:HG3	1:B:422:ARG:HH21	1.65	0.61
1:B:322:ILE:CD1	1:B:374:LEU:HD13	2.31	0.61
1:B:1703:GLU:O	1:B:1706:ALA:HB3	2.01	0.61
1:A:2078:THR:O	1:A:2079:VAL:HG13	2.01	0.61
1:B:89:ALA:O	1:B:92:ASP:HB3	2.01	0.61
1:A:416:GLN:HG3	1:A:422:ARG:HH21	1.64	0.61
1:A:366:ILE:O	1:A:366:ILE:HG12	2.00	0.61
1:B:1841:ARG:O	1:B:1844:ALA:HB3	2.00	0.61
1:B:1455:GLY:HA3	1:B:2039:SER:HB2	1.82	0.61
1:A:64:PHE:CE2	1:A:464:ALA:HB1	2.36	0.61
1:A:913:VAL:HG23	1:A:962:TRP:HB2	1.83	0.61
1:B:1442:TRP:CZ2	1:B:1497:LEU:HD23	2.36	0.60
1:A:98:ALA:HA	1:A:101:ARG:HG3	1.82	0.60
1:A:1343:PHE:O	1:A:1344:LEU:HD22	2.01	0.60
1:A:1746:ASN:ND2	1:A:1753:LEU:HD12	2.16	0.60
1:B:1408:THR:H	1:B:1409:PRO:HD3	1.65	0.60
1:B:981:SER:HA	1:B:984:GLU:HG3	1.82	0.60
1:A:1248:LEU:HD21	1:A:1277:ARG:HE	1.66	0.60
1:B:403:ILE:O	1:B:404:LEU:HD23	2.00	0.60
1:B:1299:TRP:CZ2	1:B:1304:PRO:O	2.54	0.60
1:A:1656:TYR:CD2	1:A:1687:ILE:HD13	2.35	0.60
1:B:1035:MET:SD	1:B:1091:ALA:HB3	2.42	0.60
1:B:327:SER:OG	1:B:356:ASN:ND2	2.34	0.60
1:B:123:ASP:HB3	1:B:126:THR:HB	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1439:ARG:O	1:A:1470:ARG:HB3	2.01	0.60
1:B:501:ALA:HB3	1:B:556:LEU:HD21	1.83	0.60
1:A:2006:THR:HG21	1:A:2048:ARG:HH22	1.66	0.60
1:B:215:PHE:CD2	1:B:305:LEU:HD11	2.37	0.60
1:A:247:LEU:HD11	1:A:405:GLN:HB2	1.82	0.60
1:B:1429:LEU:HD11	1:B:1443:LEU:HD11	1.82	0.60
1:B:1652:TYR:CD1	1:B:1823:VAL:HB	2.37	0.60
1:A:45:TYR:HE2	1:B:124:PRO:HB2	1.66	0.60
1:A:665:LEU:HD22	1:A:670:VAL:HB	1.83	0.60
1:B:1073:ASP:O	1:B:1074:THR:HG22	2.02	0.60
1:B:112:SER:HB2	1:B:334:PRO:CG	2.32	0.60
1:A:368:ALA:HA	1:A:371:ASP:HB3	1.82	0.60
1:A:1575:ASP:HA	1:A:1599:LEU:HD23	1.83	0.60
1:B:1119:PHE:CE1	1:B:1516:HIS:CE1	2.89	0.60
1:B:359:TYR:OH	1:B:362:PRO:HG3	2.02	0.60
1:B:1580:THR:HG22	1:B:1582:LYS:N	2.16	0.60
1:A:143:ARG:HG2	1:A:143:ARG:HH11	1.67	0.60
1:B:2078:THR:O	1:B:2079:VAL:HG13	2.01	0.60
1:A:1279:PRO:HG3	1:A:1298:GLN:NE2	2.16	0.60
1:B:468:ARG:HD3	1:B:485:VAL:HG21	1.83	0.60
1:B:1672:LEU:HD12	1:B:1696:PHE:O	2.02	0.60
1:A:586:ALA:O	1:A:589:TYR:HB3	2.02	0.60
1:B:654:PRO:O	1:B:658:MET:HB2	2.01	0.60
1:A:1549:SER:O	1:A:1552:HIS:HB3	2.01	0.60
1:A:582:LEU:O	1:A:585:VAL:HG23	2.01	0.60
1:B:343:LYS:HE3	1:B:354:ALA:HB3	1.84	0.60
1:A:670:VAL:HG12	1:A:671:PHE:N	2.16	0.60
1:B:1657:TYR:HA	1:B:1661:VAL:CG2	2.32	0.60
1:A:883:ARG:HH21	1:A:1107:ARG:HD3	1.67	0.60
1:A:1038:MET:HA	1:A:1038:MET:CE	2.32	0.60
1:A:595:THR:HB	1:A:598:GLU:H	1.66	0.60
1:A:36:ASP:CB	1:A:38:ARG:HG3	2.32	0.60
1:A:1086:LEU:N	1:A:1086:LEU:HD23	2.17	0.60
1:B:1396:PHE:CE2	1:B:1397:TYR:HD2	2.20	0.60
1:B:14:PRO:HD3	1:B:226:GLU:O	2.02	0.59
1:B:646:LYS:HG2	1:B:746:GLN:HE21	1.67	0.59
1:B:1466:GLY:HA2	1:B:1469:ILE:CG1	2.32	0.59
1:B:1625:SER:O	1:B:1626:VAL:HG23	2.02	0.59
1:A:1580:THR:HG22	1:A:1582:LYS:N	2.17	0.59
1:B:384:ARG:HH11	1:B:384:ARG:CG	2.12	0.59
1:B:1035:MET:HE3	1:B:1089:VAL:CG1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:SER:OG	1:A:356:ASN:ND2	2.35	0.59
1:B:1662:ARG:NH1	1:B:1662:ARG:CG	2.49	0.59
1:A:166:LEU:HD12	1:A:251:THR:HG21	1.83	0.59
1:B:662:LEU:HD22	1:B:672:VAL:CG1	2.29	0.59
1:A:1857:ARG:NH1	1:A:1869:PRO:CB	2.66	0.59
1:B:1657:TYR:HA	1:B:1661:VAL:HG23	1.84	0.59
1:A:1475:SER:O	1:A:1486:MET:HE1	2.01	0.59
1:A:1703:GLU:O	1:A:1706:ALA:HB3	2.02	0.59
1:B:1765:ARG:HG3	1:B:1790:THR:HG23	1.85	0.59
1:B:1097:LEU:HD12	1:B:1098:GLY:N	2.17	0.59
1:B:630:CYS:HB3	1:B:640:PRO:HG3	1.85	0.59
1:B:366:ILE:HG12	1:B:366:ILE:O	2.02	0.59
1:B:322:ILE:HD12	1:B:374:LEU:HD13	1.85	0.59
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.68	0.59
1:A:1774:LEU:HD22	1:B:1785:PHE:HB2	1.85	0.59
1:A:1736:THR:HG23	1:A:1740:GLY:H	1.66	0.59
1:B:1662:ARG:HG2	1:B:1662:ARG:HH11	1.67	0.59
1:A:9:MET:HE3	1:A:345:LEU:HD12	1.85	0.59
1:B:1003:TYR:CE1	1:B:1037:HIS:CE1	2.90	0.59
1:A:1034:ALA:O	1:A:1037:HIS:HB2	2.02	0.59
1:A:615:VAL:HG22	1:A:616:LEU:H	1.68	0.59
1:B:317:ARG:O	1:B:319:PRO:HD3	2.02	0.59
1:B:399:ASN:ND2	1:B:399:ASN:N	2.51	0.59
1:B:2101:GLN:HG3	1:B:2102:PRO:CD	2.33	0.59
1:B:288:GLU:HG3	1:B:385:GLY:O	2.02	0.59
1:A:1397:TYR:CE1	1:A:1399:SER:HB2	2.37	0.59
1:B:1454:VAL:HG13	1:B:1503:MET:CE	2.33	0.59
1:B:646:LYS:HG2	1:B:746:GLN:NE2	2.18	0.59
1:A:1118:LYS:HD2	1:A:2103:HIS:CE1	2.38	0.59
1:A:200:PHE:CE2	1:B:132:MET:HE1	2.38	0.59
1:A:1785:PHE:HB2	1:B:1774:LEU:HD22	1.83	0.59
1:B:128:VAL:HG11	1:B:130:TYR:CZ	2.37	0.59
1:A:165:LEU:HB2	1:A:337:GLY:HA3	1.85	0.58
1:A:1580:THR:HG22	1:A:1581:GLY:N	2.17	0.58
1:B:13:LEU:HB3	1:B:14:PRO:HD2	1.84	0.58
1:A:1248:LEU:CD2	1:A:1277:ARG:HE	2.16	0.58
1:B:878:HIS:HB2	1:B:1007:PHE:CE1	2.38	0.58
1:B:1472:VAL:HG12	1:B:1473:LEU:N	2.17	0.58
1:B:165:LEU:HB2	1:B:337:GLY:HA3	1.85	0.58
1:B:1736:THR:O	1:B:1739:LYS:HB2	2.03	0.58
1:A:64:PHE:HB2	1:A:429:ARG:NH2	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1528:THR:HG22	1:A:1530:HIS:N	2.15	0.58
1:B:680:ILE:HG12	1:B:681:ALA:H	1.67	0.58
1:B:1539:GLY:HA2	1:B:1580:THR:O	2.02	0.58
1:A:1122:THR:HG1	1:A:1517:PHE:HE1	1.49	0.58
1:B:527:LEU:HD12	1:B:534:VAL:HG22	1.85	0.58
1:A:1073:ASP:O	1:A:1074:THR:HG22	2.03	0.58
1:B:68:HIS:HB3	1:B:71:GLN:HG3	1.85	0.58
1:B:1299:TRP:HE1	1:B:1306:PRO:HD2	1.68	0.58
1:B:1007:PHE:HE2	1:B:1030:SER:HA	1.67	0.58
1:B:612:GLU:HG2	1:B:612:GLU:O	2.04	0.58
1:B:1694:ARG:CG	1:B:1694:ARG:NH1	2.65	0.58
1:A:23:TRP:CE2	1:A:350:HIS:HD2	2.22	0.58
1:A:1991:VAL:HG21	1:A:2033:ASN:ND2	2.18	0.58
1:A:1236:ASN:HA	1:A:1502:VAL:HG21	1.86	0.58
1:A:466:PRO:HG2	1:A:467:PHE:HD1	1.68	0.58
1:B:1662:ARG:NH2	1:B:1793:GLY:O	2.36	0.58
1:B:297:THR:HB	1:B:300:GLY:N	2.19	0.58
1:B:1674:HIS:CD2	1:B:1698:THR:CG2	2.87	0.58
1:A:917:VAL:CG1	1:A:1054:PHE:HB2	2.34	0.58
1:B:1300:ASP:O	1:B:1302:ALA:N	2.36	0.58
1:A:155:ILE:HD11	1:B:166:LEU:HD11	1.85	0.58
1:A:1248:LEU:HD21	1:A:1277:ARG:HH21	1.69	0.58
1:A:595:THR:CG2	1:A:597:GLU:HG2	2.33	0.58
1:A:1122:THR:HG21	1:A:1517:PHE:HZ	1.68	0.58
1:B:1860:GLU:HB2	1:B:1865:PRO:HG2	1.84	0.58
1:B:386:GLY:O	1:B:387:ASN:HB2	2.03	0.58
1:A:321:LEU:HD23	1:A:381:LEU:HD13	1.86	0.58
1:B:1003:TYR:CE1	1:B:1037:HIS:HE1	2.21	0.58
1:B:23:TRP:CE2	1:B:350:HIS:CD2	2.92	0.58
1:A:1299:TRP:NE1	1:A:1306:PRO:HD2	2.19	0.58
1:A:1580:THR:HG22	1:A:1582:LYS:H	1.69	0.57
1:A:112:SER:HB2	1:A:334:PRO:CG	2.31	0.57
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.85	0.57
1:B:1241:LYS:O	1:B:1241:LYS:HG3	2.03	0.57
1:A:1068:LEU:HD12	1:A:1077:ALA:O	2.04	0.57
1:B:1277:ARG:HD3	1:B:1300:ASP:OD2	2.04	0.57
1:A:945:GLU:OE1	1:B:938:LEU:HB3	2.03	0.57
1:A:103:THR:HG22	1:A:104:SER:N	2.19	0.57
1:B:1456:MET:HG3	1:B:2036:PHE:HD1	1.70	0.57
1:B:889:THR:CG2	1:B:1032:LEU:HB2	2.34	0.57
1:A:1953:ARG:HG2	1:A:2005:VAL:CG1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1138:GLU:HG3	1:B:1138:GLU:O	2.03	0.57
1:B:1762:GLN:HG2	1:B:1787:LYS:O	2.05	0.57
1:A:333:GLU:CB	1:A:334:PRO:CD	2.79	0.57
1:A:1616:MET:HE2	1:A:1650:ILE:HD13	1.87	0.57
1:B:1953:ARG:HG2	1:B:2005:VAL:CG1	2.34	0.57
1:A:1917:ARG:HH12	1:A:1974:VAL:HG12	1.69	0.57
1:A:883:ARG:HE	1:A:1107:ARG:HD3	1.69	0.57
1:B:234:THR:HG21	1:B:239:ALA:HB2	1.84	0.57
1:A:1007:PHE:HE2	1:A:1030:SER:HA	1.70	0.57
1:A:476:GLU:HB2	1:A:790:ARG:HH12	1.68	0.57
1:A:1736:THR:O	1:A:1739:LYS:HB2	2.04	0.57
1:B:91:VAL:O	1:B:457:ILE:HD11	2.04	0.57
1:A:1647:SER:O	1:A:1651:VAL:HG21	2.04	0.57
1:B:1616:MET:HB3	1:B:1800:PHE:CZ	2.39	0.57
1:B:1097:LEU:HD12	1:B:1097:LEU:C	2.24	0.57
1:B:492:VAL:HG11	1:B:572:LEU:HD21	1.87	0.57
1:B:883:ARG:HH21	1:B:1107:ARG:HD3	1.68	0.57
1:A:1734:ARG:C	1:A:1736:THR:H	2.08	0.57
1:B:1538:ARG:HH12	1:B:1585:PRO:CG	2.17	0.57
1:B:257:LYS:HD3	1:B:263:PHE:O	2.04	0.57
1:A:1841:ARG:O	1:A:1844:ALA:HB3	2.03	0.57
1:B:234:THR:CG2	1:B:239:ALA:HB2	2.34	0.57
1:A:1773:ASP:OD1	1:A:1778:HIS:HD2	1.88	0.57
1:B:368:ALA:CA	1:B:371:ASP:HB3	2.34	0.57
1:A:393:PHE:CD1	1:A:399:ASN:HB3	2.40	0.57
1:B:1996:TYR:C	1:B:1996:TYR:CD2	2.78	0.57
1:A:1672:LEU:HD12	1:A:1696:PHE:O	2.04	0.57
1:A:652:SER:OG	1:A:681:ALA:HB1	2.04	0.57
1:A:293:HIS:O	1:A:326:LYS:HD2	2.04	0.57
1:A:889:THR:CG2	1:A:1032:LEU:HB2	2.35	0.57
1:B:123:ASP:HB3	1:B:126:THR:CB	2.34	0.57
1:A:1653:THR:CG2	1:A:1796:LEU:HD21	2.35	0.57
1:A:1448:CYS:C	1:A:1450:THR:H	2.08	0.57
1:B:466:PRO:HG2	1:B:467:PHE:HD1	1.70	0.57
1:A:638:ILE:O	1:A:638:ILE:HG22	2.05	0.57
1:B:1720:PHE:N	1:B:1720:PHE:HD1	2.01	0.57
1:A:403:ILE:O	1:A:404:LEU:HD23	2.04	0.57
1:B:1277:ARG:HD3	1:B:1300:ASP:CG	2.24	0.57
1:B:22:PHE:CD2	1:B:26:LEU:HD11	2.40	0.57
1:A:1657:TYR:CZ	1:A:1799:LEU:HD11	2.40	0.57
1:A:399:ASN:H	1:A:399:ASN:ND2	2.00	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:HD11	1:B:405:GLN:HB2	1.85	0.57
1:B:799:ASN:HA	1:B:802:ARG:HG3	1.86	0.57
1:B:1320:ALA:HA	1:B:1349:LEU:HD11	1.85	0.57
1:B:1565:SER:HB2	1:B:1857:ARG:HH22	1.63	0.57
1:A:1485:GLU:HB3	1:A:1506:TYR:OH	2.05	0.57
1:B:362:PRO:HB3	1:B:369:LEU:HB3	1.87	0.57
1:B:1580:THR:HG22	1:B:1582:LYS:H	1.70	0.57
1:B:913:VAL:HG23	1:B:962:TRP:HB2	1.86	0.57
1:A:14:PRO:HD3	1:A:226:GLU:O	2.04	0.56
1:B:1651:VAL:HG23	1:B:1851:LYS:HZ1	1.70	0.56
1:A:371:ASP:CG	1:A:371:ASP:O	2.43	0.56
1:A:343:LYS:HG3	1:A:344:VAL:N	2.19	0.56
1:A:1457:VAL:CG2	1:A:1473:LEU:HD22	2.32	0.56
1:B:980:ASP:CB	1:B:982:THR:HG22	2.33	0.56
1:A:309:VAL:HG12	1:A:313:CYS:HB2	1.87	0.56
1:A:148:PHE:HB3	1:A:150:PHE:CZ	2.40	0.56
1:A:527:LEU:HD12	1:A:534:VAL:HG22	1.86	0.56
1:A:1425:TRP:HA	1:A:1428:SER:HB2	1.87	0.56
1:A:615:VAL:HG22	1:A:616:LEU:N	2.20	0.56
1:B:166:LEU:HD12	1:B:251:THR:HG21	1.87	0.56
1:A:1279:PRO:HG3	1:A:1298:GLN:HE22	1.70	0.56
1:A:19:LEU:HD11	1:A:342:ILE:HD13	1.87	0.56
1:A:492:VAL:HG11	1:A:572:LEU:HD21	1.88	0.56
1:B:970:PHE:O	1:B:1067:LYS:HE2	2.05	0.56
1:A:1545:ARG:CG	1:A:1545:ARG:HH11	2.17	0.56
1:B:903:LEU:O	1:B:905:GLN:HG3	2.05	0.56
1:B:506:MET:HE3	1:B:559:ILE:CD1	2.36	0.56
1:A:248:ASN:ND2	1:A:249:ALA:H	2.03	0.56
1:B:326:LYS:HE3	1:B:336:SER:HB2	1.87	0.56
1:A:1486:MET:CE	1:A:1506:TYR:HB3	2.35	0.56
1:B:642:CYS:HA	1:B:743:VAL:HG22	1.86	0.56
1:B:1662:ARG:NH1	1:B:1662:ARG:HG2	2.18	0.56
1:B:1222:ASP:HA	1:B:1226:LEU:CD1	2.35	0.56
1:A:1299:TRP:HE1	1:A:1305:ALA:HA	1.71	0.56
1:A:1765:ARG:N	1:A:1765:ARG:HD3	2.21	0.56
1:A:68:HIS:HB3	1:A:71:GLN:HG3	1.88	0.56
1:B:1373:LEU:N	1:B:1373:LEU:HD23	2.20	0.56
1:B:1407:GLN:HG2	1:B:1409:PRO:HD2	1.83	0.56
1:A:1348:THR:HG22	1:A:1349:LEU:N	2.14	0.56
1:B:278:ALA:CB	1:B:279:PRO:CD	2.83	0.56
1:B:1514:PHE:O	1:B:1515:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1765:ARG:HD3	1:B:1765:ARG:N	2.21	0.56
1:B:1422:SER:O	1:B:1423:PHE:HB2	2.06	0.56
1:B:1423:PHE:CD1	1:B:1989:GLN:HB3	2.41	0.56
1:A:1662:ARG:NH1	1:A:1792:HIS:ND1	2.54	0.56
1:A:1244:VAL:HB	1:A:1272:TYR:HD1	1.69	0.56
1:B:19:LEU:HD11	1:B:342:ILE:HD13	1.88	0.56
1:B:309:VAL:HG12	1:B:313:CYS:HB2	1.88	0.56
1:B:993:TYR:CZ	1:B:1008:GLN:HA	2.40	0.56
1:A:1720:PHE:CD1	1:A:1720:PHE:N	2.74	0.56
1:B:1451:SER:O	1:B:2036:PHE:CE1	2.59	0.56
1:B:1669:GLU:HG2	1:B:1742:ASP:OD2	2.06	0.56
1:B:1656:TYR:O	1:B:1661:VAL:HG23	2.06	0.56
1:B:1720:PHE:N	1:B:1720:PHE:CD1	2.71	0.56
1:A:89:ALA:O	1:A:92:ASP:HB3	2.05	0.56
1:A:903:LEU:O	1:A:905:GLN:HG3	2.06	0.56
1:A:799:ASN:HA	1:A:802:ARG:HG3	1.88	0.56
1:A:1275:THR:CG2	1:A:1299:TRP:HB2	2.36	0.55
1:A:9:MET:HE1	1:A:345:LEU:HB2	1.88	0.55
1:A:1720:PHE:HD1	1:A:1720:PHE:N	2.04	0.55
1:B:1746:ASN:HD21	1:B:1753:LEU:HD12	1.71	0.55
1:A:1996:TYR:C	1:A:1996:TYR:CD2	2.79	0.55
1:B:424:LEU:CD2	1:B:441:GLY:HA3	2.36	0.55
1:B:22:PHE:CE2	1:B:26:LEU:HD11	2.40	0.55
1:A:1570:SER:OG	1:A:1602:GLU:HB3	2.07	0.55
1:A:257:LYS:HD3	1:A:263:PHE:O	2.05	0.55
1:A:670:VAL:HG12	1:A:671:PHE:H	1.72	0.55
1:B:1007:PHE:CE2	1:B:1030:SER:HA	2.41	0.55
1:B:1038:MET:HA	1:B:1038:MET:CE	2.36	0.55
1:B:371:ASP:CG	1:B:371:ASP:O	2.43	0.55
1:A:1569:THR:HG23	1:A:1602:GLU:O	2.06	0.55
1:B:1893:LEU:HB3	1:B:1925:GLN:NE2	2.20	0.55
1:B:621:ALA:CB	1:B:662:LEU:HD11	2.36	0.55
1:B:278:ALA:HB3	1:B:279:PRO:CD	2.34	0.55
1:A:36:ASP:HB3	1:A:38:ARG:CG	2.37	0.55
1:B:36:ASP:CB	1:B:38:ARG:HG3	2.35	0.55
1:B:1996:TYR:CD1	1:B:2040:ALA:HB1	2.41	0.55
1:A:1418:VAL:HG13	1:A:1425:TRP:CH2	2.42	0.55
1:A:1003:TYR:CE1	1:A:1037:HIS:CE1	2.94	0.55
1:B:1736:THR:HG21	1:B:1740:GLY:H	1.72	0.55
1:A:1484:PRO:O	1:A:1485:GLU:CB	2.53	0.55
1:B:2103:HIS:CD2	1:B:2103:HIS:H	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1777:ASN:HD22	1:B:1783:ALA:H	1.54	0.55
1:A:1996:TYR:CD1	1:A:2040:ALA:HB1	2.41	0.55
1:A:1674:HIS:ND1	1:A:1698:THR:HG21	2.21	0.55
1:A:1443:LEU:O	1:A:1473:LEU:HA	2.06	0.55
1:B:1470:ARG:HG3	1:B:1470:ARG:O	2.05	0.55
1:A:1563:LEU:HD12	1:A:1564:CYS:H	1.72	0.55
1:B:1414:VAL:HG11	1:B:1432:ILE:HD13	1.89	0.55
1:A:1097:LEU:HD12	1:A:1098:GLY:N	2.22	0.55
1:B:1299:TRP:CH2	1:B:1333:ASN:ND2	2.75	0.55
1:A:22:PHE:CD2	1:A:26:LEU:HD11	2.41	0.55
1:B:1473:LEU:HG	1:B:1503:MET:HA	1.88	0.55
1:A:1616:MET:HB3	1:A:1800:PHE:HZ	1.72	0.55
1:A:81:MET:HG3	1:A:228:VAL:HG11	1.89	0.55
1:A:386:GLY:O	1:A:387:ASN:HB2	2.05	0.55
1:B:1560:GLN:HA	1:B:1563:LEU:HB3	1.87	0.55
1:A:1768:GLU:OE1	1:A:1768:GLU:HA	2.06	0.55
1:A:1470:ARG:HG3	1:A:1470:ARG:O	2.07	0.55
1:A:1482:PRO:C	1:A:1484:PRO:HD3	2.26	0.55
1:A:429:ARG:HH11	1:A:429:ARG:HB3	1.70	0.55
1:A:1530:HIS:HB2	1:A:1552:HIS:HB2	1.87	0.55
1:A:146:PHE:O	1:B:256:SER:HB3	2.07	0.55
1:B:23:TRP:CE2	1:B:350:HIS:HD2	2.25	0.55
1:A:111:VAL:HG22	1:A:188:LEU:HB2	1.88	0.55
1:B:82:LEU:HD13	1:B:188:LEU:HD21	1.88	0.55
1:B:98:ALA:O	1:B:101:ARG:HG3	2.07	0.55
1:A:297:THR:HB	1:A:300:GLY:N	2.20	0.55
1:A:1857:ARG:HH11	1:A:1869:PRO:CB	2.19	0.55
1:A:40:TRP:CH2	1:A:194:PRO:HA	2.42	0.55
1:B:1416:LEU:HD23	1:B:1429:LEU:HG	1.88	0.55
1:B:615:VAL:HG22	1:B:686:PHE:CD2	2.42	0.55
1:B:393:PHE:CD1	1:B:399:ASN:HB3	2.42	0.55
1:B:1448:CYS:C	1:B:1450:THR:H	2.11	0.55
1:B:644:ASN:HB2	1:B:648:THR:O	2.06	0.55
1:A:1476:ASN:HA	1:A:1486:MET:SD	2.47	0.54
1:A:1035:MET:SD	1:A:1091:ALA:HB3	2.47	0.54
1:B:1570:SER:OG	1:B:1602:GLU:HB3	2.07	0.54
1:A:1300:ASP:O	1:A:1302:ALA:N	2.38	0.54
1:B:1917:ARG:NH1	1:B:1974:VAL:HG12	2.23	0.54
1:A:878:HIS:HB2	1:A:1007:PHE:CE1	2.42	0.54
1:A:1097:LEU:HD12	1:A:1097:LEU:C	2.27	0.54
1:A:1766:PHE:CD2	1:A:1791:PHE:CE1	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:LEU:HD11	1:B:512:ARG:HD2	1.89	0.54
1:B:1227:LYS:HE2	1:B:1516:HIS:O	2.07	0.54
1:A:166:LEU:HD23	1:A:166:LEU:O	2.07	0.54
1:A:1783:ALA:H	1:B:1777:ASN:HD22	1.54	0.54
1:B:1223:ALA:HB1	1:B:1224:PRO:HD2	1.89	0.54
1:B:40:TRP:CH2	1:B:194:PRO:HA	2.42	0.54
1:B:1766:PHE:CD2	1:B:1791:PHE:CE1	2.96	0.54
1:A:1115:ILE:CD1	1:A:2111:LEU:HG	2.31	0.54
1:A:278:ALA:CB	1:A:279:PRO:CD	2.84	0.54
1:B:917:VAL:CG1	1:B:1054:PHE:HB2	2.37	0.54
1:A:506:MET:HE3	1:A:559:ILE:CD1	2.37	0.54
