



Full wwPDB EM Validation Report ⓘ

Jan 16, 2025 – 07:02 am GMT

PDB ID : 8CPZ
EMDB ID : EMD-16791
Title : Photorhabdus luminescens TcdA1 prepore-to-pore intermediate, K1179W mutant
Authors : Nganga, P.N.; Roderer, D.; Belyy, A.; Prumbaum, D.; Raunser, S.
Deposited on : 2023-03-03
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

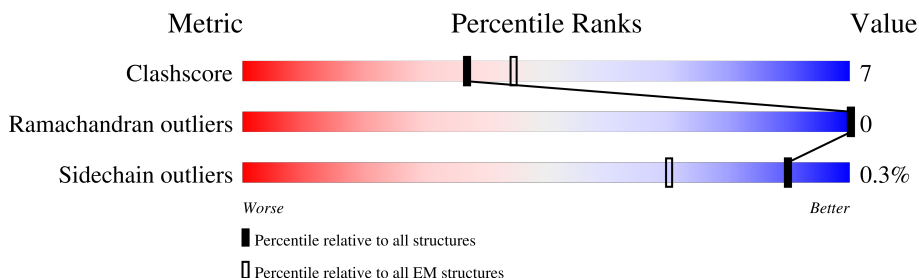
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2535	
1	B	2535	
1	C	2535	
1	D	2535	
1	E	2535	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 84420 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 TcdA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	B	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	C	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	D	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	E	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q9RN43
A	-17	ALA	-	expression tag	UNP Q9RN43
A	-16	HIS	-	expression tag	UNP Q9RN43
A	-15	HIS	-	expression tag	UNP Q9RN43
A	-14	HIS	-	expression tag	UNP Q9RN43
A	-13	HIS	-	expression tag	UNP Q9RN43
A	-12	HIS	-	expression tag	UNP Q9RN43
A	-11	HIS	-	expression tag	UNP Q9RN43
A	-10	SER	-	expression tag	UNP Q9RN43
A	-9	SER	-	expression tag	UNP Q9RN43
A	-8	GLY	-	expression tag	UNP Q9RN43
A	-7	LEU	-	expression tag	UNP Q9RN43
A	-6	GLU	-	expression tag	UNP Q9RN43
A	-5	VAL	-	expression tag	UNP Q9RN43
A	-4	LEU	-	expression tag	UNP Q9RN43
A	-3	PHE	-	expression tag	UNP Q9RN43
A	-2	GLN	-	expression tag	UNP Q9RN43
A	-1	GLY	-	expression tag	UNP Q9RN43
A	0	PRO	-	expression tag	UNP Q9RN43
A	1179	TRP	LYS	engineered mutation	UNP Q9RN43

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP Q9RN43
B	-17	ALA	-	expression tag	UNP Q9RN43
B	-16	HIS	-	expression tag	UNP Q9RN43
B	-15	HIS	-	expression tag	UNP Q9RN43
B	-14	HIS	-	expression tag	UNP Q9RN43
B	-13	HIS	-	expression tag	UNP Q9RN43
B	-12	HIS	-	expression tag	UNP Q9RN43
B	-11	HIS	-	expression tag	UNP Q9RN43
B	-10	SER	-	expression tag	UNP Q9RN43
B	-9	SER	-	expression tag	UNP Q9RN43
B	-8	GLY	-	expression tag	UNP Q9RN43
B	-7	LEU	-	expression tag	UNP Q9RN43
B	-6	GLU	-	expression tag	UNP Q9RN43
B	-5	VAL	-	expression tag	UNP Q9RN43
B	-4	LEU	-	expression tag	UNP Q9RN43
B	-3	PHE	-	expression tag	UNP Q9RN43
B	-2	GLN	-	expression tag	UNP Q9RN43
B	-1	GLY	-	expression tag	UNP Q9RN43
B	0	PRO	-	expression tag	UNP Q9RN43
B	1179	TRP	LYS	engineered mutation	UNP Q9RN43
C	-18	MET	-	initiating methionine	UNP Q9RN43
C	-17	ALA	-	expression tag	UNP Q9RN43
C	-16	HIS	-	expression tag	UNP Q9RN43
C	-15	HIS	-	expression tag	UNP Q9RN43
C	-14	HIS	-	expression tag	UNP Q9RN43
C	-13	HIS	-	expression tag	UNP Q9RN43
C	-12	HIS	-	expression tag	UNP Q9RN43
C	-11	HIS	-	expression tag	UNP Q9RN43
C	-10	SER	-	expression tag	UNP Q9RN43
C	-9	SER	-	expression tag	UNP Q9RN43
C	-8	GLY	-	expression tag	UNP Q9RN43
C	-7	LEU	-	expression tag	UNP Q9RN43
C	-6	GLU	-	expression tag	UNP Q9RN43
C	-5	VAL	-	expression tag	UNP Q9RN43
C	-4	LEU	-	expression tag	UNP Q9RN43
C	-3	PHE	-	expression tag	UNP Q9RN43
C	-2	GLN	-	expression tag	UNP Q9RN43
C	-1	GLY	-	expression tag	UNP Q9RN43
C	0	PRO	-	expression tag	UNP Q9RN43
C	1179	TRP	LYS	engineered mutation	UNP Q9RN43
D	-18	MET	-	initiating methionine	UNP Q9RN43
D	-17	ALA	-	expression tag	UNP Q9RN43

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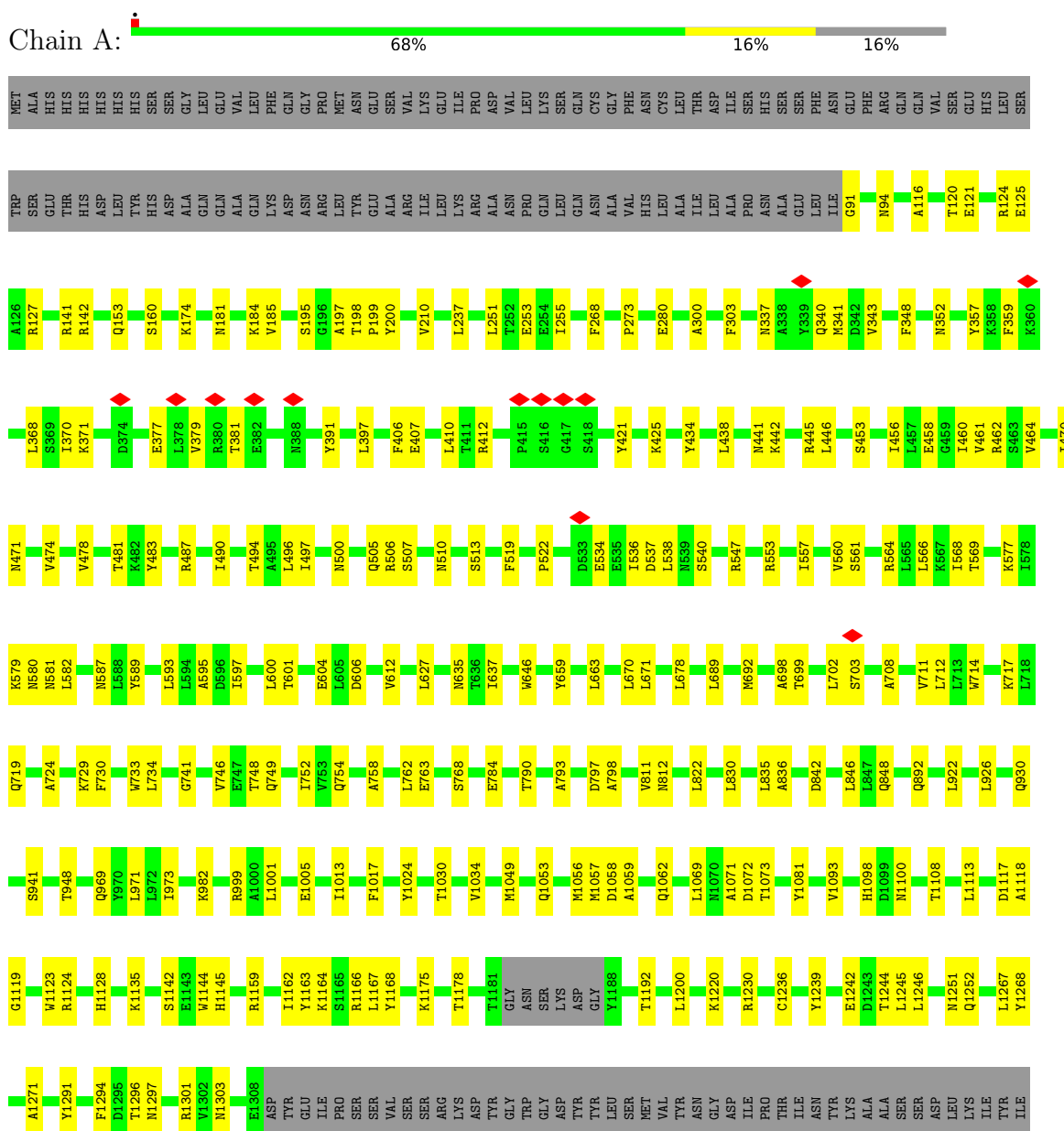
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	HIS	-	expression tag	UNP Q9RN43
D	-15	HIS	-	expression tag	UNP Q9RN43
D	-14	HIS	-	expression tag	UNP Q9RN43
D	-13	HIS	-	expression tag	UNP Q9RN43
D	-12	HIS	-	expression tag	UNP Q9RN43
D	-11	HIS	-	expression tag	UNP Q9RN43
D	-10	SER	-	expression tag	UNP Q9RN43
D	-9	SER	-	expression tag	UNP Q9RN43
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D	-7	LEU	-	expression tag	UNP Q9RN43
D	-6	GLU	-	expression tag	UNP Q9RN43
D	-5	VAL	-	expression tag	UNP Q9RN43
D	-4	LEU	-	expression tag	UNP Q9RN43
D	-3	PHE	-	expression tag	UNP Q9RN43
D	-2	GLN	-	expression tag	UNP Q9RN43
D	-1	GLY	-	expression tag	UNP Q9RN43
D	0	PRO	-	expression tag	UNP Q9RN43
D	1179	TRP	LYS	engineered mutation	UNP Q9RN43
E	-18	MET	-	initiating methionine	UNP Q9RN43
E	-17	ALA	-	expression tag	UNP Q9RN43
E	-16	HIS	-	expression tag	UNP Q9RN43
E	-15	HIS	-	expression tag	UNP Q9RN43
E	-14	HIS	-	expression tag	UNP Q9RN43
E	-13	HIS	-	expression tag	UNP Q9RN43
E	-12	HIS	-	expression tag	UNP Q9RN43
E	-11	HIS	-	expression tag	UNP Q9RN43
E	-10	SER	-	expression tag	UNP Q9RN43
E	-9	SER	-	expression tag	UNP Q9RN43
E	-8	GLY	-	expression tag	UNP Q9RN43
E	-7	LEU	-	expression tag	UNP Q9RN43
E	-6	GLU	-	expression tag	UNP Q9RN43
E	-5	VAL	-	expression tag	UNP Q9RN43
E	-4	LEU	-	expression tag	UNP Q9RN43
E	-3	PHE	-	expression tag	UNP Q9RN43
E	-2	GLN	-	expression tag	UNP Q9RN43
E	-1	GLY	-	expression tag	UNP Q9RN43
E	0	PRO	-	expression tag	UNP Q9RN43
E	1179	TRP	LYS	engineered mutation	UNP Q9RN43

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: TcdA1

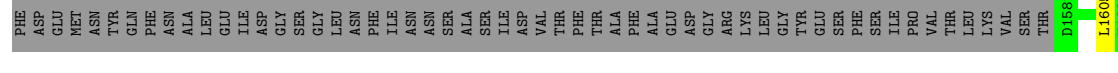
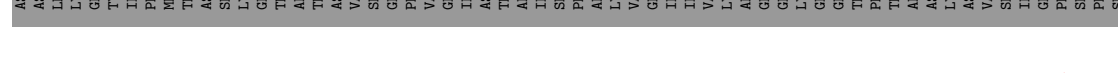
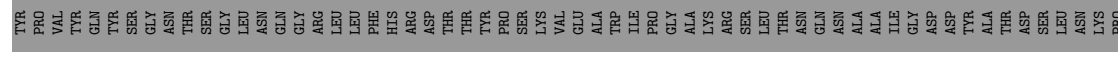
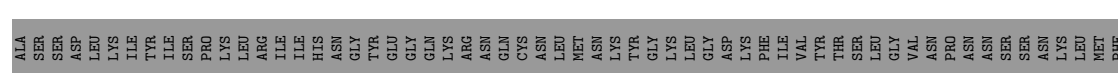
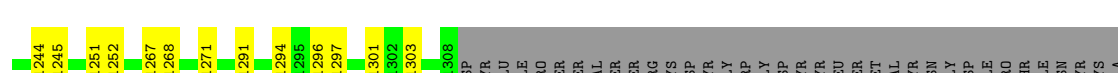
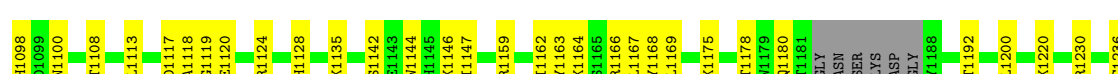
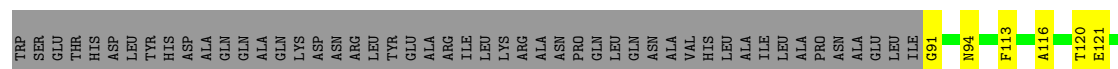