1:B:228:VAL:O	1:B:228:VAL:HG23	2.07	0.54
1:B:1802:GLU:O	1:B:1804:GLY:N	2.39	0.54
1:B:1051:PRO:HA	1:B:1101:SER:HB3	1.90	0.54
1:B:293:HIS:O	1:B:326:LYS:HD2	2.06	0.54
1:B:1734:ARG:O	1:B:1736:THR:N	2.40	0.54
1:B:420:LEU:HD11	1:B:512:ARG:CB	2.37	0.54
1:A:1996:TYR:HD1	1:A:2040:ALA:HB1	1.72	0.54
1:B:1563:LEU:HD12	1:B:1564:CYS:H	1.72	0.54
1:A:1801:GLU:O	1:A:1803:GLY:N	2.41	0.54
1:B:1470:ARG:O	1:B:1472:VAL:HG23	2.07	0.54
1:B:1472:VAL:HG13	1:B:1502:VAL:O	2.08	0.54
1:A:1222:ASP:HA	1:A:1226:LEU:CD1	2.38	0.54
1:A:2101:GLN:HG3	1:A:2102:PRO:CD	2.38	0.54
1:A:1857:ARG:CG	1:A:1871:ILE:HD11	2.38	0.54
1:A:215:PHE:HD2	1:A:305:LEU:HD11	1.68	0.54
1:B:1570:SER:HB3	1:B:1853:VAL:HG22	1.89	0.54
1:A:940:ALA:HB3	1:B:945:GLU:OE2	2.07	0.54
1:A:1606:ARG:NH2	1:A:1860:GLU:HG3	2.20	0.54
1:B:1422:SER:HB2	1:B:1424:ARG:HG3	1.90	0.54
1:A:1698:THR:OG1	1:A:1723:SER:HB3	2.06	0.54
1:A:1973:MET:HB3	1:A:1995:LYS:HE3	1.89	0.54
1:B:343:LYS:HG3	1:B:344:VAL:N	2.22	0.54
1:A:353:TRP:CZ2	1:A:383:ILE:HD12	2.43	0.54
1:B:1229:CYS:HB3	1:B:1403:LEU:HD22	1.90	0.54
1:A:359:TYR:OH	1:A:362:PRO:HG3	2.08	0.54
1:A:2102:PRO:HD2	1:A:2103:HIS:CD2	2.42	0.54
1:A:1996:TYR:HD2	1:A:1997:SER:N	2.06	0.54
1:A:2019:PHE:CD1	1:A:2060:TRP:NE1	2.76	0.54
1:A:1769:ILE:HG22	1:A:1770:GLY:N	2.22	0.54
1:A:1003:TYR:CE1	1:A:1037:HIS:HE1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1446:VAL:HA	1:A:1476:ASN:ND2	2.23	0.54
1:A:856:CYS:SG	1:B:856:CYS:CB	2.96	0.54
1:A:851:PRO:CB	1:B:122:ARG:HB3	2.37	0.54
1:A:1893:LEU:HB3	1:A:1925:GLN:NE2	2.22	0.54
1:A:295:THR:HG22	1:A:331:HIS:HD2	1.72	0.54
1:B:96:ASN:ND2	1:B:98:ALA:HB3	2.19	0.54
1:A:228:VAL:HG23	1:A:228:VAL:O	2.08	0.54
1:B:1656:TYR:CE2	1:B:1687:ILE:HD13	2.43	0.54
1:B:1773:ASP:OD1	1:B:1778:HIS:HD2	1.91	0.54
1:A:1408:THR:HB	1:A:1439:ARG:HH12	1.72	0.53
1:B:642:CYS:HA	1:B:743:VAL:CG2	2.37	0.53
1:A:1035:MET:HE3	1:A:1089:VAL:CG1	2.38	0.53
1:A:278:ALA:HB3	1:A:279:PRO:CD	2.35	0.53
1:B:1538:ARG:NH2	1:B:1585:PRO:HG2	2.21	0.53
1:A:502:GLN:HG3	1:A:556:LEU:CD1	2.35	0.53
1:B:123:ASP:HB3	1:B:126:THR:OG1	2.09	0.53
1:A:162:SER:OG	1:A:163:SER:N	2.41	0.53
1:B:1996:TYR:HD2	1:B:1997:SER:N	2.06	0.53
1:B:148:PHE:HB3	1:B:150:PHE:CZ	2.43	0.53
1:B:1068:LEU:HD12	1:B:1077:ALA:O	2.08	0.53
1:A:48:PRO:HD3	1:A:201:MET:HE3	1.89	0.53
1:A:22:PHE:CE2	1:A:26:LEU:HD11	2.43	0.53
1:B:368:ALA:HA	1:B:371:ASP:HB3	1.90	0.53
1:B:621:ALA:HB2	1:B:662:LEU:HD11	1.90	0.53
1:B:254:ASP:O	1:B:255:GLY:O	2.27	0.53
1:A:1275:THR:HG21	1:A:1299:TRP:HB2	1.90	0.53
1:B:1394:ARG:HA	1:B:1400:VAL:HG22	1.88	0.53
1:B:691:ALA:HB3	1:B:692:PRO:HD3	1.91	0.53
1:B:120:LEU:HD21	1:B:845:PRO:HG3	1.89	0.53
1:A:1748:LEU:O	1:A:1749:ALA:O	2.26	0.53
1:A:685:TYR:CD1	1:A:686:PHE:N	2.76	0.53
1:B:1333:ASN:ND2	1:B:1334:MET:SD	2.82	0.53
1:B:623:VAL:HG12	1:B:624:GLY:N	2.23	0.53
1:B:1618:PRO:CD	1:B:1629:LEU:HD11	2.38	0.53
1:B:201:MET:HA	1:B:206:LEU:HB2	1.89	0.53
1:A:351:GLY:C	1:A:383:ILE:HG22	2.28	0.53
1:A:945:GLU:OE2	1:B:940:ALA:HB3	2.09	0.53
1:B:586:ALA:O	1:B:589:TYR:HB3	2.07	0.53
1:A:234:THR:CG2	1:A:239:ALA:HB2	2.38	0.53
1:B:874:TYR:HB2	1:B:1006:PHE:CD2	2.43	0.53
1:B:1248:LEU:HD21	1:B:1277:ARG:HE	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1390:VAL:HG13	1:B:1501:LEU:HD21	1.89	0.53
1:A:1315:LEU:HB3	1:A:1344:LEU:CD1	2.38	0.53
1:B:2101:GLN:HG3	1:B:2102:PRO:HD2	1.89	0.53
1:B:432:GLU:HG3	1:B:433:ALA:N	2.24	0.53
1:A:1394:ARG:HA	1:A:1400:VAL:HG22	1.90	0.53
1:B:209:ASP:OD2	1:B:213:ARG:NE	2.42	0.53
1:B:1418:VAL:HG13	1:B:1425:TRP:CH2	2.41	0.53
1:B:301:ASP:HB2	1:B:302:PRO:HD3	1.90	0.53
1:A:2006:THR:O	1:A:2010:CYS:HB2	2.08	0.53
1:B:159:THR:CG2	1:B:398:SER:HB3	2.39	0.53
1:A:100:LEU:O	1:A:103:THR:OG1	2.24	0.53
1:A:1656:TYR:HD2	1:A:1660:VAL:HG21	1.72	0.53
1:A:542:ASP:H	1:A:545:VAL:CG1	2.22	0.53
1:B:972:THR:CG2	1:B:1081:VAL:HG23	2.38	0.53
1:A:234:THR:HG21	1:A:239:ALA:HB2	1.89	0.53
1:B:495:ILE:CD1	1:B:578:ILE:HB	2.39	0.53
1:A:275:SER:C	1:A:276:LEU:HD23	2.29	0.53
1:B:1338:LEU:CD1	1:B:1406:GLN:HG3	2.38	0.53
1:A:165:LEU:HD23	1:A:400:VAL:CG2	2.25	0.53
1:A:2103:HIS:HB2	1:A:2106:LEU:HD21	1.90	0.53
1:B:963:GLU:HA	1:B:963:GLU:OE1	2.09	0.53
1:B:1418:VAL:HG12	1:B:1418:VAL:O	2.08	0.53
1:B:214:SER:HB3	1:B:327:SER:HB3	1.91	0.53
1:A:91:VAL:O	1:A:457:ILE:HD11	2.09	0.53
1:B:1136:LEU:HD21	1:B:1218:SER:HA	1.89	0.53
1:B:963:GLU:O	1:B:965:PRO:HD3	2.08	0.53
1:A:963:GLU:HA	1:A:963:GLU:OE1	2.09	0.53
1:A:963:GLU:O	1:A:965:PRO:HD3	2.09	0.53
1:A:423:LEU:HD23	1:A:812:PRO:HG3	1.89	0.53
1:B:1607:ASP:OD1	1:B:1611:ARG:HB3	2.09	0.53
1:A:1416:LEU:HD11	1:A:1425:TRP:HB3	1.90	0.53
1:A:254:ASP:O	1:A:255:GLY:O	2.26	0.53
1:A:542:ASP:N	1:A:545:VAL:HG12	2.23	0.53
1:A:252:ASN:HD21	1:A:272:LEU:HB2	1.74	0.53
1:B:1469:ILE:HG22	1:B:1471:CYS:SG	2.49	0.53
1:A:887:PRO:HB2	1:A:890:GLY:H	1.73	0.53
1:B:1413:PRO:HA	1:B:1440:PRO:HB2	1.91	0.53
1:B:1734:ARG:C	1:B:1736:THR:H	2.11	0.53
1:A:1640:TRP:CZ2	1:A:1825:PRO:HD3	2.44	0.53
1:A:1348:THR:HG21	1:A:1378:TRP:HZ2	1.70	0.53
1:B:1669:GLU:O	1:B:1693:CYS:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1554:ALA:CB	1:B:1882:PRO:HB3	2.39	0.53
1:A:1252:GLY:CA	1:A:1318:ASN:HD22	2.22	0.53
1:B:765:ALA:HB1	1:B:768:GLN:HG2	1.89	0.53
1:B:1461:ARG:HG3	1:B:1461:ARG:O	2.09	0.53
1:A:856:CYS:SG	1:B:856:CYS:SG	3.06	0.52
1:B:1996:TYR:HD1	1:B:2040:ALA:HB1	1.74	0.52
1:A:98:ALA:O	1:A:101:ARG:HG3	2.08	0.52
1:B:1276:ASP:O	1:B:1298:GLN:HA	2.09	0.52
1:B:1874:THR:HG22	1:B:1874:THR:O	2.09	0.52
1:A:429:ARG:NH1	1:A:429:ARG:HB3	2.23	0.52
1:B:2019:PHE:CD1	1:B:2060:TRP:NE1	2.78	0.52
1:A:91:VAL:HG21	1:A:834:ILE:HD13	1.92	0.52
1:A:132:MET:HE1	1:B:200:PHE:HE2	1.73	0.52
1:A:159:THR:CG2	1:A:398:SER:HB3	2.40	0.52
1:B:1121:PHE:HE1	1:B:1512:GLY:C	2.13	0.52
1:A:1648:VAL:HB	1:A:1649:PRO:HD3	1.91	0.52
1:A:1418:VAL:O	1:A:1418:VAL:HG12	2.09	0.52
1:B:165:LEU:HD22	1:B:392:SER:HB2	1.91	0.52
1:B:638:ILE:HD11	1:B:657:ALA:O	2.09	0.52
1:B:429:ARG:HB3	1:B:429:ARG:HH11	1.73	0.52
1:B:502:GLN:HG3	1:B:556:LEU:CD1	2.37	0.52
1:A:2103:HIS:H	1:A:2103:HIS:CD2	2.27	0.52
1:B:765:ALA:HB2	1:B:783:PRO:HB3	1.91	0.52
1:B:219:GLY:O	1:B:298:LYS:HB2	2.09	0.52
1:A:1051:PRO:HA	1:A:1101:SER:HB3	1.90	0.52
1:A:39:ARG:NH1	1:A:57:LEU:HD22	2.24	0.52
1:A:1252:GLY:HA2	1:A:1318:ASN:HD22	1.73	0.52
1:A:166:LEU:HD11	1:B:155:ILE:HD11	1.90	0.52
1:A:1553:TYR:CD1	1:A:1880:PHE:HB2	2.45	0.52
1:B:1009:LEU:HD13	1:B:1023:GLN:O	2.10	0.52
1:B:1855:GLN:NE2	1:B:1858:GLU:HA	2.24	0.52
1:B:1338:LEU:HG	1:B:1342:GLY:H	1.75	0.52
1:A:1616:MET:CE	1:A:1650:ILE:HD13	2.40	0.52
1:B:166:LEU:O	1:B:166:LEU:HD23	2.09	0.52
1:B:506:MET:HB3	1:B:559:ILE:CD1	2.39	0.52
1:B:2103:HIS:HB2	1:B:2106:LEU:HD21	1.90	0.52
1:B:564:ILE:HD13	1:B:590:ALA:HB2	1.92	0.52
1:B:275:SER:C	1:B:276:LEU:HD23	2.30	0.52
1:B:2019:PHE:CE1	1:B:2060:TRP:NE1	2.77	0.52
1:A:1221:LEU:HG	1:A:1221:LEU:O	2.10	0.52
1:A:1917:ARG:NH1	1:A:1974:VAL:HG12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2006:THR:CG2	1:B:2048:ARG:HH22	2.22	0.52
1:A:796:PHE:O	1:A:800:VAL:HG23	2.09	0.52
1:B:1973:MET:HB3	1:B:1995:LYS:HE3	1.91	0.52
1:B:808:VAL:HG12	1:B:809:SER:N	2.25	0.52
1:A:1677:SER:HB2	1:A:1704:LYS:HE2	1.92	0.52
1:A:1736:THR:HG21	1:A:1740:GLY:H	1.71	0.52
1:A:112:SER:O	1:A:137:ARG:NH2	2.43	0.52
1:A:1003:TYR:CE2	1:A:1037:HIS:CE1	2.92	0.52
1:B:1568:TYR:CZ	1:B:1643:GLU:HG3	2.45	0.52
1:B:1585:PRO:HB3	1:B:1598:MET:HE1	1.92	0.52
1:A:1007:PHE:CE2	1:A:1030:SER:HA	2.44	0.52
1:A:691:ALA:HB3	1:A:692:PRO:HD3	1.91	0.52
1:A:424:LEU:CD2	1:A:441:GLY:HA3	2.40	0.52
1:A:765:ALA:HB1	1:A:768:GLN:HG2	1.92	0.52
1:A:1001:TYR:HB3	1:A:1003:TYR:CD1	2.44	0.52
1:B:1416:LEU:HD11	1:B:1425:TRP:HB3	1.92	0.52
1:B:1222:ASP:HA	1:B:1226:LEU:HD11	1.92	0.52
1:B:1255:TYR:O	1:B:1292:LEU:HD13	2.10	0.52
1:B:1698:THR:OG1	1:B:1723:SER:HB3	2.09	0.52
1:B:100:LEU:O	1:B:103:THR:OG1	2.20	0.52
1:A:1241:LYS:HG3	1:A:1241:LYS:O	2.10	0.52
1:A:993:TYR:CZ	1:A:1008:GLN:HA	2.45	0.52
1:A:1899:GLN:HG2	1:A:2088:ILE:HG21	1.92	0.52
1:B:1748:LEU:O	1:B:1749:ALA:O	2.28	0.52
1:A:326:LYS:HE3	1:A:336:SER:HB2	1.91	0.51
1:B:269:GLN:O	1:B:273:ILE:HG13	2.08	0.51
1:A:1302:ALA:O	1:A:1304:PRO:HD3	2.10	0.51
1:A:1524:PRO:O	1:A:1877:SER:HB2	2.10	0.51
1:B:665:LEU:HD22	1:B:670:VAL:HG21	1.92	0.51
1:B:429:ARG:HB3	1:B:429:ARG:NH1	2.26	0.51
1:B:399:ASN:ND2	1:B:399:ASN:H	2.07	0.51
1:B:2102:PRO:HD2	1:B:2103:HIS:CD2	2.42	0.51
1:A:851:PRO:HB2	1:B:122:ARG:HB3	1.90	0.51
1:B:1466:GLY:O	1:B:1469:ILE:HB	2.10	0.51
1:A:831:SER:OG	1:A:832:PRO:HD3	2.10	0.51
1:B:1593:LEU:HD23	1:B:1594:THR:HG22	1.92	0.51
1:A:1422:SER:HB2	1:A:1424:ARG:HG3	1.92	0.51
1:B:724:GLY:O	1:B:728:ARG:HB2	2.10	0.51
1:B:914:PHE:O	1:B:915:GLU:HG3	2.09	0.51
1:B:191:LEU:HD22	1:B:224:ARG:CZ	2.40	0.51
1:B:506:MET:HE1	1:B:555:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:PHE:CE1	1:A:1516:HIS:CE1	2.98	0.51
1:A:1456:MET:HG2	1:A:2036:PHE:HB2	1.92	0.51
1:A:130:TYR:HA	1:B:203:LEU:HD21	1.92	0.51
1:B:1275:THR:CG2	1:B:1299:TRP:HB2	2.39	0.51
1:A:1570:SER:HB3	1:A:1853:VAL:HG22	1.92	0.51
1:A:416:GLN:C	1:A:418:ALA:H	2.13	0.51
1:B:1227:LYS:HB2	1:B:1261:LEU:CD2	2.39	0.51
1:A:2101:GLN:HG3	1:A:2102:PRO:HD2	1.93	0.51
1:B:2070:LEU:HD11	1:B:2076:ASN:ND2	2.26	0.51
1:A:1674:HIS:CE1	1:A:1698:THR:HG21	2.45	0.51
1:A:765:ALA:HB2	1:A:783:PRO:HB3	1.92	0.51
1:B:169:GLN:OE1	1:B:250:GLY:HA2	2.10	0.51
1:B:1302:ALA:HB3	1:B:1304:PRO:HD3	1.92	0.51
1:B:1460:LEU:HD12	1:B:1463:GLU:OE1	2.11	0.51
1:B:333:GLU:CB	1:B:334:PRO:CD	2.84	0.51
1:A:1662:ARG:NH1	1:A:1662:ARG:CG	2.55	0.51
1:A:1289:LEU:HD22	1:A:1294:VAL:CB	2.36	0.51
1:A:662:LEU:O	1:A:666:LYS:HG2	2.09	0.51
1:A:1461:ARG:NH1	1:A:1502:VAL:HG22	2.26	0.51
1:B:1746:ASN:ND2	1:B:1753:LEU:HD12	2.25	0.51
1:A:605:TRP:O	1:A:606:ARG:C	2.49	0.51
1:B:887:PRO:HB2	1:B:890:GLY:H	1.76	0.51
1:B:1677:SER:HB2	1:B:1704:LYS:HE2	1.93	0.51
1:A:82:LEU:HD13	1:A:188:LEU:HD21	1.91	0.51
1:A:976:VAL:CG2	1:A:977:ASP:H	2.17	0.51
1:A:1528:THR:HG21	1:A:1530:HIS:O	2.11	0.51
1:A:1763:HIS:HA	1:A:1788:ASN:O	2.10	0.51
1:B:1501:LEU:HB2	1:B:1504:ASN:OD1	2.10	0.51
1:A:1526:LYS:HD3	1:A:1552:HIS:NE2	2.25	0.51
1:B:1544:ILE:HD12	1:B:1837:GLU:HA	1.92	0.51
1:B:1276:ASP:OD2	1:B:1281:ALA:HB3	2.11	0.51
1:B:81:MET:HG3	1:B:228:VAL:HG11	1.92	0.51
1:B:1001:TYR:CE2	1:B:1040:ILE:HD13	2.46	0.51
1:B:1418:VAL:HG22	1:B:1425:TRP:CD2	2.45	0.51
1:B:1470:ARG:O	1:B:1470:ARG:CG	2.58	0.51
1:A:1639:THR:O	1:A:1640:TRP:HD1	1.93	0.51
1:B:1585:PRO:HB3	1:B:1598:MET:CE	2.41	0.51
1:A:2019:PHE:CE1	1:A:2060:TRP:NE1	2.79	0.51
1:B:183:ALA:O	1:B:232:LEU:HD12	2.11	0.51
1:A:1411:ASP:HB2	1:A:1440:PRO:CD	2.41	0.51
1:B:111:VAL:HG22	1:B:188:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:HG3	1:A:123:ASP:H	1.76	0.51
1:B:982:THR:HG23	1:B:983:ALA:N	2.19	0.51
1:A:941:SER:N	1:B:945:GLU:OE2	2.44	0.51
1:B:2006:THR:O	1:B:2010:CYS:HB2	2.11	0.51
1:B:321:LEU:HD12	1:B:321:LEU:H	1.75	0.51
1:A:620:MET:HE3	1:A:682:PHE:O	2.11	0.51
1:B:625:LEU:HD22	1:B:629:GLU:OE1	2.11	0.51
1:B:1473:LEU:HD21	1:B:1503:MET:CG	2.32	0.51
1:B:416:GLN:C	1:B:418:ALA:H	2.15	0.51
1:B:1439:ARG:O	1:B:1470:ARG:HB3	2.11	0.50
1:B:1457:VAL:CG2	1:B:1473:LEU:HD22	2.33	0.50
1:A:45:TYR:CE2	1:B:124:PRO:HB2	2.45	0.50
1:B:1554:ALA:HB2	1:B:1882:PRO:HG3	1.93	0.50
1:B:248:ASN:HD22	1:B:249:ALA:H	1.56	0.50
1:A:970:PHE:O	1:A:1067:LYS:HE2	2.10	0.50
1:B:1651:VAL:HG23	1:B:1851:LYS:NZ	2.26	0.50
1:B:642:CYS:O	1:B:649:VAL:HG13	2.11	0.50
1:B:416:GLN:NE2	1:B:422:ARG:HH22	2.09	0.50
1:A:321:LEU:CD2	1:A:381:LEU:HD13	2.41	0.50
1:B:883:ARG:HE	1:B:1107:ARG:HD3	1.76	0.50
1:B:1560:GLN:HA	1:B:1563:LEU:CB	2.41	0.50
1:A:1223:ALA:HB1	1:A:1224:PRO:HD2	1.93	0.50
1:A:1470:ARG:HD3	1:A:1472:VAL:CG2	2.41	0.50
1:A:165:LEU:HD22	1:A:392:SER:HB2	1.93	0.50
1:A:1314:LEU:HG	1:A:1315:LEU:N	2.25	0.50
1:A:1800:PHE:C	1:A:1800:PHE:HD2	2.15	0.50
1:B:1674:HIS:HE1	1:B:1756:SER:OG	1.94	0.50
1:B:36:ASP:HB3	1:B:38:ARG:CG	2.40	0.50
1:A:1723:SER:C	1:A:1725:ASP:H	2.15	0.50
1:A:1861:GLN:O	1:A:1865:PRO:HG3	2.11	0.50
1:A:1606:ARG:HH21	1:A:1860:GLU:CG	2.23	0.50
1:B:972:THR:HG22	1:B:1081:VAL:HG21	1.92	0.50
1:B:309:VAL:HG22	1:B:374:LEU:HD11	1.94	0.50
1:B:1333:ASN:C	1:B:1335:ALA:H	2.14	0.50
1:A:1996:TYR:HD1	1:A:2040:ALA:CB	2.24	0.50
1:A:1422:SER:O	1:A:1423:PHE:HB2	2.11	0.50
1:B:925:LEU:HD22	1:B:931:VAL:HG21	1.94	0.50
1:B:995:ASP:O	1:B:998:LEU:HB2	2.10	0.50
1:A:776:GLU:HB3	1:A:778:SER:OG	2.12	0.50
1:A:59:ARG:HD2	1:A:59:ARG:N	2.26	0.50
1:B:9:MET:HE1	1:B:342:ILE:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:MET:HE2	1:A:1038:MET:HA	1.92	0.50
1:B:225:ALA:O	1:B:332:PRO:HA	2.12	0.50
1:B:579:GLY:O	1:B:715:THR:HG21	2.11	0.50
1:A:495:ILE:CD1	1:A:578:ILE:HB	2.41	0.50
1:A:1657:TYR:CZ	1:A:1662:ARG:HD2	2.47	0.50
1:A:384:ARG:NH1	1:A:384:ARG:HG3	2.17	0.50
1:B:420:LEU:HG	1:B:793:LEU:HD21	1.94	0.50
1:A:256:SER:HB3	1:B:146:PHE:O	2.12	0.50
1:A:269:GLN:O	1:A:273:ILE:HG13	2.11	0.50
1:A:287:LEU:HA	1:A:387:ASN:O	2.12	0.50
1:B:1024:TRP:HB2	1:B:1068:LEU:HD11	1.94	0.50
1:A:169:GLN:HE21	1:A:169:GLN:C	2.15	0.50
1:A:191:LEU:HD22	1:A:224:ARG:NH1	2.27	0.50
1:A:96:ASN:ND2	1:A:98:ALA:HB3	2.18	0.50
1:A:1800:PHE:C	1:A:1800:PHE:CD2	2.85	0.50
1:A:290:ILE:HD13	1:A:308:ILE:HD13	1.94	0.50
1:B:2001:ASN:O	1:B:2005:VAL:HG23	2.10	0.50
1:B:136:GLN:NE2	1:B:138:ALA:H	2.10	0.50
1:B:1981:GLU:HG3	1:B:1982:ASN:OD1	2.12	0.50
1:B:965:PRO:O	1:B:967:PRO:HD3	2.12	0.50
1:A:1241:LYS:HA	1:A:1269:ASP:HB3	1.93	0.50
1:A:1064:HIS:HB2	1:A:1093:GLY:HA3	1.94	0.50
1:A:946:VAL:O	1:A:954:ILE:HB	2.12	0.50
1:A:241:ARG:NH2	1:A:827:THR:O	2.45	0.50
1:A:621:ALA:O	1:A:650:THR:HG23	2.12	0.50
1:B:9:MET:HE2	1:B:342:ILE:HG12	1.94	0.50
1:A:1229:CYS:HB3	1:A:1403:LEU:HD22	1.94	0.50
1:B:638:ILE:HG22	1:B:638:ILE:O	2.11	0.49
1:A:301:ASP:HB2	1:A:302:PRO:HD3	1.94	0.49
1:B:366:ILE:HD11	1:B:369:LEU:HD11	1.94	0.49
1:A:838:HIS:O	1:A:839:SER:C	2.50	0.49
1:B:1459:CYS:CB	1:B:2032:ALA:HA	2.43	0.49
1:A:668:GLU:O	1:A:669:ASP:HB3	2.11	0.49
1:A:2006:THR:CG2	1:A:2048:ARG:HH22	2.25	0.49
1:A:9:MET:HE1	1:A:342:ILE:HA	1.93	0.49
1:A:1461:ARG:HG3	1:A:1461:ARG:O	2.12	0.49
1:B:1858:GLU:HG3	1:B:1859:GLU:N	2.26	0.49
1:A:734:TYR:CD2	1:A:734:TYR:C	2.86	0.49
1:B:295:THR:HG22	1:B:331:HIS:HD2	1.77	0.49
1:B:1429:LEU:CD1	1:B:1443:LEU:HD11	2.42	0.49
1:A:1533:VAL:HG23	1:A:1545:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.94	0.49
1:B:866:VAL:HG13	1:B:876:VAL:HG22	1.95	0.49
1:B:706:LYS:N	1:B:706:LYS:HD2	2.27	0.49
1:B:1312:ALA:HB1	1:B:1337:THR:O	2.12	0.49
1:B:82:LEU:HG	1:B:144:LEU:CD1	2.42	0.49
1:A:1130:LEU:HD22	1:A:1133:ASN:ND2	2.28	0.49
1:A:2017:VAL:HG21	1:A:2099:LEU:HD21	1.93	0.49
1:B:554:VAL:O	1:B:558:SER:HB2	2.12	0.49
1:A:554:VAL:O	1:A:558:SER:HB2	2.13	0.49