A1617	T1618	I1624	Q1630	D1657	I1676	L1690	F1711	K1712	K1713	G1722	D1729	S1739	L1766	Y1767	F1768	W1769	L1771	F1772	Y1773	Y1774	R1782	L1783	E1786	Q1787	N1788	F1789	D1790	E1791	N1793	R1794	K1797	Y1798	Y1799	W1800	S1801	P1802	L1606	T1607	L1608	F1609	A1610	R1611	Q1612	V1614	A1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960	L1961	L1962	L1963	L1964	L1965	L1966	L1967	L1968	L1969	L1970	L1971	L1972	L1973	L1974	L1975	L1976	L1977	L1978	L1979	L1980	L1981	L1982	L1983	L1984	L1985	L1986	L1987	L1988	L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000	L2001	L2002	L2003	L2004	L2005	L2006	L2007	L2008	L2009	L2010	L2011	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L2025	L2026	L2027	L2028	L2029	L2030	L2031	L2032	L2033	L2034	L2035	L2036	L2037	L2038	L2039	L2040	L2041	L2042	L2043	L2044	L2045	L2046	L2047	L2048	L2049	L2050	L2051	L2052	L2053	L2054	L2055	L2056	L2057	L2058	L2059	L2060	L2061	L2062	L2063	L2064	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2075	L2076	L2077	L2078	L2079	L2080	L2081	L2082	L2083	L2084	L2085	L2086	L2087	L2088	L2089	L2090	L2091	L2092	L2093	L2094	L2095	L2096	L2097	L2098	L2099	L2100	L2101	L2102	L2103	L2104	L2105	L2106	L2107	L2108	L2109	L2110	L2111	L2112	L2113	L2114	L2115	L2116	L2117	L2118	L2119	L2120	L2121	L2122	L2123	L2124	L2125	L2126	L2127	L2128	L2129	L2130	L2131	L2132	L2133	L2134	L2135	L2136	L2137	L2138	L2139	L2140	L2141	L2142	L2143	L2144	L2145	L2146	L2147	L2148	L2149	L2150	L2151	L2152	L2153	L2154	L2155	L2156	L2157	L2158	L2159	L2160	L2161	L2162	L2163	L2164	L2165	L2166	L2167	L2168	L2169	L2170	L2171	L2172	L2173	L2174	L2175	L2176	L2177	L2178	L2179	L2180	L2181	L2182	L2183	L2184	L2185	L2186	L2187	L2188	L2189	L2190	L2191	L2192	L2193	L2194	L2195	L2196	L2197	L2198	L2199	L2200	L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	L2261	L2262	L2263	L2264	L2265	L2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280	L2281	L2282	L2283	L2284	L2285	L2286	L2287	L2288	L2289	L2290	L2291	L2292	L2293	L2294	L2295	L2296	L2297	L2298	L2299	L2300	L2301	L2302	L2303	L2304	L2305	L2306	L2307	L2308	L2309	L2310	L2311	L2312	L2313	L2314	L2315	L2316	L2317	L2318	L2319	L2320	L2321	L2322	L2323	L2324	L2325	L2326	L2327	L2328	L2329	L2330	L2331	L2332	L2333	L2334	L2335	L2336	L2337	L2338	L2339	L2340	L2341	L2342	L2343	L2344	L2345	L2346	L2347	L2348	L2349	L2350	L2351	L2352	L2353	L2354	L2355	L2356	L2357	L2358	L2359	L2360	L2361	L2362	L2363	L2364	L2365	L2366	L2367	L2368	L2369	L2370	L2371	L2372	L2373	L2374	L2375	L2376	L2377	L2378	L2379	L2380	L2381	L2382	L2383	L2384	L2385	L2386	L2387	L2388	L2389	L2390	L2391	L2392	L2393	L2394	L2395	L2396	L2397	L2398	L2399	L2400	L2401	L2402	L2403	L2404	L2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● Molecule 1: TcdA1

Chain C: 68% 16% 16%



L971	L972	1973	K982	R999	A1000	L1001	E1002	E1005	I1013	F1017	Y1024	Y1034	S1035	Q1036	Y1040	F1041	E1042	I1045	M1049	Q1053	M1056	M1057	D1058	A1059	Q1062	L1069	M1070	A1071	D1072	T1073	Y1081	V1093	H1098	D1099	M1100	T1108	L1113	D1117	A1118						
G1119	E1120	R1124	H1128	S1142	E1143	W1144	H1145	K1146	I1147	R1159	I1162	Y1163	K1164	S1165	R1166	L1167	Y1168	L1169	K1175	T1178	T1181	GLY	ASN	SER	LYS	ASP	D1058	GLY	Y1188	T1192	L1200	K1220	R1230	C1236	Y1239	E1242	D1243	T1244	L1245	L1246	N1251	Q1252	L1267		
Y1268	A1271	Y1291	F1294	D1295	T1296	N1297	R1301	Y1302	N1303	E1308	ASP	TYR	GLU	ILE	PRO	SER	VAL	ASN	SER	SER	GLY	TRP	GLY	ASP	LYS	TRP	LEU	SER	MET	VAL	ASN	GLY	PRO	ASN	ILE	PRO	THR	ASN	LYS	ASN	LEU	LYS	THR	GLY	
ASN	THR	SER	GLY	LEU	ASN	ARG	GLN	GLY	GLN	GLN	ASN	ASN	GLN	CYS	ASN	PRO	LYS	VAL	GLU	MET	SER	VAL	ALA	ASN	THR	ILE	PRO	GLN	GLY	ILE	ALA	ALA	GLN	ASP	THR	ALA	THR	ASP	SER	GLN	TYR	ILE	PHE		
MET	THR	ASP	GLY	LYS	THR	ALA	THR	ASP	VAL	PRO	GLU	ILE	ASN	THR	ALA	LYS	VAL	GLN	ILE	GLY	ILE	ALA	LYS	ARG	LYS	ALA	GLY	LEU	THR	LYS	ASN	GLN	THR	ASP	ILE	GLN	PRO	SER	ASN	LYS	PRO	PHE	THR	GLN	PHE
ASN	ALA	LEU	GLU	ILE	ASP	GLY	SER	LEU	ASN	THR	ASN	ASN	SER	ILE	ASP	VAL	THR	PHE	ALA	ALA	GLY	GLY	THR	LYS	GLY	GLU	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
A1617	T1618	I1624	Q1630	D1657	I1676	L1690	F1711	K1712	K1713	G1722	D1729	S1739	A1763	L1766	Y1767	F1768	Y1769	L1770	L1771	Y1772	Y1773	Y1774	L1783	E1786	Q1787	M1788	F1789	D1790	E1791	A1792	N1793	R1794	K1797	Y1798	W1800	S1801	P1802	Y1805	Y1814	G1864					
Y1868	E1878	M1881	Y1882	Y1883	M1884	Q1885	A1886	L1887	H1888	D1892	Y1895	K1912	A1911	T1914	N1917	ALA	HIS	ASP	SER	ALA	ILE	VAL	LEU	ARG	GLN	ASN	ILE	PRO	THR	PRO	ALA	LEU	SER	ARG	ALA	ASN	THR	L1944	T1962	Q1965	R1966	I1976	T1985	Y1986	
A1987	T1988	P1989	A1990	L1995	A1998	Q2004	G2005	L2009	L2016	W2017	R2018	N2025	V2030	T2034	L2040	I2044	N2053	N2067	L2068	K2073	E2077	L2078	K2087	D2097	S2098	Y2099	Y2103	N2112	M2115	A2122	G2123	L2124	V2128	Q2129	A2130	S2131	R2132								
L2133	V2141	F2147	R2153	E2159	Y2163	V2171	R2189	E2193	I2194	Q2195	K2204	D2207	K2211	R2216	R2217	E2218	A2219	L2227	Q2235	L2241	S2246	L2250	V2253	L2254	R2255	G2256	Y2266	R2272	E2277	F2291	P2294	W2297	T2300												
W2317	H2321	L2322	D2325	K2326	R2327	A2328	L2329	E2330	T2334	L2337	A2338	Y2341	L2353	A2354	Q2355	E2356	I2357	D2358	K2359	L2360	N2372	F2377	S2390	V2391	S2392	F2393	L2396	R2399	Y2426	Q2430	L2433	K2438	L2441	C2445	E2446	A2447	L2448	H2452	D2456	S2457					
G2458	Q2459	F2460	G2467	K2468	F2469	I2477	L2482	T2483	L2484	L2504	T2507	K2516																																	

● Molecule 1: TcdA1

Chain E:  68% 16% 16%

MET	ALA	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	GLU	VAL	LEU	PHE	GLN	GLY	PRO	MET	ASN	ASN	GLU	LYS	GLU	ILE	ASP	VAL	LEU	LYS	SER	GLN	CYS	GLY	PHE	ASN	CYS	LEU	THR	ASP	ILE	SER	HIS	SER	SER	PHE	ASN	GLU	PHE	ARG	GLN	GLN	VAL	SER	SER	GLU	HIS	LEU	SER
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	230785	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.447	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	425.92, 425.92, 425.92	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.27	0/17247	0.51	0/23428
1	B	0.27	0/17247	0.51	0/23428
1	C	0.27	0/17247	0.51	0/23428
1	D	0.27	0/17247	0.51	0/23428
1	E	0.26	0/17247	0.51	0/23428
All	All	0.27	0/86235	0.51	0/117140

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	16884	0	16507	277	0
1	B	16884	0	16507	280	0
1	C	16884	0	16507	275	0
1	D	16884	0	16507	277	0
1	E	16884	0	16507	280	0
All	All	84420	0	82535	1241	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 7.