1:B:1423:PHE:O	1:B:1985:PRO:HB3	2.12	0.49
1:A:853:GLY:O	1:A:854:SER:HB2	2.12	0.49
1:A:1483:ALA:N	1:A:1484:PRO:HD3	2.27	0.49
1:B:1328:ALA:HB2	1:B:1381:LEU:HD11	1.94	0.49
1:B:1887:TYR:CD2	1:B:1967:GLY:HA3	2.44	0.49
1:B:527:LEU:HD12	1:B:534:VAL:CG2	2.43	0.49
1:A:1874:THR:O	1:A:1874:THR:HG22	2.11	0.49
1:A:1780:LEU:HD12	1:A:1781:GLY:H	1.78	0.49
1:A:595:THR:HG21	1:A:597:GLU:HG2	1.94	0.49
1:B:60:PHE:CD2	1:B:80:ARG:HD3	2.48	0.49
1:A:1766:PHE:HD2	1:A:1791:PHE:CE1	2.30	0.49
1:B:1032:LEU:O	1:B:1035:MET:HB2	2.13	0.49
1:A:416:GLN:NE2	1:A:422:ARG:HH22	2.10	0.49
1:A:309:VAL:HG22	1:A:374:LEU:HD11	1.95	0.49
1:A:1390:VAL:HG13	1:A:1501:LEU:CD2	2.42	0.49
1:A:1345:LEU:O	1:A:1346:LEU:HD23	2.13	0.49
1:B:1106:ARG:O	1:B:1108:PRO:HD3	2.13	0.49
1:B:831:SER:OG	1:B:832:PRO:HD3	2.13	0.49
1:B:1460:LEU:HD11	1:B:1980:LEU:HD13	1.95	0.49
1:B:1882:PRO:HG2	1:B:1885:LYS:HD2	1.95	0.49
1:B:1974:VAL:O	1:B:1974:VAL:HG23	2.13	0.49
1:A:1415:PHE:CD2	1:A:1444:MET:HE1	2.48	0.49
1:A:475:GLY:C	1:A:477:ALA:H	2.15	0.49
1:B:1244:VAL:HB	1:B:1272:TYR:CD1	2.43	0.49
1:B:838:HIS:O	1:B:839:SER:C	2.51	0.49
1:B:1532:PHE:CD2	1:B:1549:SER:HA	2.45	0.49
1:B:913:VAL:HG22	1:B:1058:ARG:HG2	1.95	0.49
1:A:1050:LEU:O	1:A:1101:SER:CB	2.60	0.49
1:A:236:LYS:C	1:A:238:LEU:H	2.16	0.49
1:B:491:PRO:HD2	1:B:756:ALA:HA	1.95	0.49
1:A:635:PRO:HD3	1:A:661:PHE:CE2	2.48	0.49
1:B:384:ARG:NH1	1:B:384:ARG:CG	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:VAL:HG13	1:A:1273:THR:CB	2.38	0.49
1:A:136:GLN:NE2	1:A:138:ALA:H	2.10	0.49
1:B:1430:LYS:HE3	1:B:1981:GLU:CA	2.42	0.49
1:B:305:LEU:O	1:B:309:VAL:HG23	2.13	0.49
1:A:527:LEU:HD12	1:A:534:VAL:CG2	2.43	0.49
1:A:156:THR:OG1	1:B:158:ASP:O	2.31	0.49
1:B:717:ILE:HD13	1:B:727:ALA:HB2	1.95	0.49
1:B:1603:PHE:CD2	1:B:1603:PHE:N	2.80	0.49
1:A:1602:GLU:CD	1:A:1650:ILE:HG12	2.34	0.48
1:A:348:LEU:HD13	1:A:406:PRO:HB3	1.95	0.48
1:A:1405:ARG:HH22	1:A:1470:ARG:NH2	2.11	0.48
1:A:1470:ARG:O	1:A:1470:ARG:CG	2.61	0.48
1:A:82:LEU:HG	1:A:144:LEU:CD1	2.44	0.48
1:B:78:GLN:HB3	1:B:188:LEU:HD13	1.95	0.48
1:A:1528:THR:HG23	1:A:1552:HIS:ND1	2.28	0.48
1:B:287:LEU:HA	1:B:387:ASN:O	2.13	0.48
1:A:359:TYR:OH	1:A:369:LEU:HD22	2.12	0.48
1:A:1666:GLN:HG2	1:A:1667:PRO:HD2	1.94	0.48
1:B:1653:THR:HG22	1:B:1810:VAL:CG1	2.40	0.48
1:A:1593:LEU:HD23	1:A:1594:THR:HG22	1.95	0.48
1:A:1085:ASN:C	1:A:1086:LEU:HD23	2.33	0.48
1:B:1996:TYR:HD1	1:B:2040:ALA:CB	2.25	0.48
1:B:1086:LEU:N	1:B:1086:LEU:HD23	2.27	0.48
1:B:1551:LEU:HD21	1:B:1627:LEU:HD21	1.95	0.48
1:A:1541:LEU:HD23	1:A:1541:LEU:N	2.29	0.48
1:B:111:VAL:HG23	1:B:188:LEU:HB2	1.94	0.48
1:B:290:ILE:HD13	1:B:308:ILE:HD13	1.96	0.48
1:B:1672:LEU:HB3	1:B:1744:VAL:HG22	1.95	0.48
1:A:377:VAL:HG13	1:A:381:LEU:CD1	2.44	0.48
1:B:1428:SER:O	1:B:1432:ILE:HG13	2.13	0.48
1:A:782:ILE:CD1	1:A:803:LEU:HD23	2.43	0.48
1:A:130:TYR:CA	1:B:203:LEU:HD21	2.43	0.48
1:B:1899:GLN:HG2	1:B:2088:ILE:HG21	1.94	0.48
1:A:1523:ARG:HH12	1:A:1536:LEU:HD12	1.78	0.48
1:A:1452:GLY:HA2	1:A:2039:SER:HB3	1.96	0.48
1:B:39:ARG:NH1	1:B:57:LEU:HD22	2.28	0.48
1:B:581:SER:OG	1:B:582:LEU:N	2.42	0.48
1:A:1670:SER:O	1:A:1742:ASP:HB2	2.13	0.48
1:B:191:LEU:HD22	1:B:224:ARG:NH1	2.29	0.48
1:B:1083:ASP:O	1:B:1086:LEU:N	2.46	0.48
1:B:236:LYS:HG3	1:B:237:SER:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2056:LEU:HA	1:A:2104:PRO:O	2.13	0.48
1:A:1418:VAL:HG22	1:A:1425:TRP:CD2	2.49	0.48
1:B:1001:TYR:HB3	1:B:1003:TYR:CD1	2.48	0.48
1:A:856:CYS:HB3	1:B:856:CYS:SG	2.54	0.48
1:A:1666:GLN:O	1:A:1669:GLU:HB2	2.13	0.48
1:A:913:VAL:HG22	1:A:1058:ARG:HG2	1.95	0.48
1:A:1024:TRP:HB2	1:A:1068:LEU:HD11	1.96	0.48
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.94	0.48
1:A:914:PHE:O	1:A:915:GLU:HG3	2.14	0.48
1:A:902:ALA:HB1	1:A:939:GLU:OE2	2.14	0.48
1:A:215:PHE:O	1:A:363:ASN:HB2	2.14	0.48
1:A:856:CYS:C	1:A:858:SER:H	2.17	0.48
1:A:541:THR:HA	1:A:545:VAL:HG11	1.95	0.48
1:A:2070:LEU:HD11	1:A:2076:ASN:ND2	2.28	0.48
1:B:133:ILE:HD12	1:B:143:ARG:HH21	1.79	0.48
1:B:782:ILE:CD1	1:B:803:LEU:HD23	2.43	0.48
1:A:1507:ARG:HH22	1:A:2046:GLU:CD	2.16	0.48
1:A:612:GLU:C	1:A:614:ASN:N	2.67	0.48
1:B:2098:PHE:CD2	1:B:2106:LEU:HD12	2.48	0.48
1:A:261:VAL:HG22	1:B:146:PHE:CE1	2.48	0.48
1:A:1519:LEU:HD12	1:A:1520:GLU:H	1.78	0.48
1:B:988:SER:O	1:B:991:ASP:N	2.47	0.48
1:A:183:ALA:O	1:A:232:LEU:HD12	2.14	0.48
1:B:504:GLN:N	1:B:546:LEU:HD11	2.28	0.48
1:B:1302:ALA:HB3	1:B:1304:PRO:CD	2.44	0.48
1:A:1432:ILE:HG22	1:A:1432:ILE:O	2.14	0.48
1:B:1442:TRP:CZ3	1:B:1472:VAL:HG11	2.48	0.48
1:A:861:VAL:HG22	1:A:934:GLU:CB	2.39	0.48
1:A:475:GLY:O	1:A:477:ALA:N	2.45	0.48
1:A:225:ALA:O	1:A:332:PRO:HA	2.13	0.48
1:B:1898:LEU:HA	1:B:1898:LEU:HD23	1.70	0.48
1:A:1457:VAL:HG11	1:A:1473:LEU:HD22	1.96	0.48
1:B:638:ILE:HD11	1:B:657:ALA:C	2.34	0.48
1:A:612:GLU:C	1:A:614:ASN:H	2.16	0.48
1:B:1882:PRO:HD2	1:B:1887:TYR:OH	2.13	0.48
1:B:321:LEU:HD12	1:B:321:LEU:N	2.28	0.48
1:B:902:ALA:HB1	1:B:939:GLU:OE2	2.13	0.48
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.95	0.48
1:B:1248:LEU:HD21	1:B:1277:ARG:HH21	1.79	0.48
1:A:642:CYS:CB	1:A:650:THR:HB	2.29	0.48
1:A:1315:LEU:HB3	1:A:1344:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1554:ALA:HB3	1:B:1882:PRO:HB3	1.96	0.48
1:A:506:MET:HB3	1:A:559:ILE:CD1	2.44	0.48
1:A:1567:TYR:HA	1:A:1857:ARG:HB2	1.96	0.48
1:B:81:MET:O	1:B:85:VAL:HG22	2.14	0.48
1:B:1038:MET:HE2	1:B:1038:MET:HA	1.96	0.48
1:A:423:LEU:HB2	1:A:797:LEU:HD22	1.96	0.48
1:B:1124:HIS:CD2	1:B:1512:GLY:HA2	2.48	0.48
1:A:1536:LEU:HB2	1:A:1543:SER:HB3	1.95	0.48
1:B:1912:LEU:HB2	1:B:1939:VAL:HG22	1.96	0.48
1:A:1106:ARG:O	1:A:1108:PRO:HD3	2.13	0.48
1:A:1016:GLU:HA	1:A:1043:PRO:HG3	1.96	0.48
1:A:431:LEU:HD23	1:A:431:LEU:C	2.34	0.48
1:B:639:VAL:HG12	1:B:640:PRO:O	2.14	0.47
1:B:1995:LYS:HB3	1:B:2041:MET:SD	2.54	0.47
1:B:1236:ASN:HA	1:B:1502:VAL:HG21	1.95	0.47
1:B:621:ALA:O	1:B:623:VAL:HG23	2.14	0.47
1:A:1476:ASN:O	1:A:1477:LEU:HD23	2.14	0.47
1:B:1554:ALA:C	1:B:1556:PRO:HD3	2.34	0.47
1:A:1647:SER:O	1:A:1651:VAL:CG2	2.61	0.47
1:A:1729:GLU:OE1	1:A:1758:ARG:HD2	2.14	0.47
1:A:1886:SER:HA	1:A:1911:LYS:HB2	1.95	0.47
1:B:259:GLN:CD	1:B:259:GLN:H	2.18	0.47
1:A:499:MET:HE2	1:A:582:LEU:HD22	1.95	0.47
1:A:1123:PRO:HB3	1:A:1510:ALA:HB1	1.95	0.47
1:B:1656:TYR:CZ	1:B:1687:ILE:HD13	2.49	0.47
1:B:1800:PHE:CD2	1:B:1800:PHE:C	2.88	0.47
1:B:51:MET:HB2	1:B:53:LYS:HE3	1.95	0.47
1:A:856:CYS:CB	1:B:856:CYS:HG	2.27	0.47
1:B:1723:SER:C	1:B:1725:ASP:H	2.18	0.47
1:A:2098:PHE:CD2	1:A:2106:LEU:HB2	2.48	0.47
1:B:1800:PHE:HD2	1:B:1800:PHE:C	2.17	0.47
1:A:1556:PRO:O	1:A:1558:SER:N	2.47	0.47
1:A:1912:LEU:HB2	1:A:1939:VAL:HG22	1.95	0.47
1:B:557:THR:HG21	1:B:603:SER:OG	2.14	0.47
1:B:326:LYS:CE	1:B:336:SER:HB2	2.44	0.47
1:A:1544:ILE:O	1:A:1545:ARG:HG3	2.15	0.47
1:B:982:THR:C	1:B:984:GLU:N	2.68	0.47
1:B:1983:GLN:HG2	1:B:1988:PHE:HE1	1.78	0.47
1:B:1486:MET:SD	1:B:1506:TYR:CD1	3.08	0.47
1:B:972:THR:HG22	1:B:1081:VAL:HG23	1.97	0.47
1:B:321:LEU:HD23	1:B:381:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2022:VAL:CG1	1:B:2022:VAL:O	2.62	0.47
1:A:262:THR:O	1:A:262:THR:CG2	2.63	0.47
1:B:525:GLN:HA	1:B:525:GLN:NE2	2.30	0.47
1:B:1003:TYR:CE2	1:B:1037:HIS:CE1	2.92	0.47
1:B:1418:VAL:HG22	1:B:1425:TRP:CG	2.50	0.47
1:B:685:TYR:CD1	1:B:686:PHE:N	2.83	0.47
1:A:111:VAL:HG23	1:A:188:LEU:HB2	1.97	0.47
1:B:359:TYR:CD2	1:B:376:VAL:HG11	2.50	0.47
1:A:2001:ASN:O	1:A:2005:VAL:HG23	2.14	0.47
1:B:2017:VAL:HG21	1:B:2099:LEU:HD21	1.97	0.47
1:B:1981:GLU:C	1:B:1983:GLN:H	2.18	0.47
1:A:503:TRP:CG	1:A:787:LYS:HB2	2.50	0.47
1:B:2006:THR:HG21	1:B:2048:ARG:NH2	2.29	0.47
1:B:48:PRO:HD3	1:B:201:MET:HE3	1.97	0.47
1:A:1774:LEU:O	1:B:1783:ALA:HB2	2.14	0.47
1:B:1050:LEU:O	1:B:1101:SER:CB	2.63	0.47
1:A:432:GLU:HG3	1:A:433:ALA:N	2.29	0.47
1:A:107:VAL:HG13	1:A:184:VAL:HB	1.96	0.47
1:B:59:ARG:HD2	1:B:59:ARG:N	2.29	0.47
1:A:838:HIS:O	1:A:840:GLN:N	2.48	0.47
1:B:796:PHE:O	1:B:800:VAL:HG23	2.14	0.47
1:B:128:VAL:CG1	1:B:130:TYR:CZ	2.98	0.47
1:B:670:VAL:HG12	1:B:671:PHE:H	1.79	0.47
1:A:618:GLY:N	1:A:679:GLY:O	2.47	0.47
1:A:1592:TRP:HB2	1:A:1595:ARG:HD3	1.97	0.47
1:A:1416:LEU:HD23	1:A:1429:LEU:HG	1.96	0.47
1:B:1411:ASP:HB2	1:B:1440:PRO:HG3	1.95	0.47
1:B:1236:ASN:CG	1:B:1502:VAL:HG23	2.36	0.47
1:A:1636:VAL:HA	1:A:1637:PRO:HD3	1.73	0.47
1:B:1725:ASP:OD2	1:B:1727:SER:HB3	2.15	0.47
1:A:1669:GLU:HG2	1:A:1742:ASP:CB	2.45	0.47
1:A:261:VAL:HG22	1:B:146:PHE:CZ	2.50	0.47
1:B:1656:TYR:CD2	1:B:1813:LEU:HB3	2.49	0.47
1:A:1107:ARG:HG3	1:A:1107:ARG:O	2.15	0.47
1:B:1239:SER:C	1:B:1241:LYS:H	2.18	0.47
1:B:1685:ILE:HG22	1:B:1686:ALA:N	2.30	0.47
1:A:1794:ILE:C	1:A:1795:LEU:HD23	2.35	0.47
1:B:610:ILE:HA	1:B:690:ILE:HD13	1.96	0.47
1:A:1711:ARG:HH22	1:A:1826:LEU:CD2	2.28	0.47
1:B:1894:GLY:O	1:B:1895:GLY:C	2.54	0.47
1:B:1733:LEU:HA	1:B:1733:LEU:HD23	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1303:ASN:HA	1:B:1333:ASN:HB2	1.96	0.47
1:B:1443:LEU:O	1:B:1473:LEU:HA	2.15	0.47
1:A:976:VAL:HG22	1:A:977:ASP:N	2.18	0.47
1:B:983:ALA:O	1:B:985:PHE:N	2.43	0.47
1:A:1130:LEU:HD11	1:A:1221:LEU:CD1	2.44	0.47
1:A:1248:LEU:HD21	1:A:1277:ARG:NH2	2.30	0.47
1:B:1129:CYS:O	1:B:1130:LEU:HB2	2.14	0.47
1:B:1239:SER:OG	1:B:1241:LYS:HG2	2.15	0.47
1:A:1748:LEU:HA	1:A:1748:LEU:HD23	1.69	0.47
1:A:1553:TYR:O	1:A:1554:ALA:HB2	2.15	0.47
1:B:1729:GLU:OE1	1:B:1758:ARG:HD2	2.15	0.47
1:A:866:VAL:HG13	1:A:876:VAL:HG22	1.97	0.47
1:B:1275:THR:HG21	1:B:1299:TRP:HB2	1.96	0.46
1:B:1390:VAL:HG13	1:B:1501:LEU:CD2	2.45	0.46
1:A:2098:PHE:CD2	1:A:2106:LEU:HD12	2.50	0.46
1:B:776:GLU:HB3	1:B:778:SER:OG	2.15	0.46
1:B:1415:PHE:HD2	1:B:1444:MET:HE1	1.79	0.46
1:A:1460:LEU:HD12	1:A:1463:GLU:OE1	2.15	0.46
1:A:65:PHE:CE2	1:A:83:LEU:HB3	2.49	0.46
1:B:112:SER:O	1:B:137:ARG:NH2	2.48	0.46
1:A:118:GLU:CD	1:B:118:GLU:HG3	2.34	0.46
1:B:1411:ASP:HB2	1:B:1440:PRO:CG	2.44	0.46
1:A:111:VAL:HG21	1:A:188:LEU:HD12	1.98	0.46
1:B:668:GLU:O	1:B:669:ASP:CB	2.62	0.46
1:B:2031:GLN:HB3	1:B:2034:TYR:HB3	1.98	0.46
1:A:92:ASP:HA	1:A:830:ILE:HB	1.97	0.46
1:B:1794:ILE:C	1:B:1795:LEU:HD23	2.36	0.46
1:B:39:ARG:NH1	1:B:226:GLU:OE2	2.47	0.46
1:B:384:ARG:NH1	1:B:384:ARG:HG3	2.16	0.46
1:A:1480:THR:HB	1:A:1482:PRO:HD2	1.97	0.46
1:A:1234:LEU:HD12	1:A:1234:LEU:O	2.16	0.46
1:A:1573:PHE:O	1:A:1576:VAL:HB	2.15	0.46
1:A:269:GLN:OE1	1:A:393:PHE:CE2	2.68	0.46
1:B:1616:MET:CE	1:B:1650:ILE:HD13	2.46	0.46
1:A:249:ALA:HB2	1:A:402:VAL:HB	1.97	0.46
1:A:831:SER:N	1:A:832:PRO:CD	2.79	0.46
1:A:1999:THR:HG22	1:A:2044:ILE:HD12	1.98	0.46
1:B:577:ILE:HG22	1:B:712:TRP:CD1	2.50	0.46
1:A:483:GLN:HG2	1:A:484:GLN:N	2.30	0.46
1:B:743:VAL:O	1:B:743:VAL:HG23	2.15	0.46
1:A:1226:LEU:CD2	1:A:1401:LEU:HD21	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:PHE:HB3	1:B:2105:VAL:HB	1.98	0.46
1:A:60:PHE:CD2	1:A:80:ARG:HD3	2.50	0.46
1:A:1414:VAL:HG11	1:A:1432:ILE:HD13	1.96	0.46
1:B:1220:LEU:HB3	1:B:1257:ARG:NH2	2.30	0.46
1:B:359:TYR:CG	1:B:376:VAL:HG11	2.50	0.46
1:B:2098:PHE:CE2	1:B:2106:LEU:CB	2.98	0.46
1:A:1231:ASP:O	1:A:1234:LEU:N	2.47	0.46
1:A:2098:PHE:CE2	1:A:2106:LEU:CB	2.98	0.46
1:A:1556:PRO:O	1:A:1557:ALA:C	2.53	0.46
1:B:1016:GLU:HA	1:B:1043:PRO:HG3	1.96	0.46
1:B:1786:LEU:C	1:B:1788:ASN:H	2.18	0.46
1:A:749:LEU:HD11	1:A:771:LEU:HD23	1.96	0.46
1:A:925:LEU:HD22	1:A:931:VAL:HG21	1.97	0.46
1:B:65:PHE:HA	1:B:147:PHE:CE1	2.50	0.46
1:B:1443:LEU:HD23	1:B:1443:LEU:HA	1.78	0.46
1:A:1602:GLU:OE2	1:A:1650:ILE:N	2.49	0.46
1:A:416:GLN:C	1:A:418:ALA:N	2.69	0.46
1:A:1262:LEU:HB3	1:A:1268:MET:SD	2.56	0.46
1:B:765:ALA:HB1	1:B:768:GLN:CG	2.46	0.46
1:B:1586:ASP:HA	1:B:1595:ARG:HH12	1.81	0.46
1:B:107:VAL:HG13	1:B:184:VAL:HB	1.96	0.46
1:B:1338:LEU:CD2	1:B:1406:GLN:HG3	2.46	0.46
1:A:1418:VAL:HG22	1:A:1425:TRP:CG	2.51	0.46
1:A:1220:LEU:HB3	1:A:1257:ARG:NH2	2.31	0.46
1:A:200:PHE:HE2	1:B:132:MET:HE1	1.80	0.46
1:B:1254:LEU:HD13	1:B:1316:VAL:HG12	1.98	0.46
1:B:1531:ALA:HA	1:B:1549:SER:H	1.81	0.46
1:B:1617:VAL:HG21	1:B:1626:VAL:CG1	2.46	0.46
1:B:1995:LYS:O	1:B:2041:MET:HE3	2.15	0.46
1:B:377:VAL:HG13	1:B:381:LEU:CD1	2.46	0.46
1:A:717:ILE:HD13	1:A:727:ALA:HB2	1.97	0.46
1:B:1651:VAL:HG13	1:B:1680:VAL:CA	2.31	0.46
1:B:657:ALA:O	1:B:661:PHE:HB2	2.16	0.46
1:B:166:LEU:C	1:B:166:LEU:HD23	2.36	0.46
1:A:856:CYS:HB3	1:B:856:CYS:HG	1.80	0.46
1:A:1532:PHE:HE1	1:A:1597:CYS:HB3	1.81	0.46
1:B:1239:SER:HA	1:B:1240:PRO:HD3	1.85	0.46
1:A:1725:ASP:OD2	1:A:1727:SER:HB3	2.15	0.46
1:A:1415:PHE:HD2	1:A:1444:MET:HE1	1.81	0.46
1:A:1676:GLY:HA2	1:A:1681:GLY:HA3	1.98	0.46
1:A:1689:LEU:O	1:A:1692:GLY:HA2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1472:VAL:CG1	1:A:1473:LEU:H	2.25	0.46
1:A:1347:HIS:HD2	1:A:1348:THR:O	1.99	0.46
1:A:1528:THR:CG2	1:A:1530:HIS:H	2.22	0.46
1:A:1222:ASP:HA	1:A:1226:LEU:HD11	1.96	0.46
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.50	0.46
1:B:1469:ILE:CG2	1:B:1469:ILE:O	2.64	0.46
1:A:706:LYS:HD2	1:A:706:LYS:N	2.31	0.46
1:A:1481:SER:N	1:A:1482:PRO:CD	2.79	0.46
1:B:81:MET:HG2	1:B:81:MET:H	1.62	0.46
1:A:9:MET:HE2	1:A:342:ILE:HG12	1.97	0.46
1:A:203:LEU:HD21	1:B:130:TYR:HA	1.98	0.46
1:A:1345:LEU:HD12	1:A:1402:PHE:O	2.16	0.46
1:B:1338:LEU:HD22	1:B:1406:GLN:NE2	2.31	0.45
1:A:2084:LEU:HD12	1:A:2111:LEU:O	2.15	0.45
1:A:33:VAL:HB	1:A:50:ARG:NH1	2.32	0.45
1:A:1257:ARG:O	1:A:1260:ALA:HB3	2.17	0.45
1:B:420:LEU:CD1	1:B:512:ARG:HD2	2.46	0.45
1:A:2070:LEU:HD11	1:A:2076:ASN:CG	2.36	0.45
1:B:1432:ILE:O	1:B:1432:ILE:HG22	2.16	0.45
1:A:965:PRO:O	1:A:967:PRO:HD3	2.16	0.45
1:B:988:SER:O	1:B:989:GLN:C	2.54	0.45
1:B:976:VAL:O	1:B:977:ASP:C	2.54	0.45
1:A:491:PRO:HD2	1:A:756:ALA:HA	1.97	0.45
1:B:431:LEU:C	1:B:431:LEU:HD23	2.36	0.45
1:B:1931:GLU:O	1:B:1933:ARG:N	2.50	0.45
1:B:1420:ASP:O	1:B:1425:TRP:CH2	2.70	0.45
1:B:269:GLN:OE1	1:B:393:PHE:CE2	2.69	0.45
1:A:856:CYS:O	1:A:858:SER:N	2.46	0.45
1:A:1419:GLU:OE2	1:A:1447:GLY:HA3	2.15	0.45
1:B:501:ALA:HA	1:B:766:LEU:HD11	1.98	0.45
1:B:460:VAL:CG2	1:B:465:MET:HG3	2.46	0.45
1:A:1390:VAL:HG13	1:A:1501:LEU:HD21	1.98	0.45
1:B:1603:PHE:HD2	1:B:1603:PHE:N	2.15	0.45
1:B:236:LYS:C	1:B:238:LEU:H	2.20	0.45
1:A:65:PHE:HA	1:A:147:PHE:CE1	2.51	0.45
1:A:72:ALA:HB3	1:A:842:TRP:CZ3	2.51	0.45
1:B:1064:HIS:HB2	1:B:1093:GLY:HA3	1.97	0.45
1:B:1886:SER:HA	1:B:1911:LYS:HB2	1.97	0.45
1:B:1754:GLN:OE1	1:B:1754:GLN:HA	2.16	0.45
1:A:1428:SER:O	1:A:1432:ILE:HG13	2.15	0.45
1:A:23:TRP:NE1	1:A:350:HIS:CD2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1418:VAL:HA	1:B:1425:TRP:CE3	2.51	0.45
1:B:635:PRO:O	1:B:637:GLY:N	2.50	0.45
1:A:1476:ASN:HB3	1:A:1486:MET:SD	2.56	0.45
1:B:979:ALA:HB1	1:B:983:ALA:HB3	1.98	0.45
1:A:1953:ARG:O	1:A:1957:THR:HB	2.16	0.45
1:A:133:ILE:HD12	1:A:143:ARG:HH21	1.80	0.45
1:B:1527:GLN:OE1	1:B:1872:ALA:HB1	2.15	0.45
1:A:1112:LEU:HD22	1:A:2110:VAL:HG11	1.98	0.45
1:A:142:ASN:HD22	1:B:396:GLY:HA3	1.81	0.45
1:B:1456:MET:HE3	1:B:2032:ALA:O	2.16	0.45
1:A:1466:GLY:O	1:A:1469:ILE:HB	2.17	0.45
1:B:1977:ASP:OD1	1:B:2031:GLN:HG2	2.15	0.45
1:A:1254:LEU:HD21	1:A:1318:ASN:HB2	1.98	0.45
1:A:1624:THR:HG22	1:A:1857:ARG:HH21	1.82	0.45
1:A:1857:ARG:NH1	1:A:1869:PRO:HB3	2.30	0.45
1:B:1095:LEU:O	1:B:1095:LEU:HD12	2.16	0.45
1:A:1124:HIS:NE2	1:A:1501:LEU:HD13	2.31	0.45
1:B:65:PHE:CE2	1:B:83:LEU:HB3	2.51	0.45
1:A:557:THR:HG21	1:A:603:SER:OG	2.16	0.45
1:B:1456:MET:CE	1:B:2032:ALA:HB1	2.46	0.45
1:B:623:VAL:HG13	1:B:672:VAL:HG22	1.97	0.45
1:B:1953:ARG:O	1:B:1957:THR:HB	2.16	0.45
1:B:1953:ARG:HA	1:B:2005:VAL:HG11	1.98	0.45
1:B:159:THR:HB	1:B:162:SER:HG	1.81	0.45
1:B:1107:ARG:O	1:B:1107:ARG:HG3	2.17	0.45
1:A:963:GLU:C	1:A:965:PRO:HD3	2.37	0.45
1:B:1748:LEU:HD23	1:B:1748:LEU:HA	1.66	0.45
1:A:1780:LEU:HD12	1:A:1781:GLY:N	2.32	0.45
1:A:618:GLY:O	1:A:679:GLY:O	2.34	0.45
1:A:1802:GLU:O	1:A:1802:GLU:HG2	2.17	0.45
1:B:1248:LEU:CD2	1:B:1277:ARG:HE	2.30	0.45
1:A:1545:ARG:CG	1:A:1545:ARG:NH1	2.76	0.45
1:A:1694:ARG:NH2	1:A:1735:HIS:HB3	2.31	0.45
1:B:1629:LEU:HB3	1:B:1631:HIS:CE1	2.51	0.45
1:A:1629:LEU:O	1:A:1630:GLN:C	2.55	0.45
1:B:1931:GLU:O	1:B:1934:ARG:N	2.50	0.45
1:A:493:TRP:CD2	1:A:752:VAL:HG22	2.52	0.45
1:A:2022:VAL:CG1	1:A:2022:VAL:O	2.64	0.45
1:B:1904:LEU:HD23	1:B:1904:LEU:HA	1.62	0.45
1:B:1541:LEU:HD13	1:B:1840:PHE:HB3	1.97	0.45
1:B:2098:PHE:CD2	1:B:2106:LEU:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:HB2	1:B:45:TYR:CE2	2.52	0.45
1:A:1231:ASP:O	1:A:1232:THR:C	2.55	0.45
1:A:1235:GLU:OE2	1:A:1515:ARG:NH1	2.50	0.45
1:A:1882:PRO:HD2	1:A:1887:TYR:OH	2.17	0.45
1:B:838:HIS:O	1:B:840:GLN:N	2.50	0.45
1:A:1786:LEU:HD23	1:A:1786:LEU:HA	1.73	0.45
1:B:169:GLN:C	1:B:169:GLN:HE21	2.19	0.45
1:B:98:ALA:HA	1:B:101:ARG:CG	2.46	0.45
1:A:1599:LEU:O	1:A:1622:LEU:HD12	2.16	0.45
1:B:258:GLU:HB2	1:B:259:GLN:NE2	2.32	0.45
1:B:2056:LEU:HA	1:B:2104:PRO:O	2.16	0.45
1:A:1095:LEU:HD12	1:A:1095:LEU:O	2.17	0.45
1:B:1137:GLN:HG2	1:B:1396:PHE:CZ	2.52	0.45
1:B:1973:MET:CB	1:B:1995:LYS:HE3	2.46	0.45
1:A:191:LEU:HD22	1:A:224:ARG:CZ	2.47	0.45
1:A:752:VAL:HA	1:A:753:PRO:HD3	1.87	0.45
1:A:548:ASP:OD2	1:A:611:LYS:NZ	2.50	0.45
1:A:995:ASP:O	1:A:998:LEU:HB2	2.16	0.45
1:B:1481:SER:N	1:B:1482:PRO:CD	2.80	0.45
1:A:724:GLY:O	1:A:728:ARG:HB2	2.16	0.45
1:B:475:GLY:C	1:B:477:ALA:H	2.20	0.45
1:B:734:TYR:C	1:B:734:TYR:CD2	2.89	0.45
1:A:1001:TYR:CE2	1:A:1040:ILE:HD13	2.52	0.45
1:B:1890:THR:O	1:B:1971:LEU:HB2	2.17	0.45
1:A:1818:ILE:HG12	1:A:1823:VAL:CG1	2.46	0.45
1:A:1248:LEU:HD21	1:A:1277:ARG:NE	2.30	0.45
1:A:1757:VAL:O	1:A:1760:LEU:HB2	2.17	0.45
1:A:1259:PRO:HG2	1:A:1292:LEU:HD22	1.99	0.45
1:B:2036:PHE:CD2	1:B:2036:PHE:C	2.91	0.45
1:B:1343:PHE:HE2	1:B:1390:VAL:HG21	1.82	0.45
1:B:1567:TYR:O	1:B:1856:VAL:HG23	2.16	0.45
1:A:217:ALA:HB2	1:A:363:ASN:HA	1.99	0.45
1:B:1449:SER:C	1:B:1477:LEU:HD22	2.37	0.45
1:B:1123:PRO:O	1:B:1393:LYS:NZ	2.50	0.45
1:A:2064:GLY:O	1:A:2066:VAL:N	2.50	0.45
1:A:1474:VAL:HA	1:A:1504:ASN:O	2.17	0.45
1:B:699:ARG:O	1:B:703:LEU:HD23	2.17	0.45
1:A:1931:GLU:O	1:A:1934:ARG:N	2.50	0.45
1:A:895:THR:HA	1:A:935:VAL:HG11	1.99	0.45
1:B:1689:LEU:HD23	1:B:1689:LEU:HA	1.70	0.45
1:B:1567:TYR:CE1	1:B:1606:ARG:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1541:LEU:O	1:B:1837:GLU:HG3	2.17	0.44
1:B:581:SER:HB2	1:B:683:HIS:NE2	2.32	0.44
1:B:159:THR:HG22	1:B:398:SER:HB3	1.99	0.44
1:B:103:THR:CG2	1:B:104:SER:N	2.80	0.44
1:A:75:MET:SD	1:A:79:LEU:HD23	2.56	0.44
1:B:1678:GLY:O	1:B:1682:GLN:HG3	2.16	0.44
1:A:1473:LEU:HG	1:A:1503:MET:HA	2.00	0.44
1:A:326:LYS:CE	1:A:336:SER:HB2	2.47	0.44
1:B:1442:TRP:CH2	1:B:1497:LEU:HD23	2.52	0.44
1:B:111:VAL:O	1:B:111:VAL:HG12	2.17	0.44
1:A:1449:SER:O	1:A:1477:LEU:HD22	2.17	0.44
1:A:627:TRP:CH2	1:A:640:PRO:HB2	2.52	0.44
1:A:1262:LEU:O	1:A:1268:MET:HG3	2.17	0.44
1:B:581:SER:HB2	1:B:683:HIS:CE1	2.52	0.44
1:A:595:THR:HG22	1:A:597:GLU:HG2	1.98	0.44
1:A:1971:LEU:HD21	1:A:2019:PHE:CD2	2.53	0.44
1:A:620:MET:HE1	1:A:682:PHE:HB2	1.99	0.44
1:A:1781:GLY:O	1:A:1784:VAL:HG23	2.17	0.44
1:A:158:ASP:O	1:B:156:THR:OG1	2.34	0.44
1:B:108:TRP:CD1	1:B:171:ALA:HB2	2.52	0.44
1:B:1251:ASP:O	1:B:1253:GLN:HG3	2.17	0.44
1:A:1065:ARG:HD3	1:A:1065:ARG:HA	1.82	0.44
1:B:647:ASP:OD1	1:B:647:ASP:N	2.50	0.44
1:A:118:GLU:HG3	1:B:118:GLU:CD	2.37	0.44
1:A:2043:ARG:HD3	1:A:2043:ARG:HA	1.69	0.44
1:B:1245:VAL:O	1:B:1315:LEU:HD12	2.16	0.44
1:A:643:HIS:HA	1:A:649:VAL:HG22	1.99	0.44
1:B:1818:ILE:HG12	1:B:1823:VAL:CG1	2.48	0.44
1:A:2015:TYR:HD2	1:A:2099:LEU:HD22	1.78	0.44
1:B:1893:LEU:HB3	1:B:1925:GLN:CD	2.38	0.44
1:B:321:LEU:H	1:B:321:LEU:CD1	2.31	0.44
1:A:1617:VAL:HG12	1:A:1619:ALA:H	1.82	0.44
1:B:2111:LEU:HA	1:B:2111:LEU:HD23	1.83	0.44
1:B:1567:TYR:C	1:B:1856:VAL:HG23	2.37	0.44
1:A:1476:ASN:HA	1:A:1486:MET:CE	2.47	0.44
1:A:850:PHE:HB3	1:A:851:PRO:HD2	2.00	0.44
1:A:166:LEU:C	1:A:166:LEU:HD23	2.38	0.44
1:B:831:SER:N	1:B:832:PRO:CD	2.80	0.44
1:A:1250:GLY:N	1:A:1276:ASP:OD2	2.50	0.44
1:A:409:ARG:HA	1:A:410:PRO:HD3	1.73	0.44
1:B:13:LEU:HD13	1:B:22:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ASN:HB2	1:B:334:PRO:HD2	1.98	0.44
1:A:305:LEU:O	1:A:309:VAL:HG23	2.17	0.44
1:A:1456:MET:CG	1:A:2036:PHE:HB2	2.46	0.44
1:A:1112:LEU:O	1:A:1114:PRO:HD3	2.17	0.44
1:B:605:TRP:O	1:B:606:ARG:C	2.56	0.44
1:B:907:LEU:HA	1:B:907:LEU:HD12	1.87	0.44
1:B:62:ALA:HB1	1:B:67:VAL:HG23	2.00	0.44
1:B:1445:ALA:O	1:B:1476:ASN:ND2	2.51	0.44
1:B:2103:HIS:HA	1:B:2104:PRO:HD3	1.78	0.44
1:A:1515:ARG:HD3	1:A:1515:ARG:HA	1.55	0.44
1:B:582:LEU:O	1:B:585:VAL:HG23	2.18	0.44
1:A:81:MET:O	1:A:85:VAL:HG22	2.18	0.44
1:B:2070:LEU:HD11	1:B:2076:ASN:CG	2.37	0.44
1:B:9:MET:CE	1:B:342:ILE:HA	2.48	0.44
1:B:1768:GLU:CA	1:B:1768:GLU:OE1	2.64	0.44
1:A:6:ILE:HG21	1:A:345:LEU:HD11	2.00	0.44
1:B:1986:GLU:HA	1:B:1989:GLN:HG2	2.00	0.44
1:A:1995:LYS:O	1:A:2041:MET:HE3	2.17	0.44
1:A:815:LEU:HB2	1:A:816:PHE:CD1	2.53	0.44
1:A:1571:LEU:O	1:A:1851:LYS:HD2	2.17	0.44
1:A:1487:HIS:O	1:A:1487:HIS:CD2	2.71	0.44
1:A:1487:HIS:HA	1:A:1488:PRO:HD3	1.80	0.44
1:A:309:VAL:C	1:A:311:ALA:H	2.21	0.44
1:A:309:VAL:HG13	1:A:313:CYS:SG	2.58	0.44
1:B:353:TRP:CZ2	1:B:383:ILE:HD12	2.53	0.44
1:B:1993:LYS:N	1:B:1994:PRO:CD	2.81	0.44
1:B:1766:PHE:HD2	1:B:1791:PHE:CE1	2.36	0.44
1:A:1973:MET:CB	1:A:1995:LYS:HE3	2.47	0.44
1:B:963:GLU:C	1:B:965:PRO:HD3	2.38	0.44
1:A:2066:VAL:HG22	1:A:2088:ILE:HD12	2.00	0.44
1:A:2036:PHE:C	1:A:2036:PHE:CD2	2.90	0.44
1:A:1249:ALA:N	1:A:1276:ASP:OD1	2.40	0.44
1:A:1052:THR:HG22	1:A:1053:ARG:HG3	1.98	0.44
1:A:1290:GLU:HG2	1:A:1291:GLN:N	2.33	0.44
1:A:213:ARG:HG3	1:A:213:ARG:HH11	1.81	0.44
1:B:1221:LEU:O	1:B:1221:LEU:HG	2.18	0.44
1:B:1416:LEU:CD2	1:B:1429:LEU:HG	2.47	0.44
1:A:1657:TYR:CE1	1:A:1799:LEU:HD11	2.53	0.44
1:A:359:TYR:CG	1:A:376:VAL:HG11	2.53	0.44
1:B:1475:SER:HB3	1:B:1505:VAL:CG1	2.47	0.44
1:B:19:LEU:HA	1:B:19:LEU:HD23	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:895:THR:HA	1:B:935:VAL:HG11	2.00	0.44
1:A:190:VAL:HG12	1:A:192:LEU:HG	2.00	0.44
1:A:587:CYS:O	1:A:591:ASP:N	2.50	0.44
1:A:642:CYS:HA	1:A:743:VAL:CG2	2.48	0.44
1:A:189:ASN:O	1:A:226:GLU:HB2	2.17	0.44
1:A:27:ILE:C	1:A:29:GLY:H	2.20	0.44
1:A:331:HIS:HE1	1:A:333:GLU:HA	1.83	0.44
1:A:889:THR:CG2	1:A:1032:LEU:CB	2.96	0.44
1:B:1971:LEU:HD21	1:B:2019:PHE:CD2	2.52	0.44
1:A:499:MET:HG3	1:A:502:GLN:NE2	2.32	0.44
1:A:1818:ILE:HG12	1:A:1823:VAL:HG11	1.99	0.44
1:A:1231:ASP:HB3	1:A:1515:ARG:HD2	2.00	0.44
1:A:1882:PRO:HA	1:A:1883:PRO:HD3	1.85	0.44
1:A:1955:LEU:O	1:A:1958:GLU:HB2	2.17	0.44
1:A:1762:GLN:O	1:A:1763:HIS:HB2	2.18	0.44
1:A:169:GLN:OE1	1:A:250:GLY:HA2	2.17	0.44
1:B:587:CYS:O	1:B:591:ASP:N	2.51	0.44
1:A:259:GLN:H	1:A:259:GLN:CD	2.20	0.44
1:A:120:LEU:C	1:A:127:LEU:HD13	2.38	0.44
1:A:1754:GLN:HA	1:A:1754:GLN:OE1	2.17	0.44
1:B:1338:LEU:HD13	1:B:1406:GLN:CG	2.48	0.43
1:B:23:TRP:NE1	1:B:350:HIS:CD2	2.86	0.43
1:A:123:ASP:CB	1:A:126:THR:HB	2.42	0.43
1:A:1216:LEU:HD13	1:A:1217:LEU:H	1.83	0.43
1:B:1118:LYS:HD2	1:B:2103:HIS:ND1	2.33	0.43
1:A:1953:ARG:HA	1:A:2005:VAL:HG11	1.99	0.43
1:B:91:VAL:HG21	1:B:834:ILE:HD13	1.99	0.43
1:B:1466:GLY:HA2	1:B:1469:ILE:CD1	2.48	0.43
1:A:984:GLU:O	1:A:985:PHE:CB	2.64	0.43
1:A:159:THR:HG22	1:A:398:SER:HB3	2.00	0.43
1:B:143:ARG:NH1	1:B:143:ARG:HG2	2.33	0.43
1:B:914:PHE:HB2	1:B:1057:ILE:HB	2.00	0.43
1:B:925:LEU:CD2	1:B:931:VAL:HG21	2.48	0.43
1:B:190:VAL:HG12	1:B:192:LEU:HG	1.99	0.43
1:B:416:GLN:C	1:B:418:ALA:N	2.70	0.43
1:B:302:PRO:HG3	1:B:363:ASN:ND2	2.33	0.43
1:A:1887:TYR:CD2	1:A:1967:GLY:HA3	2.46	0.43
1:B:1553:TYR:O	1:B:1554:ALA:HB2	2.18	0.43
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.31	0.43
1:A:1609:SER:C	1:A:1611:ARG:H	2.21	0.43
1:A:470:TYR:C	1:A:470:TYR:CD1	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:GLY:O	1:A:715:THR:HG21	2.19	0.43
1:A:525:GLN:HA	1:A:525:GLN:NE2	2.32	0.43
1:A:1483:ALA:HB1	1:A:1508:ASP:HA	2.01	0.43
1:B:2043:ARG:HA	1:B:2043:ARG:HD3	1.71	0.43
1:A:1857:ARG:NH1	1:A:1869:PRO:HB2	2.33	0.43
1:A:1786:LEU:C	1:A:1788:ASN:H	2.21	0.43
1:A:1995:LYS:HB3	1:A:2041:MET:SD	2.58	0.43
1:B:1769:ILE:HG22	1:B:1770:GLY:N	2.32	0.43
1:B:948:ASP:OD1	1:B:948:ASP:C	2.57	0.43
1:A:1442:TRP:CH2	1:A:1497:LEU:HD23	2.54	0.43
1:A:1036:LEU:O	1:A:1037:HIS:C	2.57	0.43
1:B:627:TRP:CZ3	1:B:640:PRO:HB2	2.53	0.43
1:A:366:ILE:CG1	1:A:366:ILE:O	2.66	0.43
1:A:856:CYS:C	1:A:858:SER:N	2.72	0.43
1:A:639:VAL:HG12	1:A:640:PRO:O	2.18	0.43
1:A:1299:TRP:NE1	1:A:1304:PRO:O	2.51	0.43
1:A:1993:LYS:H	1:A:1994:PRO:CD	2.32	0.43
1:A:542:ASP:OD1	1:A:542:ASP:C	2.56	0.43
1:A:1624:THR:HG22	1:A:1857:ARG:NH2	2.33	0.43
1:A:343:LYS:HE3	1:A:354:ALA:HB3	2.00	0.43
1:A:830:ILE:O	1:A:831:SER:C	2.56	0.43
1:A:811:ASN:HA	1:A:812:PRO:HD3	1.82	0.43
1:A:1619:ALA:O	1:A:1620:GLU:HB2	2.18	0.43
1:A:1238:ALA:O	1:A:1462:LYS:HG3	2.17	0.43
1:A:1662:ARG:NH1	1:A:1662:ARG:HG2	2.33	0.43
1:B:98:ALA:CA	1:B:101:ARG:HG3	2.47	0.43
1:A:1469:ILE:CG2	1:A:1469:ILE:O	2.66	0.43
1:B:259:GLN:N	1:B:259:GLN:CD	2.72	0.43
1:B:1569:THR:HG23	1:B:1602:GLU:O	2.19	0.43
1:B:1234:LEU:HD21	1:B:1268:MET:HE3	2.01	0.43
1:A:2006:THR:HG21	1:A:2048:ARG:NH2	2.32	0.43
1:B:185:VAL:HB	1:B:231:VAL:HG23	2.00	0.43
1:A:870:SER:HA	1:A:871:PRO:HD3	1.88	0.43
1:A:1049:TYR:CZ	1:A:1103:VAL:HG23	2.54	0.43
1:B:1675:SER:O	1:B:1681:GLY:HA3	2.19	0.43
1:B:1648:VAL:HB	1:B:1649:PRO:HD3	1.99	0.43
1:A:336:SER:OG	1:A:337:GLY:N	2.51	0.43
1:B:23:TRP:CE2	1:B:27:ILE:HG12	2.53	0.43
1:B:637:GLY:O	1:B:685:TYR:HE2	2.00	0.43
1:B:982:THR:O	1:B:984:GLU:N	2.49	0.43
1:A:1118:LYS:HA	1:A:2106:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1882:PRO:HG2	1:A:1885:LYS:HD2	2.01	0.43
1:B:228:VAL:CG2	1:B:228:VAL:O	2.67	0.43
1:B:290:ILE:CG2	1:B:322:ILE:HG12	2.49	0.43
1:A:1864:ALA:HA	1:A:1865:PRO:HD3	1.82	0.43
1:A:1929:VAL:HG13	1:A:1939:VAL:HG11	1.99	0.43
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.62	0.43
1:B:1112:LEU:O	1:B:1114:PRO:HD3	2.17	0.43
1:B:946:VAL:O	1:B:954:ILE:HB	2.18	0.43
1:B:1333:ASN:C	1:B:1335:ALA:N	2.72	0.43
1:B:14:PRO:HA	1:B:53:LYS:O	2.19	0.43
1:B:161:CYS:HB3	1:B:331:HIS:CE1	2.53	0.43
1:B:654:PRO:HG3	1:B:685:TYR:OH	2.18	0.43
1:A:78:GLN:HB3	1:A:188:LEU:HD13	2.01	0.43
1:A:1476:ASN:CB	1:A:1486:MET:SD	3.06	0.43
1:B:6:ILE:HG21	1:B:345:LEU:HD11	2.01	0.43
1:B:752:VAL:HA	1:B:753:PRO:HD3	1.89	0.43
1:B:1995:LYS:HA	1:B:2041:MET:HE3	2.01	0.43
1:A:782:ILE:HA	1:A:783:PRO:HD3	1.88	0.43
1:A:1757:VAL:HG11	1:A:1784:VAL:HG21	2.01	0.43
1:A:1251:ASP:O	1:A:1253:GLN:HG3	2.19	0.43
1:A:51:MET:HB2	1:A:53:LYS:HE3	2.01	0.43
1:B:283:ASP:C	1:B:285:GLU:H	2.22	0.43
1:A:23:TRP:CH2	1:A:347:SER:HA	2.54	0.43
1:B:137:ARG:O	1:B:140:MET:HG2	2.19	0.43
1:B:416:GLN:OE1	1:B:817:PRO:HG2	2.18	0.43
1:B:363:ASN:HA	1:B:364:PRO:HD3	1.81	0.43
1:B:499:MET:HG3	1:B:502:GLN:NE2	2.34	0.43
1:B:252:ASN:N	1:B:272:LEU:HD13	2.33	0.43
1:A:1083:ASP:O	1:A:1086:LEU:N	2.51	0.43
1:A:524:ASP:OD1	1:A:534:VAL:N	2.52	0.43
1:B:1984:THR:C	1:B:1986:GLU:H	2.22	0.43
1:B:2066:VAL:HG22	1:B:2088:ILE:HD12	2.00	0.43
1:A:2031:GLN:HB3	1:A:2034:TYR:HB3	1.99	0.43
1:A:108:TRP:CD1	1:A:171:ALA:HB2	2.54	0.43
1:A:129:GLY:HA3	1:B:202:LYS:HB2	2.00	0.43
1:B:161:CYS:HB3	1:B:331:HIS:HE1	1.84	0.43
1:A:206:LEU:HA	1:A:206:LEU:HD23	1.64	0.43
1:A:1235:GLU:HG2	1:A:1235:GLU:H	1.58	0.43
1:A:1390:VAL:HG22	1:A:1501:LEU:HD21	2.00	0.43
1:B:309:VAL:C	1:B:311:ALA:H	2.22	0.43
1:B:1137:GLN:NE2	1:B:1396:PHE:CE1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:LEU:HD12	1:B:954:ILE:N	2.34	0.43
1:B:1389:LEU:HD23	1:B:1389:LEU:HA	1.83	0.43
1:A:295:THR:HG22	1:A:331:HIS:CD2	2.53	0.43
1:B:23:TRP:CZ2	1:B:27:ILE:HG12	2.54	0.43
1:A:217:ALA:C	1:A:219:GLY:H	2.21	0.43
1:B:1477:LEU:HD11	1:B:2043:ARG:CD	2.43	0.43
1:B:1515:ARG:HD3	1:B:1515:ARG:HA	1.30	0.43
1:B:200:PHE:HB3	1:B:206:LEU:CG	2.48	0.43
1:B:1525:GLU:OE1	1:B:1874:THR:HG23	2.19	0.43
1:A:1345:LEU:HD13	1:A:1403:LEU:HD13	2.01	0.43
1:A:548:ASP:OD1	1:A:550:VAL:N	2.50	0.43
1:A:863:LYS:HB3	1:A:930:THR:HG21	2.01	0.43
1:A:1842:TYR:CE2	1:A:1848:HIS:HB3	2.53	0.43
1:B:1555:LEU:HA	1:B:1555:LEU:HD12	1.93	0.43
1:B:1921:ARG:HB2	1:B:1921:ARG:HE	1.65	0.43
1:B:470:TYR:CD1	1:B:470:TYR:C	2.92	0.43
1:A:1420:ASP:O	1:A:1425:TRP:CZ3	2.71	0.42
1:A:1657:TYR:CZ	1:A:1662:ARG:CD	3.02	0.42
1:B:259:GLN:HB2	1:B:263:PHE:CD1	2.54	0.42
1:B:1119:PHE:CZ	1:B:1514:PHE:HB3	2.54	0.42
1:A:662:LEU:C	1:A:664:GLN:N	2.71	0.42
1:B:1955:LEU:O	1:B:1958:GLU:HB2	2.19	0.42
1:B:1469:ILE:CG2	1:B:1471:CYS:SG	3.07	0.42
1:A:248:ASN:HD22	1:A:249:ALA:H	1.65	0.42
1:B:1085:ASN:C	1:B:1086:LEU:HD23	2.40	0.42
1:A:262:THR:O	1:A:262:THR:HG22	2.18	0.42
1:B:497:SER:HB2	1:B:762:ALA:HB2	2.00	0.42
1:B:1780:LEU:HD12	1:B:1781:GLY:H	1.83	0.42
1:A:1815:LYS:O	1:A:1819:GLN:HG3	2.18	0.42
1:B:1536:LEU:HG	1:B:1543:SER:O	2.19	0.42
1:B:111:VAL:HG21	1:B:188:LEU:HD12	2.01	0.42
1:A:1032:LEU:O	1:A:1035:MET:HB2	2.19	0.42
1:B:1477:LEU:O	1:B:1507:ARG:CG	2.67	0.42
1:B:1818:ILE:HG12	1:B:1823:VAL:HG11	2.00	0.42
1:A:119:ALA:HB2	1:A:850:PHE:CE2	2.53	0.42
1:B:1977:ASP:O	1:B:1978:ALA:HB2	2.19	0.42
1:A:470:TYR:CD2	1:A:801:GLY:HA3	2.55	0.42
1:A:1661:VAL:HG21	1:A:1810:VAL:HG22	2.01	0.42
1:B:178:GLY:O	1:B:179:GLU:C	2.58	0.42
1:A:1468:ARG:HA	1:A:1468:ARG:HD3	1.85	0.42
1:B:1468:ARG:HD3	1:B:1468:ARG:HA	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:LYS:HB3	1:B:930:THR:HG21	2.01	0.42