All (1241) 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:689:LEU:HD11	1:B:712:LEU:HB3	1.62	0.82
1:C:1296:THR:HG23	1:C:1301:ARG:HH12	1.46	0.81
1:C:689:LEU:HD11	1:C:712:LEU:HB3	1.61	0.81
1:E:689:LEU:HD11	1:E:712:LEU:HB3	1.62	0.81
1:D:1296:THR:HG23	1:D:1301:ARG:HH12	1.45	0.81
1:A:1296:THR:HG23	1:A:1301:ARG:HH12	1.46	0.80
1:B:1296:THR:HG23	1:B:1301:ARG:HH12	1.46	0.80
1:A:689:LEU:HD11	1:A:712:LEU:HB3	1.62	0.79
1:A:2445:CYS:SG	1:B:2327:ARG:NH1	2.56	0.79
1:D:2445:CYS:SG	1:E:2327:ARG:NH1	2.56	0.79
1:A:2327:ARG:NH1	1:E:2445:CYS:SG	2.55	0.79
1:B:2445:CYS:SG	1:C:2327:ARG:NH1	2.56	0.78
1:E:1296:THR:HG23	1:E:1301:ARG:HH12	1.46	0.78
1:D:689:LEU:HD11	1:D:712:LEU:HB3	1.63	0.78
1:B:1108:THR:HG1	1:B:1128:HIS:HE2	1.31	0.78
1:C:2445:CYS:SG	1:D:2327:ARG:NH1	2.57	0.78
1:E:1108:THR:HG1	1:E:1128:HIS:HE2	1.31	0.77
1:C:1059:ALA:HA	1:C:1062:GLN:HE21	1.50	0.75
1:E:1059:ALA:HA	1:E:1062:GLN:HE21	1.50	0.75
1:B:1797:LYS:HG3	1:B:1801:SER:HB2	1.69	0.74
1:B:1059:ALA:HA	1:B:1062:GLN:HE21	1.51	0.74
1:D:1059:ALA:HA	1:D:1062:GLN:HE21	1.51	0.74
1:A:1059:ALA:HA	1:A:1062:GLN:HE21	1.51	0.74
1:C:1108:THR:HG1	1:C:1128:HIS:HE2	1.34	0.73
1:C:1797:LYS:HG3	1:C:1801:SER:HB2	1.70	0.73
1:D:1093:VAL:HG21	1:D:1605:LEU:HD23	1.70	0.73
1:D:1797:LYS:HG3	1:D:1801:SER:HB2	1.68	0.73
1:E:1797:LYS:HG3	1:E:1801:SER:HB2	1.69	0.73
1:B:1093:VAL:HG21	1:B:1605:LEU:HD23	1.70	0.72
1:C:460:ILE:HG12	1:C:496:LEU:HD21	1.70	0.72
1:B:460:ILE:HG12	1:B:496:LEU:HD21	1.71	0.72
1:D:460:ILE:HG12	1:D:496:LEU:HD21	1.69	0.72
1:A:460:ILE:HG12	1:A:496:LEU:HD21	1.71	0.72
1:C:210:VAL:HG11	1:C:922:LEU:HB3	1.72	0.72
1:A:1797:LYS:HG3	1:A:1801:SER:HB2	1.70	0.72
1:C:1093:VAL:HG21	1:C:1605:LEU:HD23	1.71	0.72
1:B:2277:GLU:HA	1:B:2317:MET:HE1	1.73	0.71
1:E:460:ILE:HG12	1:E:496:LEU:HD21	1.70	0.71
1:D:1163:TYR:HB2	1:D:1245:LEU:HD21	1.72	0.71
1:C:462:ARG:HH11	1:C:506:ARG:HH11	1.37	0.71
1:E:1163:TYR:HB2	1:E:1245:LEU:HD21	1.72	0.71
1:A:300:ALA:HA	1:A:303:PHE:CD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ALA:HA	1:B:303:PHE:CD2	2.27	0.70
1:D:300:ALA:HA	1:D:303:PHE:CD2	2.27	0.70
1:E:210:VAL:HG11	1:E:922:LEU:HB3	1.74	0.70
1:A:698:ALA:HB1	1:B:2253:TRP:HA	1.71	0.70
1:C:300:ALA:HA	1:C:303:PHE:CD2	2.26	0.70
1:C:698:ALA:HB1	1:D:2253:TRP:HA	1.73	0.70
1:B:698:ALA:HB1	1:C:2253:TRP:HA	1.72	0.70
1:C:1163:TYR:HB2	1:C:1245:LEU:HD21	1.72	0.70
1:E:1093:VAL:HG21	1:E:1605:LEU:HD23	1.72	0.70
1:A:462:ARG:HH11	1:A:506:ARG:HH11	1.39	0.70
1:A:1093:VAL:HG21	1:A:1605:LEU:HD23	1.73	0.70
1:A:2277:GLU:HA	1:A:2317:MET:HE1	1.73	0.70
1:D:2277:GLU:HA	1:D:2317:MET:HE1	1.74	0.69
1:A:210:VAL:HG11	1:A:922:LEU:HB3	1.73	0.69
1:D:462:ARG:HH11	1:D:506:ARG:HH11	1.40	0.69
1:B:210:VAL:HG11	1:B:922:LEU:HB3	1.74	0.69
1:B:1163:TYR:HB2	1:B:1245:LEU:HD21	1.72	0.69
1:D:210:VAL:HG11	1:D:922:LEU:HB3	1.73	0.69
1:E:300:ALA:HA	1:E:303:PHE:CD2	2.27	0.69
1:A:1108:THR:HG1	1:A:1128:HIS:HE2	1.40	0.69
1:A:2253:TRP:HA	1:E:698:ALA:HB1	1.75	0.69
1:B:746:VAL:HB	1:B:749:GLN:HB2	1.74	0.69
1:E:462:ARG:HH11	1:E:506:ARG:HH11	1.41	0.69
1:E:746:VAL:HB	1:E:749:GLN:HB2	1.75	0.69
1:A:1163:TYR:HB2	1:A:1245:LEU:HD21	1.73	0.69
1:D:746:VAL:HB	1:D:749:GLN:HB2	1.74	0.69
1:B:462:ARG:HH11	1:B:506:ARG:HH11	1.41	0.68
1:A:746:VAL:HB	1:A:749:GLN:HB2	1.76	0.68
1:C:2277:GLU:HA	1:C:2317:MET:HE1	1.76	0.68
1:C:746:VAL:HB	1:C:749:GLN:HB2	1.73	0.67
1:E:2277:GLU:HA	1:E:2317:MET:HE1	1.75	0.67
1:C:2356:GLU:HA	1:C:2359:LYS:HG2	1.76	0.66
1:E:2356:GLU:HA	1:E:2359:LYS:HG2	1.77	0.66
1:B:2356:GLU:HA	1:B:2359:LYS:HG2	1.77	0.66
1:C:505:GLN:HE22	1:C:582:LEU:HD13	1.61	0.66
1:D:121:GLU:HG2	1:D:124:ARG:HH21	1.61	0.66
1:D:2356:GLU:HA	1:D:2359:LYS:HG2	1.77	0.66
1:C:121:GLU:HG2	1:C:124:ARG:HH21	1.61	0.65
1:E:2068:LEU:HD22	1:E:2227:LEU:HG	1.78	0.65
1:C:1069:LEU:HD23	1:C:1786:GLU:HG3	1.78	0.65
1:A:2255:ARG:NH2	1:E:703:SER:O	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:ALA:HB1	1:E:2253:TRP:HA	1.79	0.65
1:A:121:GLU:HG2	1:A:124:ARG:HH21	1.62	0.64
1:A:659:TYR:HB2	1:A:754:GLN:HG2	1.79	0.64
1:B:703:SER:O	1:C:2255:ARG:NH2	2.28	0.64
1:D:2068:LEU:HD22	1:D:2227:LEU:HG	1.79	0.64
1:A:2068:LEU:HD22	1:A:2227:LEU:HG	1.78	0.64
1:D:659:TYR:HB2	1:D:754:GLN:HG2	1.78	0.64
1:A:703:SER:O	1:B:2255:ARG:NH2	2.28	0.64
1:D:698:ALA:HB2	1:E:2256:GLY:HA3	1.79	0.64
1:A:2356:GLU:HA	1:A:2359:LYS:HG2	1.78	0.64
1:A:91:GLY:N	1:A:94:ASN:HD22	1.96	0.63
1:A:505:GLN:HE22	1:A:582:LEU:HD13	1.64	0.63
1:B:2068:LEU:HD22	1:B:2227:LEU:HG	1.79	0.63
1:B:659:TYR:HB2	1:B:754:GLN:HG2	1.80	0.63
1:E:91:GLY:N	1:E:94:ASN:HD22	1.96	0.63
1:C:703:SER:O	1:D:2255:ARG:NH2	2.29	0.63
1:E:568:ILE:HD11	1:E:606:ASP:HB2	1.81	0.63
1:A:519:PHE:O	1:A:553:ARG:NH2	2.31	0.63
1:A:1069:LEU:HD23	1:A:1786:GLU:HG3	1.80	0.63
1:B:121:GLU:HG2	1:B:124:ARG:HH21	1.64	0.63
1:D:505:GLN:HE22	1:D:582:LEU:HD13	1.64	0.63
1:E:2025:ASN:OD1	1:E:2272:ARG:NH1	2.30	0.63
1:D:1864:GLY:HA3	1:D:1883:TYR:CE1	2.34	0.63
1:E:121:GLU:HG2	1:E:124:ARG:HH21	1.62	0.63
1:E:519:PHE:O	1:E:553:ARG:NH2	2.31	0.63
1:C:670:LEU:HA	1:C:699:THR:HG21	1.81	0.62
1:A:1864:GLY:HA3	1:A:1883:TYR:CE1	2.34	0.62
1:A:368:LEU:N	1:A:381:THR:O	2.27	0.62
1:C:698:ALA:HB2	1:D:2256:GLY:HA3	1.81	0.62
1:D:703:SER:O	1:E:2255:ARG:NH2	2.28	0.62
1:E:1069:LEU:HD23	1:E:1786:GLU:HG3	1.81	0.62
1:C:91:GLY:N	1:C:94:ASN:HD22	1.97	0.62
1:C:659:TYR:HB2	1:C:754:GLN:HG2	1.80	0.62
1:E:1783:LEU:HD12	1:E:1788:ASN:HB3	1.81	0.62
1:A:2073:LYS:HZ1	1:E:2219:ALA:HA	1.64	0.62
1:B:368:LEU:N	1:B:381:THR:O	2.27	0.62
1:B:505:GLN:HE22	1:B:582:LEU:HD13	1.64	0.62
1:E:1864:GLY:HA3	1:E:1883:TYR:CE1	2.34	0.62
1:A:698:ALA:HB2	1:B:2256:GLY:HA3	1.81	0.62
1:B:1885:GLN:HA	1:B:1888:HIS:CE1	2.35	0.62
1:C:568:ILE:HD11	1:C:606:ASP:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:LYS:HE2	1:B:1611:ARG:HG2	1.81	0.61
1:A:2256:GLY:HA3	1:E:698:ALA:HB2	1.81	0.61
1:B:1864:GLY:HA3	1:B:1883:TYR:CE1	2.34	0.61
1:B:2067:ASN:HB3	1:B:2227:LEU:HD21	1.82	0.61
1:D:1069:LEU:HD23	1:D:1786:GLU:HG3	1.81	0.61
1:A:458:GLU:OE2	1:A:506:ARG:NH1	2.30	0.61
1:B:1783:LEU:HD12	1:B:1788:ASN:HB3	1.81	0.61
1:A:1885:GLN:HA	1:A:1888:HIS:CE1	2.35	0.61
1:B:2016:LEU:O	1:C:2327:ARG:NH2	2.34	0.61
1:E:505:GLN:HE22	1:E:582:LEU:HD13	1.66	0.61
1:C:2068:LEU:HD22	1:C:2227:LEU:HG	1.80	0.61
1:D:1783:LEU:HD12	1:D:1788:ASN:HB3	1.82	0.61
1:B:2219:ALA:HA	1:C:2073:LYS:HZ1	1.66	0.61
1:C:1783:LEU:HD12	1:C:1788:ASN:HB3	1.82	0.61
1:B:91:GLY:N	1:B:94:ASN:HD22	1.97	0.61
1:B:2153:ARG:NH1	1:B:2159:GLU:OE1	2.31	0.61
1:D:1885:GLN:HA	1:D:1888:HIS:CE1	2.35	0.61
1:D:2438:LYS:HG3	1:D:2446:GLU:HG3	1.83	0.61
1:E:2504:LEU:HD21	1:E:2507:ILE:HD11	1.82	0.61
1:C:2016:LEU:O	1:D:2327:ARG:NH2	2.34	0.61
1:C:2504:LEU:HD21	1:C:2507:ILE:HD11	1.82	0.61
1:C:1864:GLY:HA3	1:C:1883:TYR:CE1	2.35	0.61
1:C:2218:GLU:OE1	1:D:2073:LYS:NZ	2.34	0.61
1:A:568:ILE:HD11	1:A:606:ASP:HB2	1.83	0.61
1:B:2438:LYS:HG3	1:B:2446:GLU:HG3	1.83	0.61
1:B:2504:LEU:HD21	1:B:2507:ILE:HD11	1.81	0.61
1:C:519:PHE:O	1:C:553:ARG:NH2	2.34	0.61
1:E:1885:GLN:HA	1:E:1888:HIS:CE1	2.35	0.61
1:B:568:ILE:HD11	1:B:606:ASP:HB2	1.81	0.60
1:C:253:GLU:O	1:C:442:LYS:NZ	2.28	0.60
1:A:1611:ARG:HG2	1:E:1164:LYS:HE2	1.83	0.60
1:D:2504:LEU:HD21	1:D:2507:ILE:HD11	1.83	0.60
1:E:2393:PHE:HA	1:E:2396:LEU:HD12	1.83	0.60
1:A:1783:LEU:HD12	1:A:1788:ASN:HB3	1.83	0.60
1:B:2460:PHE:CE1	1:C:2330:GLU:HB3	2.36	0.60
1:D:670:LEU:HA	1:D:699:THR:HG21	1.84	0.60
1:D:2025:ASN:OD1	1:D:2272:ARG:NH1	2.30	0.60
1:A:2330:GLU:HB3	1:E:2460:PHE:CE1	2.36	0.60
1:B:698:ALA:HB2	1:C:2256:GLY:HA3	1.82	0.60
1:B:830:LEU:HD21	1:B:835:LEU:HD12	1.84	0.60
1:D:1794:ARG:NH2	1:D:1798:TYR:OH	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2393:PHE:HA	1:D:2396:LEU:HD12	1.82	0.60
1:E:2438:LYS:HG3	1:E:2446:GLU:HG3	1.82	0.60
1:B:458:GLU:OE2	1:B:506:ARG:NH1	2.31	0.60
1:C:1885:GLN:HA	1:C:1888:HIS:CE1	2.36	0.60
1:E:659:TYR:HB2	1:E:754:GLN:HG2	1.83	0.60
1:E:830:LEU:HD21	1:E:835:LEU:HD12	1.83	0.60
1:B:2393:PHE:HA	1:B:2396:LEU:HD12	1.83	0.60
1:C:2025:ASN:OD1	1:C:2272:ARG:NH1	2.32	0.60
1:C:2438:LYS:HG3	1:C:2446:GLU:HG3	1.82	0.60
1:D:2460:PHE:CE1	1:E:2330:GLU:HB3	2.37	0.60
1:A:2460:PHE:CE1	1:B:2330:GLU:HB3	2.37	0.60
1:B:1069:LEU:HD23	1:B:1786:GLU:HG3	1.83	0.60
1:C:2460:PHE:CE1	1:D:2330:GLU:HB3	2.37	0.60
1:D:519:PHE:O	1:D:553:ARG:NH2	2.34	0.60
1:D:1607:THR:HG21	1:D:1768:PHE:HZ	1.66	0.60
1:B:670:LEU:HA	1:B:699:THR:HG21	1.82	0.60
1:D:568:ILE:HD11	1:D:606:ASP:HB2	1.83	0.60
1:A:2504:LEU:HD21	1:A:2507:ILE:HD11	1.82	0.59
1:C:337:ASN:ND2	1:C:421:TYR:O	2.25	0.59
1:B:2218:GLU:OE1	1:C:2073:LYS:NZ	2.33	0.59
1:D:91:GLY:N	1:D:94:ASN:HD22	2.00	0.59
1:A:830:LEU:HD21	1:A:835:LEU:HD12	1.84	0.59
1:A:2016:LEU:O	1:B:2327:ARG:NH2	2.35	0.59
1:C:741:GLY:HA2	1:E:2005:GLY:HA2	1.85	0.59
1:D:830:LEU:HD21	1:D:835:LEU:HD12	1.83	0.59
1:A:670:LEU:HA	1:A:699:THR:HG21	1.83	0.59
1:D:2219:ALA:HA	1:E:2073:LYS:HZ1	1.67	0.59
1:D:2016:LEU:O	1:E:2327:ARG:NH2	2.34	0.59
1:A:2005:GLY:HA2	1:D:741:GLY:HA2	1.85	0.59
1:A:2393:PHE:HA	1:A:2396:LEU:HD12	1.85	0.59
1:A:2218:GLU:OE1	1:B:2073:LYS:NZ	2.35	0.58
1:C:540:SER:HB2	1:D:848:GLN:NE2	2.18	0.58
1:E:368:LEU:N	1:E:381:THR:O	2.27	0.58
1:A:741:GLY:HA2	1:C:2005:GLY:HA2	1.86	0.58
1:B:540:SER:HB2	1:C:848:GLN:NE2	2.18	0.58
1:C:2067:ASN:HB3	1:C:2227:LEU:HD21	1.84	0.58
1:E:337:ASN:ND2	1:E:421:TYR:O	2.25	0.58
1:A:848:GLN:NE2	1:E:540:SER:HB2	2.18	0.58
1:B:2005:GLY:HA2	1:E:741:GLY:HA2	1.85	0.58
1:E:1607:THR:HG21	1:E:1768:PHE:HZ	1.67	0.58
1:C:830:LEU:HD21	1:C:835:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1607:THR:HG21	1:C:1768:PHE:HZ	1.67	0.58
1:D:540:SER:HB2	1:E:848:GLN:NE2	2.18	0.58
1:A:2438:LYS:HG3	1:A:2446:GLU:HG3	1.86	0.58
1:B:741:GLY:HA2	1:D:2005:GLY:HA2	1.86	0.58
1:E:198:THR:O	1:E:445:ARG:NH1	2.37	0.58
1:A:540:SER:HB2	1:B:848:GLN:NE2	2.18	0.58
1:B:1607:THR:HG21	1:B:1768:PHE:HZ	1.67	0.58
1:D:2218:GLU:OE1	1:E:2073:LYS:NZ	2.34	0.58
1:D:2246:SER:HA	1:D:2250:LEU:HD23	1.85	0.58
1:A:2112:ASN:HA	1:A:2115:MET:HG2	1.86	0.58
1:C:2393:PHE:HA	1:C:2396:LEU:HD12	1.84	0.58
1:A:1607:THR:HG21	1:A:1768:PHE:HZ	1.69	0.58
1:B:519:PHE:O	1:B:553:ARG:NH2	2.37	0.58
1:B:2246:SER:HA	1:B:2250:LEU:HD23	1.85	0.58
1:E:458:GLU:OE2	1:E:506:ARG:NH1	2.30	0.58
1:E:2040:LEU:O	1:E:2044:ILE:HG12	2.04	0.58
1:A:2327:ARG:NH2	1:E:2016:LEU:O	2.36	0.58
1:B:1794:ARG:NH2	1:B:1798:TYR:OH	2.37	0.58
1:C:505:GLN:NE2	1:C:582:LEU:HD13	2.19	0.58
1:D:2153:ARG:NH1	1:D:2159:GLU:OE1	2.32	0.57
1:C:458:GLU:OE2	1:C:506:ARG:NH1	2.31	0.57
1:C:1966:ARG:HD2	1:C:1976:ILE:HG13	1.86	0.57
1:C:2219:ALA:HA	1:D:2073:LYS:HZ1	1.69	0.57
1:D:612:VAL:HG22	1:D:637:ILE:HD12	1.86	0.57
1:D:2067:ASN:HB3	1:D:2227:LEU:HD21	1.86	0.57
1:D:2112:ASN:HA	1:D:2115:MET:HG2	1.86	0.57
1:A:2246:SER:HA	1:A:2250:LEU:HD23	1.85	0.57
1:B:505:GLN:NE2	1:B:582:LEU:HD13	2.19	0.57
1:B:2040:LEU:O	1:B:2044:ILE:HG12	2.05	0.57
1:C:2246:SER:HA	1:C:2250:LEU:HD23	1.84	0.57
1:D:505:GLN:NE2	1:D:582:LEU:HD13	2.20	0.57
1:E:670:LEU:HA	1:E:699:THR:HG21	1.85	0.57
1:E:2246:SER:HA	1:E:2250:LEU:HD23	1.86	0.57
1:A:2040:LEU:O	1:A:2044:ILE:HG12	2.05	0.57
1:B:2353:LEU:HD23	1:B:2357:ILE:HD11	1.87	0.57
1:C:1220:LYS:HE2	1:C:1267:LEU:HB3	1.85	0.57
1:C:2040:LEU:O	1:C:2044:ILE:HG12	2.05	0.57
1:C:2112:ASN:HA	1:C:2115:MET:HG2	1.85	0.57
1:C:2153:ARG:NH1	1:C:2159:GLU:OE1	2.32	0.57
1:E:2067:ASN:HB3	1:E:2227:LEU:HD21	1.87	0.57
1:E:2112:ASN:HA	1:E:2115:MET:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:ASP:OD1	1:B:798:ALA:N	2.38	0.57
1:B:2112:ASN:HA	1:B:2115:MET:HG2	1.87	0.57
1:A:2353:LEU:HD23	1:A:2357:ILE:HD11	1.87	0.56
1:B:646:TRP:CZ2	1:B:768:SER:HB3	2.40	0.56
1:D:2040:LEU:O	1:D:2044:ILE:HG12	2.05	0.56
1:A:836:ALA:HB2	1:A:846:LEU:HD12	1.87	0.56
1:A:2153:ARG:NH1	1:A:2159:GLU:OE1	2.32	0.56
1:C:2353:LEU:HD23	1:C:2357:ILE:HD11	1.88	0.56
1:D:337:ASN:ND2	1:D:421:TYR:O	2.25	0.56
1:D:458:GLU:OE2	1:D:506:ARG:NH1	2.32	0.56
1:D:646:TRP:CZ2	1:D:768:SER:HB3	2.40	0.56
1:D:797:ASP:OD1	1:D:798:ALA:N	2.38	0.56
1:D:1164:LYS:HE2	1:E:1611:ARG:HG2	1.85	0.56
1:D:2353:LEU:HD23	1:D:2357:ILE:HD11	1.87	0.56
1:E:1072:ASP:OD1	1:E:1073:THR:N	2.38	0.56
1:E:2353:LEU:HD23	1:E:2357:ILE:HD11	1.87	0.56
1:A:1966:ARG:HD2	1:A:1976:ILE:HG13	1.87	0.56
1:B:1072:ASP:OD1	1:B:1073:THR:N	2.38	0.56
1:E:836:ALA:HB2	1:E:846:LEU:HD12	1.87	0.56
1:B:1966:ARG:HD2	1:B:1976:ILE:HG13	1.87	0.56
1:E:797:ASP:OD1	1:E:798:ALA:N	2.38	0.56
1:E:2153:ARG:NH1	1:E:2159:GLU:OE1	2.33	0.56
1:C:797:ASP:OD1	1:C:798:ALA:N	2.38	0.56
1:C:2103:TYR:CE1	1:C:2189:ARG:HG2	2.40	0.56
1:D:836:ALA:HB2	1:D:846:LEU:HD12	1.88	0.56
1:A:337:ASN:ND2	1:A:421:TYR:O	2.25	0.56
1:B:836:ALA:HB2	1:B:846:LEU:HD12	1.88	0.56
1:B:2433:LEU:HA	1:B:2484:LEU:HA	1.88	0.56
1:D:1072:ASP:OD1	1:D:1073:THR:N	2.39	0.56
1:A:646:TRP:CZ2	1:A:768:SER:HB3	2.41	0.56
1:A:2067:ASN:HB3	1:A:2227:LEU:HD21	1.87	0.56
1:B:337:ASN:ND2	1:B:421:TYR:O	2.25	0.56
1:C:646:TRP:CZ2	1:C:768:SER:HB3	2.41	0.56
1:D:1271:ALA:HB1	1:E:1611:ARG:HD3	1.88	0.56
1:A:797:ASP:OD1	1:A:798:ALA:N	2.38	0.56
1:C:612:VAL:HG22	1:C:637:ILE:HD12	1.88	0.56
1:A:341:MET:HE2	1:A:359:PHE:CE1	2.42	0.55
1:A:505:GLN:NE2	1:A:582:LEU:HD13	2.20	0.55
1:C:836:ALA:HB2	1:C:846:LEU:HD12	1.88	0.55
1:C:2341:TYR:OH	1:C:2390:SER:O	2.20	0.55
1:D:2433:LEU:HA	1:D:2484:LEU:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:646:TRP:CZ2	1:E:768:SER:HB3	2.41	0.55
1:C:1164:LYS:HE2	1:D:1611:ARG:HG2	1.87	0.55
1:D:2204:LYS:HG2	1:E:2087:LYS:HD2	1.88	0.55
1:E:2433:LEU:HA	1:E:2484:LEU:HA	1.87	0.55
1:A:1252:GLN:HB3	1:A:1297:ASN:OD1	2.06	0.55
1:E:557:ILE:HB	1:E:561:SER:OG	2.07	0.55
1:E:1966:ARG:HD2	1:E:1976:ILE:HG13	1.87	0.55
1:A:2025:ASN:OD1	1:A:2272:ARG:NH1	2.33	0.55
1:B:1058:ASP:O	1:B:1062:GLN:HG3	2.06	0.55
1:E:505:GLN:NE2	1:E:582:LEU:HD13	2.20	0.55
1:A:1072:ASP:OD1	1:A:1073:THR:N	2.39	0.55
1:B:341:MET:HE1	1:B:359:PHE:CE1	2.42	0.55
1:C:198:THR:O	1:C:445:ARG:NH1	2.39	0.55
1:D:1117:ASP:OD1	1:D:1118:ALA:N	2.38	0.55
1:A:612:VAL:HG22	1:A:637:ILE:HD12	1.87	0.55
1:D:341:MET:HE2	1:D:359:PHE:CE1	2.42	0.55
1:E:120:THR:O	1:E:124:ARG:HG3	2.07	0.55
1:E:253:GLU:O	1:E:442:LYS:NZ	2.30	0.55
1:A:2103:TYR:CE1	1:A:2189:ARG:HG2	2.42	0.55