1:A:743:VAL:O	1:A:743:VAL:HG23	2.20	0.42
1:B:1315:LEU:HD23	1:B:1344:LEU:HD11	2.00	0.42
1:A:808:VAL:HG12	1:A:809:SER:H	1.84	0.42
1:A:1090:VAL:HG22	1:A:1095:LEU:HB2	2.02	0.42
1:A:2041:MET:HA	1:A:2044:ILE:HG13	2.02	0.42
1:A:1896:PHE:CE2	1:A:2019:PHE:CE1	3.07	0.42
1:B:557:THR:HA	1:B:560:GLN:HE21	1.84	0.42
1:B:1786:LEU:HD23	1:B:1786:LEU:HA	1.82	0.42
1:A:708:ARG:HD3	1:A:727:ALA:O	2.19	0.42
1:B:475:GLY:O	1:B:477:ALA:N	2.51	0.42
1:A:1894:GLY:O	1:A:1895:GLY:C	2.57	0.42
1:B:1636:VAL:HG22	1:B:1636:VAL:O	2.19	0.42
1:A:1411:ASP:OD2	1:A:1439:ARG:HB2	2.19	0.42
1:A:39:ARG:NH1	1:A:226:GLU:OE2	2.51	0.42
1:B:27:ILE:C	1:B:29:GLY:H	2.21	0.42
1:A:2095:LEU:CD1	1:A:2099:LEU:HG	2.49	0.42
1:B:1993:LYS:H	1:B:1994:PRO:CD	2.31	0.42
1:B:972:THR:CG2	1:B:1081:VAL:CG2	2.96	0.42
1:A:48:PRO:HD3	1:A:201:MET:CE	2.50	0.42
1:B:1551:LEU:HD21	1:B:1627:LEU:CD2	2.48	0.42
1:B:1676:GLY:O	1:B:1682:GLN:HG2	2.20	0.42
1:A:202:LYS:HB2	1:B:129:GLY:HA3	2.02	0.42
1:A:1598:MET:O	1:A:1598:MET:HG2	2.20	0.42
1:A:347:SER:HB2	1:A:352:VAL:O	2.19	0.42
1:B:263:PHE:HE2	1:B:303:GLN:HE21	1.66	0.42
1:B:1670:SER:OG	1:B:1741:VAL:HA	2.19	0.42
1:A:1787:LYS:HB2	1:A:1789:VAL:HG23	2.01	0.42
1:A:321:LEU:HD12	1:A:321:LEU:H	1.84	0.42
1:B:40:TRP:CZ3	1:B:194:PRO:HA	2.55	0.42
1:B:40:TRP:HB3	1:B:847:ALA:CB	2.49	0.42
1:A:606:ARG:HA	1:A:694:LEU:HD11	2.00	0.42
1:A:925:LEU:CD2	1:A:931:VAL:HG21	2.49	0.42
1:B:895:THR:O	1:B:898:THR:HB	2.20	0.42
1:A:1585:PRO:HB3	1:A:1598:MET:CE	2.49	0.42
1:A:988:SER:O	1:A:989:GLN:C	2.56	0.42
1:B:1757:VAL:O	1:B:1760:LEU:HB2	2.19	0.42
1:A:289:TYR:CD2	1:A:289:TYR:C	2.93	0.42
1:A:1734:ARG:C	1:A:1736:THR:N	2.72	0.42
1:A:189:ASN:HB2	1:A:334:PRO:HD2	1.99	0.42
1:B:165:LEU:HD23	1:B:400:VAL:CG2	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:PRO:O	1:B:368:ALA:HB3	2.20	0.42
1:A:1656:TYR:O	1:A:1657:TYR:C	2.54	0.42
1:B:82:LEU:HG	1:B:144:LEU:HD13	2.02	0.42
1:A:1245:VAL:HB	1:A:1315:LEU:CD1	2.49	0.42
1:B:1222:ASP:N	1:B:1222:ASP:OD1	2.49	0.42
1:A:1119:PHE:HB3	1:A:2105:VAL:HB	2.01	0.42
1:B:462:PRO:HA	1:B:465:MET:O	2.19	0.42
1:A:321:LEU:HD23	1:A:381:LEU:CD1	2.48	0.42
1:A:1996:TYR:CD2	1:A:1997:SER:N	2.85	0.42
1:A:765:ALA:HB1	1:A:768:GLN:CG	2.49	0.42
1:A:211:THR:HG22	1:A:212:CYS:N	2.34	0.42
1:A:644:ASN:HB3	1:A:770:VAL:HG11	2.01	0.42
1:A:1433:LEU:HD11	1:A:1465:GLY:C	2.40	0.42
1:B:1815:LYS:O	1:B:1819:GLN:HG3	2.20	0.42
1:B:423:LEU:HB2	1:B:797:LEU:HD22	2.01	0.42
1:B:2049:ARG:HD2	1:B:2049:ARG:HA	1.84	0.42
1:B:55:LYS:HB3	1:B:55:LYS:HE2	1.69	0.42
1:A:27:ILE:HD13	1:A:27:ILE:HA	1.81	0.42
1:B:1382:PHE:HA	1:B:1387:LEU:HD12	2.01	0.42
1:A:1637:PRO:O	1:A:1639:THR:N	2.52	0.42
1:A:98:ALA:HA	1:A:101:ARG:CG	2.49	0.42
1:A:257:LYS:NZ	1:A:261:VAL:O	2.51	0.42
1:A:228:VAL:CG2	1:A:228:VAL:O	2.67	0.42
1:A:1603:PHE:HZ	1:A:1628:LEU:HD22	1.84	0.42
1:A:163:SER:O	1:A:167:ALA:N	2.47	0.42
1:A:353:TRP:O	1:A:355:PRO:HD3	2.19	0.42
1:B:305:LEU:HD22	1:B:322:ILE:CD1	2.50	0.42
1:A:1240:PRO:HB3	1:A:1267:VAL:O	2.20	0.42
1:B:1711:ARG:HG2	1:B:1712:PHE:CE1	2.55	0.42
1:B:416:GLN:HE21	1:B:448:LEU:CD1	2.33	0.42
1:A:1514:PHE:O	1:A:1515:ARG:NH1	2.53	0.42
1:B:193:LYS:HA	1:B:194:PRO:HD3	1.85	0.42
1:A:1239:SER:C	1:A:1241:LYS:H	2.23	0.42
1:A:620:MET:CE	1:A:682:PHE:O	2.66	0.42
1:B:876:VAL:HG12	1:B:876:VAL:O	2.20	0.42
1:A:1879:THR:HG1	1:A:1903:TRP:HH2	1.65	0.42
1:B:409:ARG:HA	1:B:410:PRO:HD3	1.74	0.42
1:B:5:VAL:HG21	1:B:242:VAL:HG22	2.01	0.42
1:A:948:ASP:C	1:A:948:ASP:OD1	2.58	0.42
1:A:672:VAL:HG12	1:A:672:VAL:O	2.18	0.42
1:A:384:ARG:NH1	1:A:384:ARG:CG	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PRO:HA	1:A:366:ILE:CG2	2.49	0.42
1:A:166:LEU:CD1	1:A:251:THR:HG21	2.49	0.42
1:A:595:THR:HG22	1:A:596:GLN:N	2.35	0.42
1:B:527:LEU:HD11	1:B:554:VAL:HG11	2.01	0.42
1:A:795:PHE:CE1	1:A:799:ASN:ND2	2.86	0.42
1:A:1451:SER:O	1:A:2036:PHE:CE1	2.73	0.42
1:A:495:ILE:HG12	1:A:758:VAL:HG13	2.02	0.42
1:B:1763:HIS:HA	1:B:1788:ASN:O	2.20	0.42
1:B:1801:GLU:O	1:B:1803:GLY:N	2.53	0.42
1:A:283:ASP:C	1:A:285:GLU:H	2.23	0.42
1:B:1941:VAL:O	1:B:1941:VAL:HG12	2.18	0.42
1:A:899:LEU:HA	1:A:899:LEU:HD12	1.82	0.42
1:B:1303:ASN:OD1	1:B:1332:GLY:HA3	2.19	0.42
1:A:420:LEU:HD11	1:A:512:ARG:HB3	2.01	0.42
1:A:1116:LEU:HD22	1:A:2098:PHE:CE1	2.55	0.42
1:B:1234:LEU:HD12	1:B:1234:LEU:O	2.19	0.42
1:B:1671:VAL:HG23	1:B:1743:LEU:HD13	2.02	0.42
1:A:1123:PRO:HA	1:A:1512:GLY:HA3	2.01	0.42
1:B:270:GLU:HG3	1:B:311:ALA:HB2	2.01	0.42
1:A:19:LEU:HA	1:A:19:LEU:HD23	1.68	0.42
1:B:1038:MET:CE	1:B:1041:LEU:HD23	2.50	0.42
1:A:1557:ALA:O	1:A:1560:GLN:HB3	2.20	0.42
1:B:1757:VAL:HG11	1:B:1784:VAL:HG21	2.01	0.42
1:A:178:GLY:O	1:A:179:GLU:C	2.57	0.42
1:A:1862:GLY:O	1:A:1863:PRO:C	2.59	0.42
1:A:114:SER:O	1:A:117:SER:HB3	2.19	0.42
1:B:1303:ASN:C	1:B:1333:ASN:HB2	2.41	0.41
1:A:1480:THR:CG2	1:A:1482:PRO:HD2	2.50	0.41
1:A:253:THR:O	1:A:254:ASP:C	2.59	0.41
1:A:503:TRP:HB3	1:A:787:LYS:HD2	2.02	0.41
1:B:2064:GLY:O	1:B:2066:VAL:N	2.53	0.41
1:B:147:PHE:C	1:B:147:PHE:CD2	2.93	0.41
1:B:1537:SER:H	1:B:1543:SER:HB2	1.85	0.41
1:B:119:ALA:HB2	1:B:850:PHE:CZ	2.55	0.41
1:A:1656:TYR:CE2	1:A:1687:ILE:HD13	2.55	0.41
1:B:979:ALA:O	1:B:980:ASP:C	2.58	0.41
1:A:359:TYR:CD2	1:A:376:VAL:HG11	2.55	0.41
1:A:366:ILE:HD11	1:A:369:LEU:HD11	2.01	0.41
1:A:254:ASP:HB2	1:A:257:LYS:HE2	2.02	0.41
1:A:1993:LYS:N	1:A:1994:PRO:CD	2.82	0.41
1:A:9:MET:CE	1:A:342:ILE:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:VAL:HG12	1:B:130:TYR:CE2	2.54	0.41
1:A:776:GLU:HB3	1:A:778:SER:H	1.84	0.41
1:A:1873:LEU:HD22	1:A:1874:THR:N	2.34	0.41
1:B:1966:GLY:HA2	1:B:2013:LEU:HA	2.02	0.41
1:A:630:CYS:C	1:A:632:GLN:N	2.73	0.41
1:A:1413:PRO:HA	1:A:1440:PRO:O	2.21	0.41
1:A:118:GLU:OE2	1:B:118:GLU:HG3	2.20	0.41
1:A:111:VAL:CG2	1:A:188:LEU:HD12	2.50	0.41
1:A:1272:TYR:HB3	1:A:1294:VAL:HG22	2.01	0.41
1:B:273:ILE:O	1:B:277:TYR:HD1	2.01	0.41
1:B:322:ILE:HD11	1:B:374:LEU:HD13	2.01	0.41
1:B:1241:LYS:HA	1:B:1269:ASP:HB3	2.02	0.41
1:B:1996:TYR:CD2	1:B:1997:SER:N	2.85	0.41
1:B:830:ILE:O	1:B:831:SER:C	2.59	0.41
1:B:1049:TYR:CZ	1:B:1103:VAL:HG23	2.55	0.41
1:B:1060:ASP:OD1	1:B:1062:VAL:HG23	2.20	0.41
1:A:894:LEU:HD12	1:A:894:LEU:HA	1.81	0.41
1:A:1442:TRP:CZ3	1:A:1472:VAL:HG11	2.55	0.41
1:A:23:TRP:CE2	1:A:27:ILE:HG12	2.55	0.41
1:A:367:PRO:O	1:A:368:ALA:HB3	2.20	0.41
1:B:1405:ARG:HH22	1:B:1470:ARG:NH2	2.19	0.41
1:B:889:THR:CG2	1:B:1032:LEU:CB	2.98	0.41
1:A:302:PRO:HG3	1:A:363:ASN:ND2	2.35	0.41
1:B:162:SER:OG	1:B:163:SER:N	2.50	0.41
1:A:795:PHE:O	1:A:798:SER:HB2	2.20	0.41
1:A:40:TRP:CZ3	1:A:194:PRO:HA	2.55	0.41
1:B:1766:PHE:O	1:B:1792:HIS:HB2	2.20	0.41
1:A:259:GLN:N	1:A:259:GLN:CD	2.74	0.41
1:A:896:TRP:CG	1:A:907:LEU:HD11	2.56	0.41
1:B:894:LEU:HA	1:B:894:LEU:HD12	1.83	0.41
1:A:1242:MET:HG3	1:A:1313:ASP:HB3	2.02	0.41
1:A:13:LEU:HD13	1:A:22:PHE:CD1	2.55	0.41
1:B:33:VAL:HG11	1:B:223:CYS:SG	2.60	0.41
1:A:1277:ARG:HD3	1:A:1300:ASP:OD2	2.19	0.41
1:B:1706:ALA:O	1:B:1707:TYR:C	2.59	0.41
1:A:954:ILE:HD13	1:A:954:ILE:HA	1.91	0.41
1:B:1115:ILE:HD11	1:B:2111:LEU:HD12	2.02	0.41
1:B:423:LEU:HD23	1:B:812:PRO:HG3	2.02	0.41
1:B:1712:PHE:HA	1:B:1713:PRO:HD3	1.84	0.41
1:B:1519:LEU:HD12	1:B:1520:GLU:H	1.85	0.41
1:B:1879:THR:HG1	1:B:1903:TRP:HH2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1296:GLN:H	1:A:1296:GLN:HG2	1.64	0.41
1:A:489:LYS:HE2	1:A:489:LYS:HB3	1.77	0.41
1:B:13:LEU:HB2	1:B:22:PHE:CD1	2.55	0.41
1:A:111:VAL:O	1:A:111:VAL:HG12	2.20	0.41
1:B:1122:THR:HA	1:B:1123:PRO:HD3	1.92	0.41
1:A:257:LYS:HG3	1:A:257:LYS:H	1.68	0.41
1:A:1998:GLY:O	1:A:2002:LEU:HD12	2.20	0.41
1:B:1836:VAL:HG13	1:B:1854:ILE:HD13	2.03	0.41
1:A:527:LEU:HD11	1:A:554:VAL:HG11	2.02	0.41
1:A:469:GLY:CA	1:A:805:LEU:HD21	2.51	0.41
1:A:749:LEU:HA	1:A:749:LEU:HD23	1.88	0.41
1:B:178:GLY:O	1:B:180:CYS:N	2.53	0.41
1:A:1568:TYR:CE2	1:A:1855:GLN:HB2	2.56	0.41
1:A:1921:ARG:HB2	1:A:1921:ARG:HE	1.67	0.41
1:A:1216:LEU:O	1:A:1220:LEU:HD12	2.21	0.41
1:B:1538:ARG:HH12	1:B:1585:PRO:HG2	1.86	0.41
1:B:257:LYS:NZ	1:B:261:VAL:O	2.49	0.41
1:A:1234:LEU:CD2	1:A:1262:LEU:HD22	2.48	0.41
1:A:1669:GLU:CG	1:A:1742:ASP:OD2	2.69	0.41
1:A:263:PHE:HE2	1:A:303:GLN:HE21	1.68	0.41
1:A:252:ASN:N	1:A:272:LEU:HD13	2.36	0.41
1:A:460:VAL:CG2	1:A:465:MET:HG3	2.46	0.41
1:B:322:ILE:CG2	1:B:323:GLY:N	2.83	0.41
1:A:561:ILE:HG23	1:A:589:TYR:CE2	2.56	0.41
1:B:1617:VAL:N	1:B:1800:PHE:HZ	2.19	0.41
1:A:953:LEU:HD12	1:A:954:ILE:N	2.35	0.41
1:A:258:GLU:HB2	1:A:259:GLN:NE2	2.36	0.41
1:B:744:LEU:HA	1:B:747:GLU:OE1	2.21	0.41
1:A:1671:VAL:HG23	1:A:1743:LEU:HB2	2.02	0.41
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.79	0.41
1:B:635:PRO:O	1:B:636:PRO:C	2.59	0.41
1:B:980:ASP:OD1	1:B:980:ASP:N	2.53	0.41
1:B:1315:LEU:O	1:B:1344:LEU:HD13	2.21	0.41
1:B:214:SER:O	1:B:301:ASP:OD2	2.38	0.41
1:B:581:SER:HA	1:B:738:ASN:HD21	1.85	0.41
1:A:541:THR:O	1:A:542:ASP:HB3	2.20	0.41
1:B:1433:LEU:HA	1:B:1433:LEU:HD12	1.79	0.41
1:A:1789:VAL:CG1	1:A:1790:THR:N	2.83	0.41
1:A:288:GLU:OE2	1:A:383:ILE:HG13	2.21	0.41
1:A:623:VAL:HA	1:A:671:PHE:O	2.21	0.41
1:A:637:GLY:O	1:A:654:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:SER:O	1:A:902:ALA:CB	2.68	0.41
1:A:147:PHE:C	1:A:147:PHE:CD2	2.94	0.41
1:A:2112:ALA:O	1:A:2113:GLU:HG2	2.21	0.41
1:B:513:LEU:HA	1:B:513:LEU:HD23	1.77	0.41
1:A:1096:PHE:CD2	1:A:1096:PHE:N	2.89	0.41
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.68	0.41
1:A:1011:LEU:HA	1:A:1011:LEU:HD12	1.85	0.41
1:B:333:GLU:O	1:B:336:SER:HB3	2.21	0.41
1:B:1343:PHE:CZ	1:B:1405:ARG:HD2	2.56	0.41
1:B:1457:VAL:HG11	1:B:1473:LEU:HD22	2.02	0.41
1:B:1429:LEU:HD11	1:B:1443:LEU:HD21	2.03	0.41
1:B:1567:TYR:HA	1:B:1857:ARG:HG3	2.02	0.41
1:B:1312:ALA:HB1	1:B:1337:THR:HG22	2.00	0.41
1:B:33:VAL:HB	1:B:50:ARG:NH1	2.34	0.41
1:A:64:PHE:CB	1:A:429:ARG:HH21	2.23	0.41
1:B:277:TYR:HB3	1:B:278:ALA:H	1.58	0.41
1:A:300:GLY:O	1:A:301:ASP:C	2.59	0.41
1:A:416:GLN:HE21	1:A:448:LEU:CD1	2.34	0.41
1:A:639:VAL:HG12	1:A:640:PRO:HD2	2.02	0.41
1:A:1669:GLU:HG2	1:A:1742:ASP:OD2	2.21	0.41
1:B:2006:THR:CG2	1:B:2048:ARG:HH12	2.34	0.41
1:B:1998:GLY:O	1:B:2002:LEU:HD12	2.20	0.41
1:A:624:GLY:H	1:A:671:PHE:HB3	1.86	0.41
1:A:598:GLU:OE1	1:A:706:LYS:NZ	2.48	0.41
1:B:795:PHE:CE1	1:B:799:ASN:ND2	2.87	0.41
1:A:193:LYS:HA	1:A:194:PRO:HD3	1.86	0.41
1:A:1893:LEU:HB3	1:A:1925:GLN:CD	2.41	0.41
1:B:561:ILE:HG23	1:B:589:TYR:CE2	2.56	0.41
1:B:494:PHE:O	1:B:495:ILE:HD13	2.20	0.41
1:B:704:ASP:O	1:B:706:LYS:HD2	2.20	0.41
1:B:1755:ALA:HA	1:B:1758:ARG:NH1	2.36	0.41
1:A:528:LYS:HB3	1:A:529:PRO:HD3	2.03	0.41
1:B:1243:LYS:HA	1:B:1271:ASP:HB2	2.02	0.41
1:B:453:MET:HE2	1:B:453:MET:HB3	1.89	0.41
1:B:1842:TYR:CE2	1:B:1848:HIS:HB3	2.56	0.41
1:A:389:GLY:O	1:A:390:ILE:HG13	2.21	0.41
1:A:1583:LEU:HD23	1:A:1583:LEU:HA	1.88	0.41
1:A:1408:THR:HG22	1:A:1409:PRO:HD2	2.03	0.41
1:B:634:CYS:HA	1:B:635:PRO:HD3	1.89	0.41
1:A:1766:PHE:O	1:A:1792:HIS:HB2	2.21	0.41
1:A:1480:THR:HG22	1:A:1482:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ARG:HD2	1:B:429:ARG:HA	1.91	0.41
1:B:1257:ARG:O	1:B:1260:ALA:HB3	2.21	0.41
1:B:1951:GLY:O	1:B:1954:SER:HB2	2.20	0.41
1:B:1991:VAL:HG21	1:B:2033:ASN:HD22	1.84	0.41
1:B:6:ILE:HG21	1:B:345:LEU:CD1	2.51	0.41
1:A:907:LEU:HA	1:A:907:LEU:HD12	1.88	0.41
1:A:674:GLU:HG2	1:A:674:GLU:H	1.28	0.41
1:B:1456:MET:HE2	1:B:1460:LEU:HD22	2.02	0.40
1:B:295:THR:HG22	1:B:331:HIS:CD2	2.55	0.40
1:B:1453:VAL:HG12	1:B:1457:VAL:HG23	2.03	0.40
1:B:1473:LEU:CG	1:B:1503:MET:HA	2.51	0.40
1:A:270:GLU:HG3	1:A:311:ALA:HB2	2.03	0.40
1:B:1643:GLU:O	1:B:1644:GLU:C	2.60	0.40
1:B:253:THR:O	1:B:254:ASP:C	2.59	0.40
1:B:366:ILE:CG1	1:B:366:ILE:O	2.68	0.40
1:A:1514:PHE:O	1:A:1515:ARG:HD3	2.21	0.40
1:B:1741:VAL:CG1	1:B:1742:ASP:N	2.84	0.40
1:A:1974:VAL:HG23	1:A:1974:VAL:O	2.21	0.40
1:B:1139:GLU:OE2	1:B:1216:LEU:CD1	2.68	0.40
1:A:1857:ARG:HG3	1:A:1871:ILE:HD11	2.03	0.40
1:A:1689:LEU:O	1:A:1692:GLY:N	2.48	0.40
1:B:1931:GLU:HA	1:B:1931:GLU:OE1	2.21	0.40
1:A:1240:PRO:HD2	1:A:1462:LYS:HZ1	1.87	0.40
1:B:1780:LEU:HD12	1:B:1781:GLY:N	2.36	0.40
1:A:1243:LYS:HD2	1:A:1312:ALA:N	2.37	0.40
1:A:161:CYS:HB3	1:A:331:HIS:CE1	2.56	0.40
1:A:23:TRP:CZ2	1:A:27:ILE:HG12	2.57	0.40
1:A:82:LEU:HG	1:A:144:LEU:HD13	2.02	0.40
1:A:1315:LEU:HB3	1:A:1344:LEU:HD11	2.02	0.40
1:A:612:GLU:O	1:A:614:ASN:N	2.54	0.40
1:A:305:LEU:HD23	1:A:308:ILE:HD12	2.03	0.40
1:B:1118:LYS:N	1:B:1517:PHE:O	2.47	0.40
1:B:641:ALA:HB1	1:B:683:HIS:CB	2.49	0.40
1:B:122:ARG:O	1:B:123:ASP:C	2.58	0.40
1:A:734:TYR:CD2	1:A:734:TYR:O	2.74	0.40
1:A:1433:LEU:HD21	1:A:1465:GLY:HA3	2.03	0.40
1:B:1659:LEU:HD23	1:B:1767:LEU:CD1	2.51	0.40
1:B:654:PRO:O	1:B:658:MET:CB	2.68	0.40
1:B:623:VAL:CG1	1:B:624:GLY:N	2.85	0.40
1:A:1347:HIS:CD2	1:A:1348:THR:O	2.74	0.40
1:A:429:ARG:HA	1:A:429:ARG:HD2	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLY:O	1:A:298:LYS:HB2	2.20	0.40
1:B:420:LEU:HD12	1:B:512:ARG:HH11	1.86	0.40
1:A:1118:LYS:HD2	1:A:2103:HIS:ND1	2.35	0.40
1:A:81:MET:HG2	1:A:81:MET:H	1.62	0.40
1:B:1573:PHE:O	1:B:1576:VAL:HB	2.21	0.40
1:B:1863:PRO:O	1:B:1865:PRO:HD3	2.21	0.40
1:A:1674:HIS:ND1	1:A:1698:THR:CG2	2.83	0.40
1:B:2041:MET:HA	1:B:2044:ILE:HG13	2.03	0.40
1:B:490:ARG:HA	1:B:491:PRO:HD3	1.96	0.40
1:B:1636:VAL:HG23	1:B:1640:TRP:HB2	2.03	0.40
1:A:2090:SER:O	1:A:2094:VAL:HG23	2.22	0.40
1:B:588:GLY:HA3	1:B:730:PHE:CE1	2.57	0.40
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.68	0.40
1:B:1456:MET:CE	1:B:1460:LEU:HD22	2.52	0.40
1:B:189:ASN:O	1:B:226:GLU:HB2	2.21	0.40
1:B:1314:LEU:HG	1:B:1315:LEU:N	2.36	0.40
1:B:300:GLY:O	1:B:301:ASP:C	2.59	0.40
1:B:1122:THR:HG1	1:B:1517:PHE:HE1	1.68	0.40
1:A:666:LYS:O	1:A:668:GLU:N	2.55	0.40
1:B:1553:TYR:O	1:B:1882:PRO:HG3	2.21	0.40
1:B:2017:VAL:HG12	1:B:2018:ILE:N	2.37	0.40
1:B:252:ASN:HD21	1:B:272:LEU:HB2	1.81	0.40
1:A:159:THR:O	1:A:160:ALA:HB3	2.21	0.40
1:B:1617:VAL:HG21	1:B:1626:VAL:HG11	2.04	0.40
1:A:654:PRO:HD3	1:A:686:PHE:HE1	1.86	0.40
1:B:876:VAL:HA	1:B:884:VAL:HG11	2.03	0.40
1:A:1238:ALA:HB1	1:A:1467:HIS:CD2	2.56	0.40
1:A:825:ARG:HG2	1:A:826:GLY:N	2.36	0.40
1:A:588:GLY:O	1:A:594:LEU:HB2	2.21	0.40
1:A:1733:LEU:HD23	1:A:1733:LEU:HA	1.68	0.40
1:A:509:SER:O	1:A:512:ARG:HG3	2.22	0.40
1:A:273:ILE:O	1:A:277:TYR:HD1	2.05	0.40
1:B:912:VAL:HG22	1:B:913:VAL:N	2.36	0.40
1:B:2022:VAL:HG13	1:B:2026:ARG:HG2	2.04	0.40
1:B:971:ASP:OD1	1:B:973:ARG:HB2	2.21	0.40
1:B:1726:THR:CG2	1:B:1726:THR:O	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1948/2512 (78%)	1586 (81%)	282 (14%)	80 (4%)	3	27
1	B	1992/2512 (79%)	1622 (81%)	296 (15%)	74 (4%)	4	29
All	All	3940/5024 (78%)	3208 (81%)	578 (15%)	154 (4%)	4	28