1:B:1164:LYS:HE2	1:C:1611:ARG:HG2	1.87	0.55
1:B:1252:GLN:HB3	1:B:1297:ASN:OD1	2.07	0.55
1:D:368:LEU:N	1:D:381:THR:O	2.27	0.55
1:B:1868:TYR:HB3	1:B:1976:ILE:HD12	1.89	0.55
1:C:120:THR:O	1:C:124:ARG:HG3	2.07	0.55
1:C:368:LEU:HG	1:C:370:ILE:HD11	1.89	0.55
1:A:2433:LEU:HA	1:A:2484:LEU:HA	1.88	0.55
1:C:1252:GLN:HB3	1:C:1297:ASN:OD1	2.07	0.55
1:D:1630:GLN:HG2	1:D:1772:PHE:CE2	2.42	0.55
1:A:557:ILE:HB	1:A:561:SER:OG	2.07	0.54
1:B:2025:ASN:OD1	1:B:2272:ARG:NH1	2.35	0.54
1:B:2103:TYR:CE1	1:B:2189:ARG:HG2	2.43	0.54
1:C:341:MET:HE2	1:C:359:PHE:CE1	2.42	0.54
1:C:2103:TYR:CE1	1:C:2193:GLU:HG2	2.43	0.54
1:D:1966:ARG:HD2	1:D:1976:ILE:HG13	1.87	0.54
1:A:811:VAL:HG22	1:A:822:LEU:HD21	1.89	0.54
1:B:120:THR:O	1:B:124:ARG:HG3	2.07	0.54
1:C:368:LEU:N	1:C:381:THR:O	2.27	0.54
1:D:120:THR:O	1:D:124:ARG:HG3	2.06	0.54
1:D:1058:ASP:O	1:D:1062:GLN:HG3	2.07	0.54
1:A:120:THR:O	1:A:124:ARG:HG3	2.07	0.54
1:A:368:LEU:HG	1:A:370:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1794:ARG:NH2	1:A:1798:TYR:OH	2.39	0.54
1:C:1072:ASP:OD1	1:C:1073:THR:N	2.39	0.54
1:C:2337:LEU:HB3	1:C:2507:ILE:HB	1.89	0.54
1:D:1252:GLN:HB3	1:D:1297:ASN:OD1	2.07	0.54
1:E:300:ALA:HA	1:E:303:PHE:HD2	1.73	0.54
1:E:612:VAL:HG22	1:E:637:ILE:HD12	1.88	0.54
1:A:1630:GLN:HG2	1:A:1772:PHE:CE2	2.42	0.54
1:E:1252:GLN:HB3	1:E:1297:ASN:OD1	2.07	0.54
1:B:510:ASN:OD1	1:C:153:GLN:NE2	2.38	0.54
1:C:2433:LEU:HA	1:C:2484:LEU:HA	1.88	0.54
1:B:198:THR:O	1:B:445:ARG:NH1	2.41	0.54
1:B:368:LEU:HG	1:B:370:ILE:HD11	1.89	0.54
1:D:2426:TYR:HB3	1:E:2334:THR:HG21	1.88	0.54
1:A:195:SER:HB3	1:A:198:THR:OG1	2.08	0.54
1:A:300:ALA:HA	1:A:303:PHE:HD2	1.72	0.54
1:A:848:GLN:HE22	1:E:540:SER:HB2	1.73	0.54
1:C:195:SER:HB3	1:C:198:THR:OG1	2.08	0.54
1:E:1630:GLN:HG2	1:E:1772:PHE:CE2	2.42	0.54
1:A:198:THR:O	1:A:445:ARG:NH1	2.40	0.54
1:A:1271:ALA:HB1	1:B:1611:ARG:HD3	1.90	0.54
1:E:341:MET:HE2	1:E:359:PHE:CE1	2.43	0.54
1:D:368:LEU:HG	1:D:370:ILE:HD11	1.89	0.54
1:D:811:VAL:HG22	1:D:822:LEU:HD21	1.89	0.54
1:A:1058:ASP:O	1:A:1062:GLN:HG3	2.06	0.54
1:C:557:ILE:HB	1:C:561:SER:OG	2.07	0.54
1:D:557:ILE:HB	1:D:561:SER:OG	2.07	0.54
1:E:2337:LEU:HB3	1:E:2507:ILE:HB	1.90	0.54
1:A:2103:TYR:CE1	1:A:2193:GLU:HG2	2.43	0.53
1:B:612:VAL:HG22	1:B:637:ILE:HD12	1.89	0.53
1:C:2053:ASN:ND2	1:C:2241:LEU:HD11	2.23	0.53
1:D:2141:VAL:HG21	1:E:1175:LYS:HE2	1.90	0.53
1:E:2103:TYR:CE1	1:E:2189:ARG:HG2	2.44	0.53
1:C:300:ALA:HA	1:C:303:PHE:HD2	1.72	0.53
1:E:197:ALA:N	1:E:948:THR:HG21	2.23	0.53
1:A:1071:ALA:HB2	1:A:1791:GLU:OE2	2.09	0.53
1:C:2426:TYR:HB3	1:D:2334:THR:HG21	1.90	0.53
1:E:195:SER:HB3	1:E:198:THR:OG1	2.08	0.53
1:E:368:LEU:HG	1:E:370:ILE:HD11	1.89	0.53
1:E:811:VAL:HG22	1:E:822:LEU:HD21	1.90	0.53
1:B:557:ILE:HB	1:B:561:SER:OG	2.07	0.53
1:C:268:PHE:HZ	1:C:441:ASN:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1058:ASP:O	1:C:1062:GLN:HG3	2.09	0.53
1:C:1271:ALA:HB1	1:D:1611:ARG:HD3	1.90	0.53
1:D:198:THR:O	1:D:445:ARG:NH1	2.41	0.53
1:D:540:SER:HB2	1:E:848:GLN:HE22	1.74	0.53
1:D:1220:LYS:HE2	1:D:1267:LEU:HB3	1.91	0.53
1:E:2341:TYR:OH	1:E:2390:SER:O	2.21	0.53
1:C:926:LEU:HD22	1:C:930:GLN:HB3	1.91	0.53
1:D:1790:ASP:OD1	1:D:1791:GLU:N	2.42	0.53
1:D:2103:TYR:CE1	1:D:2189:ARG:HG2	2.43	0.53
1:A:197:ALA:N	1:A:948:THR:HG21	2.24	0.53
1:B:540:SER:HB2	1:C:848:GLN:HE22	1.73	0.53
1:B:719:GLN:HB3	1:B:724:ALA:HB1	1.90	0.53
1:B:2141:VAL:HG21	1:C:1175:LYS:HE2	1.91	0.53
1:B:2426:TYR:HB3	1:C:2334:THR:HG21	1.89	0.53
1:C:540:SER:HB2	1:D:848:GLN:HE22	1.74	0.53
1:B:1271:ALA:HB1	1:C:1611:ARG:HD3	1.90	0.53
1:D:197:ALA:N	1:D:948:THR:HG21	2.23	0.53
1:D:300:ALA:HA	1:D:303:PHE:HD2	1.73	0.53
1:E:2122:ALA:HA	1:E:2171:VAL:HG23	1.91	0.53
1:B:195:SER:HB3	1:B:198:THR:OG1	2.08	0.53
1:B:1790:ASP:OD1	1:B:1791:GLU:N	2.42	0.53
1:B:2204:LYS:HG2	1:C:2087:LYS:HD2	1.90	0.53
1:E:671:LEU:HD22	1:E:734:LEU:HD21	1.90	0.53
1:A:1220:LYS:HE2	1:A:1267:LEU:HB3	1.90	0.53
1:C:510:ASN:OD1	1:D:153:GLN:NE2	2.39	0.53
1:C:671:LEU:HD22	1:C:734:LEU:HD21	1.90	0.53
1:E:1058:ASP:O	1:E:1062:GLN:HG3	2.08	0.53
1:A:540:SER:HB2	1:B:848:GLN:HE22	1.74	0.53
1:A:1611:ARG:HD3	1:E:1271:ALA:HB1	1.91	0.53
1:E:462:ARG:NH1	1:E:506:ARG:HH11	2.07	0.53
1:A:2426:TYR:HB3	1:B:2334:THR:HG21	1.91	0.52
1:B:197:ALA:N	1:B:948:THR:HG21	2.23	0.52
1:C:1071:ALA:HB2	1:C:1791:GLU:OE2	2.09	0.52
1:D:195:SER:HB3	1:D:198:THR:OG1	2.08	0.52
1:D:1868:TYR:HB3	1:D:1976:ILE:HD12	1.91	0.52
1:A:2219:ALA:HA	1:B:2073:LYS:HZ1	1.73	0.52
1:B:268:PHE:HZ	1:B:441:ASN:HB2	1.75	0.52
1:B:300:ALA:HA	1:B:303:PHE:HD2	1.73	0.52
1:B:671:LEU:HD22	1:B:734:LEU:HD21	1.90	0.52
1:C:141:ARG:HH22	1:C:1005:GLU:CD	2.13	0.52
1:C:1790:ASP:OD1	1:C:1791:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:601:THR:HG22	1:E:604:GLU:OE1	2.10	0.52
1:E:1220:LYS:HE2	1:E:1267:LEU:HB3	1.91	0.52
1:E:1722:GLY:O	1:E:1739:SER:HB2	2.10	0.52
1:A:1790:ASP:OD1	1:A:1791:GLU:N	2.42	0.52
1:B:2053:ASN:ND2	1:B:2241:LEU:HD11	2.24	0.52
1:B:2122:ALA:HA	1:B:2171:VAL:HG23	1.91	0.52
1:B:2341:TYR:OH	1:B:2390:SER:O	2.22	0.52
1:D:671:LEU:HD22	1:D:734:LEU:HD21	1.90	0.52
1:D:812:ASN:HA	1:E:1998:ALA:HB2	1.91	0.52
1:E:2053:ASN:ND2	1:E:2241:LEU:HD11	2.24	0.52
1:C:1794:ARG:NH2	1:C:1798:TYR:OH	2.42	0.52
1:D:268:PHE:HZ	1:D:441:ASN:HB2	1.74	0.52
1:D:1878:GLU:HA	1:D:1881:MET:HG3	1.91	0.52
1:E:1878:GLU:HA	1:E:1881:MET:HG3	1.90	0.52
1:A:2334:THR:HG21	1:E:2426:TYR:HB3	1.90	0.52
1:B:1117:ASP:OD1	1:B:1118:ALA:N	2.39	0.52
1:B:1630:GLN:HG2	1:B:1772:PHE:CE2	2.44	0.52
1:C:197:ALA:N	1:C:948:THR:HG21	2.24	0.52
1:E:1117:ASP:OD1	1:E:1118:ALA:N	2.39	0.52
1:C:811:VAL:HG22	1:C:822:LEU:HD21	1.91	0.52
1:E:926:LEU:HD22	1:E:930:GLN:HB3	1.92	0.52
1:A:719:GLN:HB3	1:A:724:ALA:HB1	1.90	0.52
1:A:812:ASN:HA	1:B:1998:ALA:HB2	1.91	0.52
1:B:237:LEU:HD11	1:B:483:TYR:HB2	1.91	0.52
1:B:1230:ARG:NH2	1:B:1251:ASN:OD1	2.43	0.52
1:D:462:ARG:NH1	1:D:506:ARG:HH11	2.07	0.52
1:A:2141:VAL:HG21	1:B:1175:LYS:HE2	1.92	0.52
1:B:462:ARG:NH1	1:B:506:ARG:HH11	2.08	0.52
1:C:462:ARG:NH1	1:C:506:ARG:HH11	2.06	0.52
1:C:601:THR:HG22	1:C:604:GLU:OE1	2.10	0.52
1:E:719:GLN:HB3	1:E:724:ALA:HB1	1.89	0.52
1:E:2103:TYR:CE1	1:E:2193:GLU:HG2	2.45	0.52
1:A:253:GLU:O	1:A:442:LYS:NZ	2.28	0.52
1:A:268:PHE:HZ	1:A:441:ASN:HB2	1.75	0.52
1:A:601:THR:HG22	1:A:604:GLU:OE1	2.10	0.52
1:C:1630:GLN:HG2	1:C:1772:PHE:CE2	2.45	0.52
1:C:1878:GLU:HA	1:C:1881:MET:HG3	1.91	0.52
1:E:497:ILE:HG21	1:E:589:TYR:HD2	1.74	0.52
1:A:237:LEU:HD11	1:A:483:TYR:HB2	1.92	0.52
1:A:926:LEU:HD22	1:A:930:GLN:HB3	1.92	0.52
1:A:1878:GLU:HA	1:A:1881:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:THR:HG22	1:B:604:GLU:OE1	2.10	0.52
1:B:678:LEU:HD11	1:B:692:MET:HA	1.92	0.52
1:B:811:VAL:HG22	1:B:822:LEU:HD21	1.91	0.52
1:B:2266:TYR:CZ	1:B:2297:TRP:HB2	2.45	0.52
1:B:1722:GLY:O	1:B:1739:SER:HB2	2.11	0.51
1:C:1146:LYS:NZ	1:C:1147:ILE:O	2.40	0.51
1:C:1722:GLY:O	1:C:1739:SER:HB2	2.10	0.51
1:D:1071:ALA:HB2	1:D:1791:GLU:OE2	2.10	0.51
1:A:671:LEU:HD22	1:A:734:LEU:HD21	1.92	0.51
1:A:1614:VAL:O	1:A:1618:THR:HG23	2.11	0.51
1:B:537:ASP:HA	1:B:577:LYS:HA	1.91	0.51
1:B:564:ARG:NH2	1:C:842:ASP:OD1	2.43	0.51
1:B:2337:LEU:HB3	1:B:2507:ILE:HB	1.93	0.51
1:C:2338:ALA:HA	1:C:2353:LEU:HD13	1.92	0.51
1:E:1794:ARG:NH2	1:E:1798:TYR:OH	2.43	0.51
1:A:537:ASP:HA	1:A:577:LYS:HA	1.92	0.51
1:A:1722:GLY:O	1:A:1739:SER:HB2	2.10	0.51
1:B:1614:VAL:O	1:B:1618:THR:HG23	2.11	0.51
1:A:678:LEU:HD11	1:A:692:MET:HA	1.92	0.51
1:C:2004:GLN:H	1:C:2300:THR:HG22	1.76	0.51
1:D:2341:TYR:OH	1:D:2390:SER:O	2.22	0.51
1:E:1071:ALA:HB2	1:E:1791:GLU:OE2	2.11	0.51
1:A:2204:LYS:HG2	1:B:2087:LYS:HD2	1.92	0.51
1:D:601:THR:HG22	1:D:604:GLU:OE1	2.10	0.51
1:E:1230:ARG:NH2	1:E:1251:ASN:OD1	2.43	0.51
1:A:141:ARG:HH22	1:A:1005:GLU:CD	2.13	0.51
1:A:2053:ASN:ND2	1:A:2241:LEU:HD11	2.25	0.51
1:A:2266:TYR:CZ	1:A:2297:TRP:HB2	2.46	0.51
1:B:536:ILE:HD13	1:B:547:ARG:HB2	1.93	0.51
1:C:1868:TYR:HB3	1:C:1976:ILE:HD12	1.93	0.51
1:D:237:LEU:HD11	1:D:483:TYR:HB2	1.93	0.51
1:A:842:ASP:OD1	1:E:564:ARG:NH2	2.44	0.51
1:A:153:GLN:NE2	1:E:510:ASN:OD1	2.39	0.51
1:A:724:ALA:O	1:A:729:LYS:NZ	2.32	0.51
1:A:1024:TYR:O	1:A:1030:THR:OG1	2.23	0.51
1:B:141:ARG:HH22	1:B:1005:GLU:CD	2.13	0.51
1:B:1878:GLU:HA	1:B:1881:MET:HG3	1.92	0.51
1:B:2132:ARG:HH11	1:B:2163:TYR:HB3	1.76	0.51
1:D:926:LEU:HD22	1:D:930:GLN:HB3	1.93	0.51
1:D:2122:ALA:HA	1:D:2171:VAL:HG23	1.93	0.51
1:E:141:ARG:HH22	1:E:1005:GLU:CD	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:PHE:HZ	1:E:441:ASN:HB2	1.74	0.51
1:E:2266:TYR:CZ	1:E:2297:TRP:HB2	2.45	0.51
1:B:2103:TYR:CE1	1:B:2193:GLU:HG2	2.45	0.51
1:D:2337:LEU:HB3	1:D:2507:ILE:HB	1.92	0.51
1:E:370:ILE:HG13	1:E:410:LEU:HG	1.93	0.51
1:E:1790:ASP:OD1	1:E:1791:GLU:N	2.43	0.51
1:A:2122:ALA:HA	1:A:2171:VAL:HG23	1.93	0.51
1:C:719:GLN:HB3	1:C:724:ALA:HB1	1.92	0.51
1:D:2103:TYR:CE1	1:D:2193:GLU:HG2	2.46	0.51
1:A:453:SER:HB3	1:A:456:ILE:HG12	1.93	0.50
1:A:462:ARG:NH1	1:A:506:ARG:HH11	2.06	0.50
1:A:2087:LYS:HD2	1:E:2204:LYS:HG2	1.92	0.50
1:D:1722:GLY:O	1:D:1739:SER:HB2	2.10	0.50
1:D:2053:ASN:ND2	1:D:2241:LEU:HD11	2.26	0.50
1:D:2266:TYR:CZ	1:D:2297:TRP:HB2	2.47	0.50
1:A:2341:TYR:OH	1:A:2390:SER:O	2.21	0.50
1:B:497:ILE:HG21	1:B:589:TYR:HD2	1.76	0.50
1:C:370:ILE:HG13	1:C:410:LEU:HG	1.94	0.50
1:D:537:ASP:HA	1:D:577:LYS:HA	1.94	0.50
1:E:1291:TYR:HA	1:E:1294:PHE:CE2	2.47	0.50
1:C:536:ILE:HD13	1:C:547:ARG:HB2	1.94	0.50
1:D:702:LEU:HD22	1:D:708:ALA:HB2	1.93	0.50
1:C:678:LEU:HD11	1:C:692:MET:HA	1.94	0.50
1:D:1230:ARG:NH2	1:D:1251:ASN:OD1	2.45	0.50
1:A:2073:LYS:NZ	1:E:2218:GLU:OE1	2.34	0.50
1:B:460:ILE:HG21	1:B:478:VAL:HG12	1.94	0.50
1:D:370:ILE:HG13	1:D:410:LEU:HG	1.94	0.50
1:D:1291:TYR:HA	1:D:1294:PHE:CE2	2.47	0.50
1:E:470:ILE:HA	1:E:474:VAL:HG11	1.93	0.50
1:E:1614:VAL:O	1:E:1618:THR:HG23	2.11	0.50
1:B:1291:TYR:HA	1:B:1294:PHE:CE2	2.47	0.50
1:B:2033:LEU:HD11	1:B:2266:TYR:HA	1.94	0.50
1:C:812:ASN:HA	1:D:1998:ALA:HB2	1.93	0.50
1:C:1230:ARG:NH2	1:C:1251:ASN:OD1	2.45	0.50
1:A:510:ASN:OD1	1:B:153:GLN:NE2	2.40	0.50
1:A:1291:TYR:HA	1:A:1294:PHE:CE2	2.47	0.50
1:A:1998:ALA:HB2	1:E:812:ASN:HA	1.92	0.50
1:A:2337:LEU:HB3	1:A:2507:ILE:HB	1.93	0.50
1:C:470:ILE:HA	1:C:474:VAL:HG11	1.94	0.50
1:C:702:LEU:HD22	1:C:708:ALA:HB2	1.93	0.50
1:B:926:LEU:HD22	1:B:930:GLN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:MET:CE	1:C:410:LEU:HD22	2.42	0.50
1:C:2122:ALA:HA	1:C:2171:VAL:HG23	1.94	0.50
1:C:2204:LYS:HG2	1:D:2087:LYS:HD2	1.93	0.50
1:E:471:ASN:H	1:E:474:VAL:HG12	1.76	0.50
1:A:371:LYS:HG2	1:A:377:GLU:HA	1.94	0.50
1:A:2004:GLN:H	1:A:2300:THR:HG22	1.76	0.50
1:B:370:ILE:HG13	1:B:410:LEU:HG	1.93	0.50
1:C:497:ILE:HG21	1:C:589:TYR:HD2	1.76	0.50
1:D:2393:PHE:HE1	1:D:2482:LEU:HB2	1.77	0.50
1:E:198:THR:HB	1:E:199:PRO:HA	1.94	0.50
1:E:453:SER:HB3	1:E:456:ILE:HG12	1.94	0.50
1:A:341:MET:CE	1:A:410:LEU:HD22	2.42	0.49
1:B:1220:LYS:HE2	1:B:1267:LEU:HB3	1.93	0.49
1:D:141:ARG:HH22	1:D:1005:GLU:CD	2.13	0.49
1:D:371:LYS:HG2	1:D:377:GLU:HA	1.93	0.49
1:E:210:VAL:HG22	1:E:926:LEU:HD11	1.94	0.49
1:E:702:LEU:HD22	1:E:708:ALA:HB2	1.93	0.49
1:A:470:ILE:HA	1:A:474:VAL:HG11	1.93	0.49
1:B:470:ILE:HA	1:B:474:VAL:HG11	1.94	0.49
1:C:522:PRO:O	1:C:553:ARG:NH1	2.45	0.49
1:C:564:ARG:NH2	1:D:842:ASP:OD1	2.45	0.49
1:C:2266:TYR:CZ	1:C:2297:TRP:HB2	2.48	0.49
1:E:2393:PHE:HE1	1:E:2482:LEU:HB2	1.77	0.49
1:A:1230:ARG:NH2	1:A:1251:ASN:OD1	2.45	0.49
1:A:1962:THR:OG1	1:A:1966:ARG:NH2	2.45	0.49
1:C:471:ASN:H	1:C:474:VAL:HG12	1.77	0.49
1:D:471:ASN:H	1:D:474:VAL:HG12	1.77	0.49
1:A:702:LEU:HD22	1:A:708:ALA:HB2	1.93	0.49
1:A:1098:HIS:HE1	1:A:1100:ASN:HB3	1.78	0.49
1:B:1071:ALA:HB2	1:B:1791:GLU:OE2	2.11	0.49
1:C:537:ASP:HA	1:C:577:LYS:HA	1.93	0.49
1:D:470:ILE:HA	1:D:474:VAL:HG11	1.93	0.49
1:A:341:MET:HE1	1:A:410:LEU:HD22	1.93	0.49
1:A:1175:LYS:HE2	1:E:2141:VAL:HG21	1.94	0.49
1:B:1098:HIS:HE1	1:B:1100:ASN:HB3	1.78	0.49
1:C:1614:VAL:O	1:C:1618:THR:HG23	2.11	0.49
1:D:198:THR:HB	1:D:199:PRO:HA	1.94	0.49
1:D:460:ILE:HG21	1:D:478:VAL:HG12	1.95	0.49
1:E:407:GLU:HA	1:E:425:LYS:HA	1.94	0.49
1:A:1117:ASP:OD1	1:A:1118:ALA:N	2.38	0.49
1:A:2099:TYR:CE2	1:A:2195:GLN:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LYS:HG2	1:B:377:GLU:HA	1.93	0.49
1:D:1614:VAL:O	1:D:1618:THR:HG23	2.11	0.49
1:A:370:ILE:HG13	1:A:410:LEU:HG	1.94	0.49
1:A:714:TRP:CZ3	1:A:762:LEU:HD22	2.48	0.49
1:B:341:MET:CE	1:B:410:LEU:HD22	2.42	0.49
1:C:371:LYS:HG2	1:C:377:GLU:HA	1.93	0.49
1:C:1291:TYR:HA	1:C:1294:PHE:CE2	2.47	0.49
1:D:1108:THR:OG1	1:D:1128:HIS:NE2	2.37	0.49
1:E:341:MET:CE	1:E:410:LEU:HD22	2.42	0.49
1:E:371:LYS:HG2	1:E:377:GLU:HA	1.93	0.49
1:A:2132:ARG:HH11	1:A:2163:TYR:HB3	1.77	0.49
1:B:453:SER:HB3	1:B:456:ILE:HG12	1.94	0.49
1:D:536:ILE:HD13	1:D:547:ARG:HB2	1.94	0.49
1:D:1962:THR:OG1	1:D:1966:ARG:NH2	2.46	0.49
1:E:237:LEU:HD11	1:E:483:TYR:HB2	1.95	0.49
1:E:678:LEU:HD11	1:E:692:MET:HA	1.93	0.49
1:A:497:ILE:HG21	1:A:589:TYR:HD2	1.77	0.49
1:A:564:ARG:NH2	1:B:842:ASP:OD1	2.46	0.49
1:B:198:THR:HB	1:B:199:PRO:HA	1.94	0.49
1:C:453:SER:HB3	1:C:456:ILE:HG12	1.94	0.49
1:D:453:SER:HB3	1:D:456:ILE:HG12	1.93	0.49
1:D:564:ARG:NH2	1:E:842:ASP:OD1	2.46	0.49
1:A:2338:ALA:HA	1:A:2353:LEU:HD13	1.94	0.49
1:B:471:ASN:H	1:B:474:VAL:HG12	1.77	0.49
1:C:210:VAL:HG22	1:C:926:LEU:HD11	1.95	0.49
1:E:2099:TYR:CE2	1:E:2195:GLN:HB3	2.48	0.49
1:A:536:ILE:HD13	1:A:547:ARG:HB2	1.94	0.48
1:B:702:LEU:HD22	1:B:708:ALA:HB2	1.94	0.48
1:B:1962:THR:OG1	1:B:1966:ARG:NH2	2.46	0.48
1:D:2235:GLN:HG3	1:E:1995:LEU:HB2	1.96	0.48
1:E:1868:TYR:HB3	1:E:1976:ILE:HD12	1.95	0.48
1:A:471:ASN:H	1:A:474:VAL:HG12	1.78	0.48
1:B:2338:ALA:HA	1:B:2353:LEU:HD13	1.95	0.48
1:C:714:TRP:CZ3	1:C:762:LEU:HD22	2.48	0.48
1:D:341:MET:CE	1:D:410:LEU:HD22	2.42	0.48
1:D:2099:TYR:CE2	1:D:2195:GLN:HB3	2.49	0.48
1:C:1098:HIS:HE1	1:C:1100:ASN:HB3	1.78	0.48
1:C:2393:PHE:HE1	1:C:2482:LEU:HB2	1.78	0.48
1:D:1098:HIS:HE1	1:D:1100:ASN:HB3	1.79	0.48
1:E:537:ASP:HA	1:E:577:LYS:HA	1.95	0.48
1:A:198:THR:HB	1:A:199:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2393:PHE:HE1	1:B:2482:LEU:HB2	1.78	0.48
1:C:2132:ARG:HH11	1:C:2163:TYR:HB3	1.79	0.48