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	GLU
1	A	255	GLY
1	A	278	ALA
1	A	333	GLU
1	A	413	PRO
1	A	418	ALA
1	A	582	LEU
1	A	615	VAL
1	A	818	PRO
1	A	839	SER
1	A	976	VAL
1	A	1224	PRO
1	A	1303	ASN
1	A	1485	GLU
1	A	1611	ARG
1	A	1638	SER
1	A	1749	ALA
1	A	1802	GLU
1	A	1862	GLY
1	B	179	GLU
1	B	255	GLY
1	B	278	ALA
1	B	333	GLU
1	B	418	ALA
1	B	636	PRO

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Mol	Chain	Res	Type
1	B	669	ASP
1	B	839	SER
1	B	978	PRO
1	B	980	ASP
1	B	1224	PRO
1	B	1749	ALA
1	B	1800	PHE
1	B	1862	GLY
1	A	163	SER
1	A	282	PRO
1	A	318	GLU
1	A	387	ASN
1	A	476	GLU
1	A	488	SER
1	A	984	GLU
1	A	985	PHE
1	A	1056	SER
1	A	1301	PRO
1	A	1593	LEU
1	A	1735	HIS
1	A	1801	GLU
1	A	1870	PRO
1	A	2025	GLY
1	A	2079	VAL
1	A	2112	ALA
1	B	163	SER
1	B	282	PRO
1	B	318	GLU
1	B	370	GLN
1	B	387	ASN
1	B	413	PRO
1	B	476	GLU
1	B	856	CYS
1	B	974	ALA
1	B	983	ALA
1	B	984	GLU
1	B	1225	ALA
1	B	1301	PRO
1	B	1302	ALA
1	B	1593	LEU
1	B	1735	HIS
1	B	1802	GLU