1:D:719:GLN:HB3	1:D:724:ALA:HB1	1.95	0.48
1:E:1098:HIS:HE1	1:E:1100:ASN:HB3	1.78	0.48
1:A:407:GLU:HA	1:A:425:LYS:HA	1.94	0.48
1:B:2099:TYR:CE2	1:B:2195:GLN:HB3	2.48	0.48
1:C:198:THR:HB	1:C:199:PRO:HA	1.94	0.48
1:C:460:ILE:HG21	1:C:478:VAL:HG12	1.96	0.48
1:D:678:LEU:HD11	1:D:692:MET:HA	1.95	0.48
1:D:2004:GLN:H	1:D:2300:THR:HG22	1.78	0.48
1:E:460:ILE:HG21	1:E:478:VAL:HG12	1.96	0.48
1:A:2393:PHE:HE1	1:A:2482:LEU:HB2	1.77	0.48
1:D:210:VAL:HG22	1:D:926:LEU:HD11	1.96	0.48
1:E:497:ILE:HG21	1:E:589:TYR:CD2	2.49	0.48
1:A:160:SER:HA	1:A:982:LYS:HA	1.96	0.48
1:A:1124:ARG:HD2	1:A:1144:TRP:CE2	2.49	0.48
1:D:510:ASN:OD1	1:E:153:GLN:NE2	2.40	0.48
1:D:1124:ARG:HD2	1:D:1144:TRP:CE2	2.49	0.48
1:E:1124:ARG:HD2	1:E:1144:TRP:CE2	2.49	0.48
1:A:464:VAL:HG21	1:A:474:VAL:HA	1.96	0.48
1:B:197:ALA:H	1:B:948:THR:HG21	1.79	0.47
1:D:2338:ALA:HA	1:D:2353:LEU:HD13	1.95	0.47
1:A:460:ILE:HG21	1:A:478:VAL:HG12	1.96	0.47
1:D:464:VAL:HG21	1:D:474:VAL:HA	1.97	0.47
1:A:522:PRO:O	1:A:553:ARG:NH1	2.46	0.47
1:C:341:MET:HE1	1:C:410:LEU:HD22	1.96	0.47
1:C:2033:LEU:HD11	1:C:2266:TYR:HA	1.96	0.47
1:D:348:PHE:CE1	1:D:352:ASN:HB3	2.50	0.47
1:D:407:GLU:HA	1:D:425:LYS:HA	1.96	0.47
1:D:497:ILE:HG21	1:D:589:TYR:HD2	1.79	0.47
1:E:2338:ALA:HA	1:E:2353:LEU:HD13	1.95	0.47
1:C:1117:ASP:OD1	1:C:1118:ALA:N	2.39	0.47
1:D:127:ARG:HG3	1:D:127:ARG:HH11	1.79	0.47
1:E:714:TRP:CZ3	1:E:762:LEU:HD22	2.49	0.47
1:A:1868:TYR:HB3	1:A:1976:ILE:HD12	1.96	0.47
1:B:2004:GLN:H	1:B:2300:THR:HG22	1.79	0.47
1:B:1124:ARG:HD2	1:B:1144:TRP:CE2	2.50	0.47
1:B:2469:PHE:H	1:C:2327:ARG:NH2	2.13	0.47
1:C:2078:LEU:HD13	1:C:2217:ARG:HA	1.97	0.47
1:E:127:ARG:HG3	1:E:127:ARG:HH11	1.79	0.47
1:E:2132:ARG:HH11	1:E:2163:TYR:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.80	0.47
1:A:2469:PHE:H	1:B:2327:ARG:NH2	2.13	0.47
1:D:2033:LEU:HD11	1:D:2266:TYR:HA	1.96	0.47
1:E:536:ILE:HD13	1:E:547:ARG:HB2	1.96	0.47
1:A:2033:LEU:HD11	1:A:2266:TYR:HA	1.96	0.47
1:B:538:LEU:HB2	1:B:566:LEU:HD22	1.97	0.47
1:C:160:SER:HA	1:C:982:LYS:HA	1.97	0.47
1:C:1962:THR:OG1	1:C:1966:ARG:NH2	2.47	0.47
1:E:2004:GLN:H	1:E:2300:THR:HG22	1.79	0.47
1:A:348:PHE:CE1	1:A:352:ASN:HB3	2.50	0.47
1:B:407:GLU:HA	1:B:425:LYS:HA	1.97	0.47
1:B:714:TRP:CZ3	1:B:762:LEU:HD22	2.50	0.47
1:B:812:ASN:HA	1:C:1998:ALA:HB2	1.96	0.47
1:C:2469:PHE:H	1:D:2327:ARG:NH2	2.13	0.47
1:A:1001:LEU:HD23	1:A:1013:ILE:HD12	1.97	0.46
1:C:497:ILE:HG21	1:C:589:TYR:CD2	2.50	0.46
1:C:1617:ALA:HA	1:C:1624:ILE:HD11	1.97	0.46
1:D:341:MET:HE1	1:D:410:LEU:HD22	1.97	0.46
1:D:1617:ALA:HA	1:D:1624:ILE:HD11	1.97	0.46
1:B:1244:THR:HG21	1:B:1268:TYR:CD1	2.50	0.46
1:D:1001:LEU:HD23	1:D:1013:ILE:HD12	1.96	0.46
1:A:1617:ALA:HA	1:A:1624:ILE:HD11	1.97	0.46
1:B:341:MET:HE3	1:B:410:LEU:HD22	1.96	0.46
1:A:730:PHE:HE1	1:A:752:ILE:HG23	1.81	0.46
1:D:593:LEU:O	1:D:597:ILE:HG12	2.16	0.46
1:E:348:PHE:CE1	1:E:352:ASN:HB3	2.50	0.46
1:B:127:ARG:HG3	1:B:127:ARG:HH11	1.80	0.46
1:B:2321:HIS:NE2	1:B:2325:ASP:OD2	2.49	0.46
1:D:522:PRO:O	1:D:553:ARG:NH1	2.45	0.46
1:E:2033:LEU:HD11	1:E:2266:TYR:HA	1.96	0.46
1:B:474:VAL:O	1:B:478:VAL:HG13	2.16	0.46
1:C:348:PHE:CE1	1:C:352:ASN:HB3	2.50	0.46
1:D:1244:THR:HG21	1:D:1268:TYR:CD1	2.50	0.46
1:D:2132:ARG:HH11	1:D:2163:TYR:HB3	1.80	0.46
1:E:1617:ALA:HA	1:E:1624:ILE:HD11	1.98	0.46
1:B:593:LEU:O	1:B:597:ILE:HG12	2.16	0.46
1:C:237:LEU:HD11	1:C:483:TYR:HB2	1.98	0.46
1:C:407:GLU:HA	1:C:425:LYS:HA	1.96	0.46
1:E:174:LYS:HG2	1:E:185:VAL:HG21	1.96	0.46
1:E:370:ILE:HD13	1:E:379:VAL:HG13	1.98	0.46
1:E:1024:TYR:O	1:E:1030:THR:OG1	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:VAL:HG22	1:B:926:LEU:HD11	1.98	0.46
1:B:497:ILE:HG21	1:B:589:TYR:CD2	2.50	0.46
1:C:127:ARG:HG3	1:C:127:ARG:HH11	1.79	0.46
1:A:1118:ALA:O	1:D:2133:LEU:HD22	2.16	0.46
1:A:1244:THR:HG21	1:A:1268:TYR:CD1	2.51	0.46
1:B:2009:LEU:HG	1:B:2294:PRO:HB3	1.98	0.46
1:C:1113:LEU:HD11	1:C:1119:GLY:HA3	1.98	0.46
1:D:969:GLN:HB3	1:D:999:ARG:NH1	2.31	0.46
1:B:348:PHE:CE1	1:B:352:ASN:HB3	2.50	0.46
1:B:1617:ALA:HA	1:B:1624:ILE:HD11	1.97	0.46
1:C:1124:ARG:NE	1:C:1142:SER:O	2.48	0.46
1:C:2321:HIS:NE2	1:C:2325:ASP:OD2	2.49	0.46
1:E:522:PRO:O	1:E:553:ARG:NH1	2.48	0.46
1:A:497:ILE:HG21	1:A:589:TYR:CD2	2.51	0.45
1:B:357:TYR:CE2	1:B:391:TYR:HB2	2.51	0.45
1:C:1168:TYR:HD2	1:C:1200:LEU:HD11	1.81	0.45
1:C:2099:TYR:CE2	1:C:2195:GLN:HB3	2.50	0.45
1:D:357:TYR:CE2	1:D:391:TYR:HB2	2.51	0.45
1:A:2337:LEU:HD23	1:A:2507:ILE:HG13	1.99	0.45
1:C:1001:LEU:HD23	1:C:1013:ILE:HD12	1.98	0.45
1:C:2441:LEU:HG	1:C:2445:CYS:HB2	1.98	0.45
1:D:534:GLU:OE2	1:D:580:ASN:ND2	2.49	0.45
1:D:2469:PHE:H	1:E:2327:ARG:NH2	2.15	0.45
1:A:255:ILE:HD12	1:A:438:LEU:HD13	1.99	0.45
1:B:1024:TYR:CD1	1:B:1034:VAL:HG21	2.52	0.45
1:C:174:LYS:HG2	1:C:185:VAL:HG21	1.98	0.45
1:C:370:ILE:HD13	1:C:379:VAL:HG13	1.99	0.45
1:C:1892:ASP:OD1	1:C:1892:ASP:N	2.50	0.45
1:D:1711:PHE:CE2	1:D:1713:LYS:HB3	2.52	0.45
1:E:197:ALA:H	1:E:948:THR:HG21	1.79	0.45
1:A:593:LEU:O	1:A:597:ILE:HG12	2.16	0.45
1:B:370:ILE:HD13	1:B:379:VAL:HG13	1.99	0.45
1:B:1711:PHE:CE2	1:B:1713:LYS:HB3	2.52	0.45
1:C:464:VAL:HG21	1:C:474:VAL:HA	1.98	0.45
1:D:1024:TYR:CG	1:D:1034:VAL:HG21	2.52	0.45
1:E:969:GLN:HB3	1:E:999:ARG:NH1	2.31	0.45
1:E:1146:LYS:NZ	1:E:1147:ILE:O	2.42	0.45
1:E:2441:LEU:HG	1:E:2445:CYS:HB2	1.98	0.45
1:A:370:ILE:HD13	1:A:379:VAL:HG13	1.99	0.45
1:B:1001:LEU:HD23	1:B:1013:ILE:HD12	1.99	0.45
1:B:1146:LYS:NZ	1:B:1147:ILE:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1147:ILE:HD13	1:C:1169:LEU:HD11	1.99	0.45
1:D:174:LYS:HG2	1:D:185:VAL:HG21	1.98	0.45
1:D:370:ILE:HD13	1:D:379:VAL:HG13	1.99	0.45
1:E:1244:THR:HG21	1:E:1268:TYR:CD1	2.51	0.45
1:E:2337:LEU:HD23	1:E:2507:ILE:HG13	1.99	0.45
1:A:500:ASN:HB2	1:A:627:LEU:HD13	1.98	0.45
1:A:1024:TYR:CG	1:A:1034:VAL:HG21	2.52	0.45
1:A:1711:PHE:CE2	1:A:1713:LYS:HB3	2.51	0.45
1:A:2393:PHE:CE1	1:A:2482:LEU:HB2	2.52	0.45
1:B:1113:LEU:HD11	1:B:1119:GLY:HA3	1.99	0.45
1:B:1124:ARG:NE	1:B:1142:SER:O	2.49	0.45
1:B:1178:THR:HG22	1:B:1192:THR:HG23	1.99	0.45
1:C:2141:VAL:HG21	1:D:1175:LYS:HE2	1.99	0.45
1:D:1892:ASP:OD1	1:D:1892:ASP:N	2.50	0.45
1:B:181:ASN:HD21	1:B:184:LYS:HG2	1.82	0.45
1:B:2235:GLN:HG3	1:C:1995:LEU:HB2	1.98	0.45
1:C:969:GLN:HB3	1:C:999:ARG:NH1	2.31	0.45
1:C:1244:THR:HG21	1:C:1268:TYR:CD1	2.51	0.45
1:C:2393:PHE:HB3	1:C:2477:ILE:O	2.17	0.45
1:E:1711:PHE:CE2	1:E:1713:LYS:HB3	2.52	0.45
1:A:2441:LEU:HG	1:A:2445:CYS:HB2	1.98	0.45
1:B:730:PHE:HE1	1:B:752:ILE:HG23	1.82	0.45
1:B:969:GLN:HB3	1:B:999:ARG:NH1	2.32	0.45
1:B:2441:LEU:HG	1:B:2445:CYS:HB2	1.98	0.45
1:C:2393:PHE:CE1	1:C:2482:LEU:HB2	2.52	0.45
1:D:2393:PHE:HB3	1:D:2477:ILE:O	2.17	0.45
1:E:464:VAL:HG21	1:E:474:VAL:HA	1.99	0.45
1:A:357:TYR:CE2	1:A:391:TYR:HB2	2.52	0.45
1:D:197:ALA:H	1:D:948:THR:HG21	1.81	0.45
1:E:200:TYR:CE1	1:E:941:SER:HB3	2.52	0.45
1:E:1024:TYR:CD1	1:E:1034:VAL:HG21	2.51	0.45
1:A:2147:PHE:CD1	1:E:2147:PHE:HB3	2.52	0.45
1:B:1236:CYS:H	1:B:1303:ASN:ND2	2.15	0.45
1:B:1892:ASP:N	1:B:1892:ASP:OD1	2.50	0.45