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Mol	Chain	Res	Type
1	B	1858	GLU
1	B	2025	GLY
1	B	2079	VAL
1	A	216	ASP
1	A	254	ASP
1	A	310	ASN
1	A	317	ARG
1	A	319	PRO
1	A	613	ALA
1	A	854	SER
1	A	1014	ASP
1	A	1110	GLU
1	A	1225	ALA
1	A	1596	ASP
1	A	1649	PRO
1	A	1706	ALA
1	A	2021	SER
1	B	213	ARG
1	B	254	ASP
1	B	317	ARG
1	B	319	PRO
1	B	488	SER
1	B	820	GLU
1	B	1056	SER
1	B	1560	GLN
1	B	1596	ASP
1	B	1706	ALA
1	B	1863	PRO
1	B	2065	ASP
1	A	14	PRO
1	A	237	SER
1	A	238	LEU
1	A	445	SER
1	A	848	ALA
1	A	857	SER
1	A	1389	LEU
1	A	1409	PRO
1	A	1557	ALA
1	A	1734	ARG
1	A	1800	PHE
1	A	1835	LYS
1	A	2065	ASP

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Mol	Chain	Res	Type
1	A	2078	THR
1	B	14	PRO
1	B	60	PHE
1	B	162	SER
1	B	238	LEU
1	B	310	ASN
1	B	445	SER
1	B	1014	ASP
1	B	1110	GLU
1	B	1449	SER
1	B	1464	PRO
1	B	1491	SER
1	B	1548	CYS
1	B	1734	ARG
1	B	1932	TRP
1	B	1982	ASN
1	B	2021	SER
1	B	2078	THR
1	B	2102	PRO
1	A	60	PHE
1	A	162	SER
1	A	215	PHE
1	A	617	PRO
1	A	1464	PRO
1	A	1471	CYS
1	A	1597	CYS
1	A	1692	GLY
1	A	1865	PRO
1	A	2056	LEU
1	A	2102	PRO
1	B	1835	LYS
1	B	1978	ALA
1	B	1979	VAL
1	B	2056	LEU
1	A	1500	ASP
1	B	635	PRO
1	B	1467	HIS
1	A	487	GLY
1	A	853	GLY
1	B	1303	ASN
1	B	1409	PRO
1	B	487	GLY

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Mol	Chain	Res	Type
1	A	355	PRO
1	A	1240	PRO
1	B	1408	THR

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	1624/2072 (78%)	1450 (89%)	174 (11%)	8	34
1	B	1660/2072 (80%)	1473 (89%)	187 (11%)	7	32
All	All	3284/4144 (79%)	2923 (89%)	361 (11%)	8	33

All (361) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	59	ARG
1	A	81	MET
1	A	86	THR
1	A	111	VAL
1	A	117	SER
1	A	123	ASP
1	A	128	VAL
1	A	136	GLN
1	A	144	LEU
1	A	169	GLN
1	A	170	SER
1	A	172	TYR
1	A	181	SER
1	A	223	CYS
1	A	224	ARG
1	A	241	ARG
1	A	248	ASN
1	A	251	THR
1	A	263	PHE

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Mol	Chain	Res	Type
1	A	295	THR
1	A	297	THR
1	A	309	VAL
1	A	317	ARG
1	A	318	GLU
1	A	320	LEU
1	A	327	SER
1	A	329	MET
1	A	343	LYS
1	A	347	SER
1	A	356	ASN
1	A	366	ILE
1	A	371	ASP
1	A	375	GLN
1	A	383	ILE
1	A	399	ASN
1	A	400	VAL
1	A	402	VAL
1	A	407	ASN
1	A	439	GLU
1	A	446	ARG
1	A	460	VAL
1	A	470	TYR
1	A	480	GLN
1	A	489	LYS
1	A	492	VAL
1	A	502	GLN
1	A	520	ILE
1	A	525	GLN
1	A	541	THR
1	A	543	GLU
1	A	549	ILE
1	A	552	SER
1	A	556	LEU
1	A	558	SER
1	A	568	THR
1	A	569	SER
1	A	572	LEU
1	A	574	PRO
1	A	597	GLU
1	A	614	ASN
1	A	616	LEU

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Mol	Chain	Res	Type
1	A	658	MET
1	A	673	LYS
1	A	674	GLU
1	A	677	THR
1	A	689	SER
1	A	703	LEU
1	A	730	PHE
1	A	734	TYR
1	A	736	VAL
1	A	757	VAL
1	A	773	ARG
1	A	825	ARG
1	A	846	SER
1	A	849	ASP
1	A	857	SER
1	A	866	VAL
1	A	894	LEU
1	A	917	VAL
1	A	931	VAL
1	A	937	LEU
1	A	941	SER
1	A	947	SER
1	A	949	SER
1	A	953	LEU
1	A	959	VAL
1	A	972	THR
1	A	1011	LEU
1	A	1026	ASP
1	A	1038	MET
1	A	1052	THR
1	A	1055	THR
1	A	1068	LEU
1	A	1069	TYR
1	A	1070	THR
1	A	1074	THR
1	A	1084	ARG
1	A	1087	ASN
1	A	1088	THR
1	A	1095	LEU
1	A	1097	LEU
1	A	1101	SER
1	A	1105	PRO

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Mol	Chain	Res	Type
1	A	1107	ARG
1	A	1112	LEU
1	A	1122	THR
1	A	1216	LEU
1	A	1267	VAL
1	A	1275	THR
1	A	1299	TRP
1	A	1346	LEU
1	A	1376	ASP
1	A	1408	THR
1	A	1421	THR
1	A	1428	SER
1	A	1456	MET
1	A	1460	LEU
1	A	1468	ARG
1	A	1473	LEU
1	A	1476	ASN
1	A	1480	THR
1	A	1481	SER
1	A	1491	SER
1	A	1505	VAL
1	A	1525	GLU
1	A	1527	GLN
1	A	1541	LEU
1	A	1542	SER
1	A	1573	PHE
1	A	1583	LEU
1	A	1596	ASP
1	A	1597	CYS
1	A	1614	MET
1	A	1626	VAL
1	A	1638	SER
1	A	1639	THR
1	A	1651	VAL
1	A	1660	VAL
1	A	1662	ARG
1	A	1669	GLU
1	A	1697	THR
1	A	1698	THR
1	A	1722	ASN
1	A	1735	HIS
1	A	1736	THR

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Mol	Chain	Res	Type
1	A	1760	LEU
1	A	1762	GLN
1	A	1768	GLU
1	A	1790	THR
1	A	1800	PHE
1	A	1823	VAL
1	A	1841	ARG
1	A	1843	MET
1	A	1860	GLU
1	A	1861	GLN
1	A	1873	LEU
1	A	1877	SER
1	A	1922	THR
1	A	1927	ARG
1	A	1937	VAL
1	A	1944	SER
1	A	1957	THR
1	A	1996	TYR
1	A	2005	VAL
1	A	2006	THR
1	A	2022	VAL
1	A	2026	ARG
1	A	2028	ASN
1	A	2043	ARG
1	A	2044	ILE
1	A	2078	THR
1	A	2096	ASP
1	A	2111	LEU
1	B	32	MET
1	B	59	ARG
1	B	81	MET
1	B	86	THR
1	B	111	VAL
1	B	112	SER
1	B	122	ARG
1	B	123	ASP
1	B	126	THR
1	B	127	LEU
1	B	128	VAL
1	B	136	GLN
1	B	144	LEU
1	B	169	GLN

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Mol	Chain	Res	Type
1	B	170	SER
1	B	172	TYR
1	B	181	SER
1	B	223	CYS
1	B	224	ARG
1	B	241	ARG
1	B	248	ASN
1	B	251	THR
1	B	263	PHE
1	B	288	GLU
1	B	295	THR
1	B	297	THR
1	B	309	VAL
1	B	317	ARG
1	B	318	GLU
1	B	320	LEU
1	B	329	MET
1	B	334	PRO
1	B	343	LYS
1	B	347	SER
1	B	356	ASN
1	B	366	ILE
1	B	371	ASP
1	B	375	GLN
1	B	383	ILE
1	B	399	ASN
1	B	400	VAL
1	B	402	VAL
1	B	407	ASN
1	B	439	GLU
1	B	446	ARG
1	B	460	VAL
1	B	489	LYS
1	B	492	VAL
1	B	502	GLN
1	B	520	ILE
1	B	545	VAL
1	B	549	ILE
1	B	552	SER
1	B	556	LEU
1	B	558	SER
1	B	568	THR

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Mol	Chain	Res	Type
1	B	569	SER
1	B	572	LEU
1	B	574	PRO
1	B	615	VAL
1	B	635	PRO
1	B	664	GLN
1	B	670	VAL
1	B	675	VAL
1	B	676	ARG
1	B	689	SER
1	B	730	PHE
1	B	734	TYR
1	B	736	VAL
1	B	757	VAL
1	B	821	PHE
1	B	825	ARG
1	B	846	SER
1	B	866	VAL
1	B	894	LEU
1	B	917	VAL
1	B	931	VAL
1	B	937	LEU
1	B	941	SER
1	B	947	SER
1	B	949	SER
1	B	959	VAL
1	B	964	SER
1	B	971	ASP
1	B	972	THR
1	B	976	VAL
1	B	980	ASP
1	B	982	THR
1	B	1011	LEU
1	B	1026	ASP
1	B	1038	MET
1	B	1052	THR
1	B	1055	THR
1	B	1068	LEU
1	B	1069	TYR
1	B	1070	THR
1	B	1074	THR
1	B	1084	ARG

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Mol	Chain	Res	Type
1	B	1087	ASN
1	B	1088	THR
1	B	1095	LEU
1	B	1097	LEU
1	B	1101	SER
1	B	1107	ARG
1	B	1122	THR
1	B	1216	LEU
1	B	1218	SER
1	B	1235	GLU
1	B	1267	VAL
1	B	1275	THR
1	B	1299	TRP
1	B	1337	THR
1	B	1340	GLU
1	B	1346	LEU
1	B	1373	LEU
1	B	1395	SER
1	B	1421	THR
1	B	1428	SER
1	B	1456	MET
1	B	1460	LEU
1	B	1473	LEU
1	B	1480	THR
1	B	1481	SER
1	B	1486	MET
1	B	1487	HIS
1	B	1505	VAL
1	B	1515	ARG
1	B	1525	GLU
1	B	1528	THR
1	B	1548	CYS
1	B	1551	LEU
1	B	1558	SER
1	B	1573	PHE
1	B	1583	LEU
1	B	1595	ARG
1	B	1597	CYS
1	B	1598	MET
1	B	1603	PHE
1	B	1612	ARG
1	B	1614	MET

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Mol	Chain	Res	Type
1	B	1636	VAL
1	B	1639	THR
1	B	1653	THR
1	B	1661	VAL
1	B	1662	ARG
1	B	1669	GLU
1	B	1671	VAL
1	B	1687	ILE
1	B	1694	ARG
1	B	1697	THR
1	B	1698	THR
1	B	1722	ASN
1	B	1735	HIS
1	B	1736	THR
1	B	1760	LEU
1	B	1762	GLN
1	B	1768	GLU
1	B	1790	THR
1	B	1800	PHE
1	B	1823	VAL
1	B	1841	ARG
1	B	1843	MET
1	B	1856	VAL
1	B	1860	GLU
1	B	1868	LEU
1	B	1873	LEU
1	B	1877	SER
1	B	1904	LEU
1	B	1922	THR
1	B	1927	ARG
1	B	1937	VAL
1	B	1940	LEU
1	B	1944	SER
1	B	1957	THR
1	B	1979	VAL
1	B	1982	ASN
1	B	1988	PHE
1	B	1996	TYR
1	B	2005	VAL
1	B	2006	THR
1	B	2022	VAL
1	B	2026	ARG

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Mol	Chain	Res	Type
1	B	2028	ASN
1	B	2043	ARG
1	B	2044	ILE
1	B	2078	THR
1	B	2096	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	96	ASN
1	A	136	GLN
1	A	248	ASN
1	A	306	ASN
1	A	350	HIS
1	A	356	ASN
1	A	399	ASN
1	A	425	GLN
1	A	444	HIS
1	A	525	GLN
1	A	560	GLN
1	A	632	GLN
1	A	644	ASN
1	A	697	GLN
1	A	737	ASN
1	A	833	HIS
1	A	1023	GLN
1	A	1037	HIS
1	A	1111	HIS
1	A	1133	ASN
1	A	1298	GLN
1	A	1318	ASN
1	A	1388	HIS
1	A	1467	HIS
1	A	1487	HIS
1	A	1735	HIS
1	A	1777	ASN
1	A	1778	HIS
1	A	1855	GLN
1	A	2076	ASN
1	A	2086	GLN
1	A	2103	HIS

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Mol	Chain	Res	Type
1	B	25	ASN
1	B	96	ASN
1	B	136	GLN
1	B	199	GLN
1	B	248	ASN
1	B	306	ASN
1	B	350	HIS
1	B	356	ASN
1	B	399	ASN
1	B	425	GLN
1	B	502	GLN
1	B	525	GLN
1	B	560	GLN
1	B	632	GLN
1	B	643	HIS
1	B	663	GLN
1	B	697	GLN
1	B	737	ASN
1	B	738	ASN
1	B	833	HIS
1	B	1023	GLN
1	B	1037	HIS
1	B	1111	HIS
1	B	1133	ASN
1	B	1298	GLN
1	B	1333	ASN
1	B	1406	GLN
1	B	1458	ASN
1	B	1467	HIS
1	B	1674	HIS
1	B	1735	HIS
1	B	1777	ASN
1	B	1778	HIS
1	B	1855	GLN
1	B	2076	ASN
1	B	2086	GLN
1	B	2103	HIS

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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	1962/2512 (78%)	-0.10	91 (4%)	36	24	63, 118, 226, 276	0
1	B	2004/2512 (79%)	0.12	141 (7%)	19	12	54, 158, 230, 276	0
All	All	3966/5024 (78%)	0.01	232 (5%)	26	16	54, 136, 229, 276	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	581	SER	8.1
1	B	496	CYS	7.6
1	B	579	GLY	7.6
1	A	1297	GLY	7.5
1	B	498	GLY	7.3
1	B	672	VAL	7.2
1	A	1387	LEU	6.7
1	A	1406	GLN	6.3
1	B	580	HIS	6.2
1	B	2078	THR	6.1
1	B	497	SER	6.0
1	B	671	PHE	5.5
1	B	583	GLY	5.4
1	A	2078	THR	5.3
1	B	1863	PRO	5.2
1	A	1398	GLY	5.1
1	A	1415	PHE	5.1
1	A	1386	SER	5.0
1	A	1407	GLN	5.0
1	B	703	LEU	4.9
1	A	1486	MET	4.8
1	A	2079	VAL	4.8
1	A	1441	VAL	4.7
1	B	2069	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	674	GLU	4.4
1	B	622	ALA	4.3
1	B	410	PRO	4.3
1	B	2076	ASN	4.3
1	B	392	SER	4.2
1	B	673	LYS	4.2
1	A	419	ALA	4.1
1	B	667	ARG	4.1
1	A	1269	ASP	4.1
1	B	2080	ILE	4.0
1	B	1140	LEU	4.0
1	A	982	THR	3.9
1	A	2029	ALA	3.9
1	B	1286	GLN	3.9
1	B	1136	LEU	3.8
1	A	414	PRO	3.8
1	B	1486	MET	3.8
1	B	1296	GLN	3.8
1	A	336	SER	3.8
1	B	10	SER	3.8
1	B	1437	SER	3.7
1	B	1297	GLY	3.7
1	B	414	PRO	3.7
1	A	1442	TRP	3.7
1	B	928	THR	3.7
1	A	1468	ARG	3.7
1	B	1384	GLY	3.7
1	A	1385	ALA	3.6
1	B	1276	ASP	3.6
1	A	983	ALA	3.6
1	A	1464	PRO	3.6
1	A	1135	ALA	3.6
1	B	617	PRO	3.5
1	A	2080	ILE	3.5
1	B	717	ILE	3.5
1	B	670	VAL	3.5
1	B	2068	VAL	3.5
1	A	1384	GLY	3.5
1	A	1296	GLN	3.4
1	B	1439	ARG	3.4
1	B	161	CYS	3.4
1	B	391	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1437	SER	3.4
1	B	1869	PRO	3.4
1	B	669	ASP	3.4
1	B	413	PRO	3.3
1	B	1143	CYS	3.3
1	A	981	SER	3.3
1	B	1441	VAL	3.3
1	A	1465	GLY	3.2
1	B	2079	VAL	3.2
1	A	2081	GLY	3.2
1	B	408	SER	3.1
1	B	646	LYS	3.1
1	B	1340	GLU	3.1
1	B	1523	ARG	3.1
1	A	293	HIS	3.1
1	A	1382	PHE	3.1
1	A	1510	ALA	3.1
1	B	2077	ASP	3.1
1	B	1864	ALA	3.1
1	B	293	HIS	3.1
1	B	1275	THR	3.0
1	B	1458	ASN	3.0
1	B	1876	LEU	3.0
1	B	560	GLN	3.0
1	A	1388	HIS	3.0
1	B	316	ARG	3.0
1	A	1509	GLY	3.0
1	B	1455	GLY	3.0
1	B	661	PHE	3.0
1	A	364	PRO	2.9
1	A	1305	ALA	2.9
1	B	336	SER	2.9
1	B	666	LYS	2.9
1	B	653	GLY	2.9
1	A	392	SER	2.9
1	B	1987	PHE	2.8
1	B	624	GLY	2.8
1	B	324	SER	2.8
1	B	658	MET	2.8
1	A	1482	PRO	2.8
1	A	2034	TYR	2.8
1	B	298	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	2071	GLU	2.8
1	A	2077	ASP	2.8
1	A	978	PRO	2.8
1	A	975	ALA	2.8
1	B	665	LEU	2.7
1	A	1426	VAL	2.7
1	B	1979	VAL	2.7
1	A	1349	LEU	2.7
1	A	2070	LEU	2.7
1	B	664	GLN	2.7
1	B	488	SER	2.7
1	A	49	ARG	2.7
1	A	976	VAL	2.7
1	A	1429	LEU	2.7
1	A	1430	LYS	2.6
1	B	1280	GLN	2.6
1	A	1134	THR	2.6
1	B	625	LEU	2.6
1	A	980	ASP	2.6
1	A	2069	VAL	2.6
1	B	1586	ASP	2.6
1	B	2070	LEU	2.6
1	A	496	CYS	2.6
1	B	762	ALA	2.6
1	A	1484	PRO	2.6
1	A	2076	ASN	2.6
1	B	337	GLY	2.6
1	B	647	ASP	2.5
1	B	539	LEU	2.5
1	A	1491	SER	2.5
1	A	1436	ALA	2.5
1	B	499	MET	2.5
1	B	1231	ASP	2.5
1	B	1981	GLU	2.5
1	B	1468	ARG	2.5
1	A	1348	THR	2.5
1	B	541	THR	2.5
1	B	1243	LYS	2.5
1	A	1974	VAL	2.5
1	B	1412	SER	2.5
1	B	790	ARG	2.4
1	B	644	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	419	ALA	2.4
1	A	1255	TYR	2.4
1	B	1484	PRO	2.4
1	A	1304	PRO	2.4
1	B	663	GLN	2.4
1	A	1487	HIS	2.4
1	B	360	HIS	2.4
1	B	1284	ALA	2.4
1	B	1978	ALA	2.4
1	B	369	LEU	2.4
1	A	1300	ASP	2.4
1	A	1286	GLN	2.4
1	A	1467	HIS	2.4
1	B	721	GLN	2.4
1	A	1287	ALA	2.4
1	A	1513	ALA	2.4
1	B	389	GLY	2.4
1	B	495	ILE	2.3
1	A	1383	ALA	2.3
1	B	1320	ALA	2.3
1	B	1141	GLN	2.3
1	B	294	GLY	2.3
1	B	1327	PRO	2.3
1	A	1306	PRO	2.3
1	B	364	PRO	2.3
1	B	654	PRO	2.3
1	A	1397	TYR	2.3
1	B	1408	THR	2.3
1	B	1570	SER	2.3
1	A	1278	ASN	2.3
1	B	409	ARG	2.3
1	A	1298	GLN	2.3
1	B	374	LEU	2.3
1	A	977	ASP	2.3
1	A	161	CYS	2.3
1	B	621	ALA	2.2
1	B	1313	ASP	2.2
1	A	337	GLY	2.2
1	A	1033	ASP	2.2
1	B	35	ALA	2.2
1	B	1485	GLU	2.2
1	A	1408	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1434	ALA	2.2
1	B	975	ALA	2.2
1	B	1976	ARG	2.2
1	A	1291	GLN	2.2
1	B	1294	VAL	2.2
1	B	1339	LYS	2.2
1	B	660	GLU	2.2
1	B	49	ARG	2.2
1	B	722	TRP	2.2
1	B	1587	SER	2.2
1	A	1341	GLY	2.1
1	B	2082	GLY	2.1
1	B	1602	GLU	2.1
1	B	370	GLN	2.1
1	A	1681	GLY	2.1
1	A	1238	ALA	2.1
1	A	1235	GLU	2.1
1	A	1240	PRO	2.1
1	B	331	HIS	2.1
1	B	483	GLN	2.1
1	A	1377	GLN	2.1
1	B	634	CYS	2.1
1	B	685	TYR	2.1
1	B	1557	ALA	2.1
1	B	1584	SER	2.1
1	B	557	THR	2.1
1	B	788	ASP	2.1
1	B	412	PRO	2.1
1	A	1431	ASP	2.1
1	B	482	VAL	2.1
1	B	2020	SER	2.1
1	B	1139	GLU	2.1
1	B	2024	CYS	2.0
1	A	1279	PRO	2.0
1	A	889	THR	2.0
1	A	1409	PRO	2.0
1	B	655	GLN	2.0
1	B	1386	SER	2.0
1	B	1434	ALA	2.0
1	A	391	ASN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.