1:C:357:TYR:CE2	1:C:391:TYR:HB2	2.52	0.45
1:C:724:ALA:O	1:C:729:LYS:NZ	2.32	0.45
1:C:1024:TYR:CG	1:C:1034:VAL:HG21	2.52	0.45
1:D:507:SER:HB3	1:D:513:SER:HB2	1.99	0.45
1:D:2441:LEU:HG	1:D:2445:CYS:HB2	1.99	0.45
1:E:474:VAL:O	1:E:478:VAL:HG13	2.17	0.45
1:E:2393:PHE:CE1	1:E:2482:LEU:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASN:HD21	1:A:184:LYS:HG2	1.82	0.44
1:B:522:PRO:O	1:B:553:ARG:NH1	2.50	0.44
1:B:659:TYR:CE2	1:B:758:ALA:HB2	2.52	0.44
1:C:593:LEU:O	1:C:597:ILE:HG12	2.17	0.44
1:C:1124:ARG:HD2	1:C:1144:TRP:CE2	2.52	0.44
1:C:1711:PHE:CE2	1:C:1713:LYS:HB3	2.52	0.44
1:C:2133:LEU:HD22	1:E:1118:ALA:O	2.16	0.44
1:E:141:ARG:NH2	1:E:1005:GLU:OE2	2.44	0.44
1:E:507:SER:HB3	1:E:513:SER:HB2	2.00	0.44
1:E:593:LEU:O	1:E:597:ILE:HG12	2.16	0.44
1:A:210:VAL:HG22	1:A:926:LEU:HD11	1.99	0.44
1:B:340:GLN:OE1	1:B:412:ARG:NH2	2.50	0.44
1:B:1766:LEU:O	1:B:1770:GLU:HB2	2.17	0.44
1:B:2133:LEU:HD22	1:D:1118:ALA:O	2.17	0.44
1:C:2219:ALA:HA	1:D:2073:LYS:NZ	2.33	0.44
1:D:2393:PHE:CE1	1:D:2482:LEU:HB2	2.52	0.44
1:E:1056:MET:HG3	1:E:1081:TYR:CE1	2.52	0.44
1:E:1135:LYS:HA	1:E:1135:LYS:HD3	1.81	0.44
1:B:534:GLU:OE2	1:B:580:ASN:ND2	2.50	0.44
1:B:1147:ILE:HD13	1:B:1169:LEU:HD11	1.99	0.44
1:B:2129:GLN:NE2	1:D:1120:GLU:OE2	2.51	0.44
1:C:251:LEU:HD13	1:C:446:LEU:HD13	1.99	0.44
1:C:2360:LEU:HB3	1:C:2377:PHE:HE1	1.82	0.44
1:D:538:LEU:HB2	1:D:566:LEU:HD22	1.99	0.44
1:E:2018:ARG:NH2	1:E:2473:GLU:OE2	2.51	0.44
1:A:1056:MET:HG3	1:A:1081:TYR:CE1	2.53	0.44
1:B:160:SER:HA	1:B:982:LYS:HA	1.98	0.44
1:B:1056:MET:HG3	1:B:1081:TYR:CE1	2.53	0.44
1:B:2393:PHE:CE1	1:B:2482:LEU:HB2	2.53	0.44
1:E:160:SER:HA	1:E:982:LYS:HA	1.98	0.44
1:E:195:SER:OG	1:E:948:THR:HG22	2.18	0.44
1:A:2207:ASP:O	1:A:2211:LYS:HG2	2.18	0.44
1:A:2393:PHE:HB3	1:A:2477:ILE:O	2.18	0.44
1:B:1024:TYR:O	1:B:1030:THR:OG1	2.27	0.44
1:B:2078:LEU:HD13	1:B:2217:ARG:HA	2.00	0.44
1:B:2219:ALA:HA	1:C:2073:LYS:NZ	2.33	0.44
1:E:181:ASN:HD21	1:E:184:LYS:HG2	1.83	0.44
1:E:1001:LEU:HD23	1:E:1013:ILE:HD12	1.99	0.44
1:A:197:ALA:H	1:A:948:THR:HG21	1.82	0.44
1:A:2219:ALA:HA	1:B:2073:LYS:NZ	2.32	0.44
1:E:1962:THR:OG1	1:E:1966:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ARG:HE	1:B:973:ILE:HD11	1.82	0.44
1:B:784:GLU:HG3	1:B:790:THR:HA	1.98	0.44
1:B:2147:PHE:HB3	1:C:2147:PHE:CD1	2.52	0.44
1:C:197:ALA:H	1:C:948:THR:HG21	1.82	0.44
1:C:255:ILE:HD12	1:C:438:LEU:HD13	1.99	0.44
1:C:2207:ASP:O	1:C:2211:LYS:HG2	2.18	0.44
1:D:2030:VAL:O	1:D:2034:THR:HG23	2.18	0.44
1:D:2147:PHE:HB3	1:E:2147:PHE:CD1	2.52	0.44
1:D:2219:ALA:HA	1:E:2073:LYS:NZ	2.33	0.44
1:E:357:TYR:CE2	1:E:391:TYR:HB2	2.52	0.44
1:E:2078:LEU:HD13	1:E:2217:ARG:HA	2.00	0.44
1:A:474:VAL:O	1:A:478:VAL:HG13	2.18	0.44
1:B:174:LYS:HG2	1:B:185:VAL:HG21	2.00	0.44
1:C:507:SER:HB3	1:C:513:SER:HB2	2.00	0.44
1:D:784:GLU:HG3	1:D:790:THR:HA	1.99	0.44
1:D:2078:LEU:HD13	1:D:2217:ARG:HA	2.00	0.44
1:D:2321:HIS:NE2	1:D:2325:ASP:OD2	2.51	0.44
1:A:507:SER:HB3	1:A:513:SER:HB2	2.00	0.44
1:A:2235:GLN:HG3	1:B:1995:LEU:HB2	2.00	0.44
1:B:124:ARG:HG2	1:B:1911:ALA:HB1	2.00	0.44
1:C:273:PRO:HG3	1:C:434:TYR:CE1	2.52	0.44
1:C:1178:THR:HG22	1:C:1192:THR:HG23	2.00	0.44
1:C:2129:GLN:NE2	1:E:1120:GLU:OE2	2.51	0.44
1:E:1124:ARG:NE	1:E:1142:SER:O	2.51	0.44
1:E:1892:ASP:OD1	1:E:1892:ASP:N	2.50	0.44
1:E:2207:ASP:O	1:E:2211:LYS:HG2	2.18	0.44
1:A:784:GLU:HG3	1:A:790:THR:HA	2.00	0.43
1:A:969:GLN:HB3	1:A:999:ARG:NH1	2.32	0.43
1:A:1113:LEU:HD11	1:A:1119:GLY:HA3	2.00	0.43
1:A:2133:LEU:HD22	1:C:1118:ALA:O	2.17	0.43
1:B:273:PRO:HG3	1:B:434:TYR:CE1	2.53	0.43
1:B:2360:LEU:HB3	1:B:2377:PHE:HE1	1.83	0.43
1:C:255:ILE:HG12	1:C:442:LYS:HE3	2.00	0.43
1:C:474:VAL:O	1:C:478:VAL:HG13	2.18	0.43
1:D:659:TYR:CE2	1:D:758:ALA:HB2	2.53	0.43
1:D:1002:GLU:OE1	1:E:1888:HIS:NE2	2.50	0.43
1:E:487:ARG:HE	1:E:635:ASN:HD21	1.66	0.43
1:A:174:LYS:HG2	1:A:185:VAL:HG21	1.99	0.43
1:B:464:VAL:HG21	1:B:474:VAL:HA	2.01	0.43
1:E:730:PHE:HE1	1:E:752:ILE:HG23	1.83	0.43
1:E:2009:LEU:HG	1:E:2294:PRO:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ILE:HD12	1:A:494:THR:HG22	2.00	0.43
1:A:2030:VAL:O	1:A:2034:THR:HG23	2.18	0.43
1:A:2327:ARG:NH2	1:E:2469:PHE:H	2.16	0.43
1:C:1135:LYS:HA	1:C:1135:LYS:HD3	1.82	0.43
1:C:1766:LEU:O	1:C:1770:GLU:HB2	2.17	0.43
1:D:255:ILE:HG12	1:D:442:LYS:HE3	2.00	0.43
1:D:1773:TYR:HD2	1:D:1774:TYR:CD1	2.36	0.43
1:D:2337:LEU:HD23	1:D:2507:ILE:HG13	1.99	0.43
1:E:2321:HIS:NE2	1:E:2325:ASP:OD2	2.51	0.43
1:E:2393:PHE:HB3	1:E:2477:ILE:O	2.19	0.43
1:A:1178:THR:HG22	1:A:1192:THR:HG23	2.01	0.43
1:A:1236:CYS:H	1:A:1303:ASN:ND2	2.17	0.43
1:A:2321:HIS:NE2	1:A:2325:ASP:OD2	2.52	0.43
1:A:2452:HIS:CE1	1:A:2456:ASP:HB2	2.54	0.43
1:B:195:SER:OG	1:B:948:THR:HG22	2.18	0.43
1:C:534:GLU:OE2	1:C:580:ASN:ND2	2.51	0.43
1:C:2337:LEU:HD23	1:C:2507:ILE:HG13	2.00	0.43
1:D:113:PHE:HE1	1:D:1035:SER:HG	1.64	0.43
1:D:474:VAL:O	1:D:478:VAL:HG13	2.18	0.43
1:E:255:ILE:HG12	1:E:442:LYS:HE3	2.00	0.43
1:A:280:GLU:OE2	1:B:1895:TYR:HB2	2.19	0.43
1:A:534:GLU:OE2	1:A:580:ASN:ND2	2.51	0.43
1:B:1048:THR:HG23	1:B:1061:LEU:HD11	2.00	0.43
1:B:2030:VAL:O	1:B:2034:THR:HG23	2.18	0.43
1:C:2147:PHE:HB3	1:D:2147:PHE:CD1	2.52	0.43
1:D:1053:GLN:HE21	1:D:1057:MET:HG3	1.83	0.43
1:D:1159:ARG:HD3	1:D:1303:ASN:ND2	2.33	0.43
1:E:659:TYR:CE2	1:E:758:ALA:HB2	2.53	0.43
1:A:1766:LEU:O	1:A:1770:GLU:HB2	2.18	0.43
1:B:280:GLU:OE2	1:C:1895:TYR:HB2	2.18	0.43
1:B:487:ARG:HE	1:B:635:ASN:HD21	1.66	0.43
1:B:2452:HIS:CE1	1:B:2456:ASP:HB2	2.54	0.43
1:D:181:ASN:HD21	1:D:184:LYS:HG2	1.83	0.43
1:D:497:ILE:HG21	1:D:589:TYR:CD2	2.54	0.43
1:D:2360:LEU:HB3	1:D:2377:PHE:HE1	1.83	0.43
1:D:2448:LEU:HB2	1:D:2458:GLY:HA3	2.00	0.43
1:E:255:ILE:HD12	1:E:438:LEU:HD13	1.99	0.43
1:E:569:THR:HG21	1:E:587:ASN:HB3	2.01	0.43
1:E:1168:TYR:HD2	1:E:1200:LEU:HD11	1.83	0.43
1:A:1773:TYR:HD2	1:A:1774:TYR:CD1	2.37	0.43
1:A:1895:TYR:HB2	1:E:280:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2207:ASP:O	1:B:2211:LYS:HG2	2.18	0.43
1:C:124:ARG:HD3	1:C:1914:THR:OG1	2.18	0.43
1:C:280:GLU:OE2	1:D:1895:TYR:HB2	2.19	0.43
1:C:730:PHE:HE1	1:C:752:ILE:HG23	1.82	0.43
1:C:1236:CYS:H	1:C:1303:ASN:ND2	2.16	0.43
1:D:1236:CYS:H	1:D:1303:ASN:ND2	2.16	0.43
1:D:1887:LEU:HD12	1:D:1887:LEU:HA	1.90	0.43
1:E:694:PRO:HA	1:E:705:GLU:OE1	2.19	0.43
1:A:659:TYR:CE2	1:A:758:ALA:HB2	2.53	0.43
1:A:1159:ARG:HD3	1:A:1303:ASN:ND2	2.33	0.43
1:A:1793:ASN:O	1:A:1797:LYS:HB2	2.19	0.43
1:A:2078:LEU:HD13	1:A:2217:ARG:HA	2.01	0.43
1:B:1118:ALA:O	1:E:2133:LEU:HD22	2.18	0.43
1:C:142:ARG:HE	1:C:973:ILE:HD11	1.84	0.43
1:C:659:TYR:CE2	1:C:758:ALA:HB2	2.53	0.43
1:C:1166:ARG:HB2	1:D:1614:VAL:HG11	2.01	0.43
1:C:2009:LEU:HG	1:C:2294:PRO:HB3	2.01	0.43
1:C:2452:HIS:CE1	1:C:2456:ASP:HB2	2.54	0.43
1:D:340:GLN:OE1	1:D:412:ARG:NH2	2.51	0.43
1:D:1168:TYR:HD2	1:D:1200:LEU:HD11	1.83	0.43
1:E:490:ILE:HD12	1:E:494:THR:HG22	2.01	0.43
1:E:558:ASP:OD1	1:E:558:ASP:N	2.47	0.43
1:E:1766:LEU:O	1:E:1770:GLU:HB2	2.19	0.43
1:E:2030:VAL:O	1:E:2034:THR:HG23	2.18	0.43
1:A:273:PRO:HG3	1:A:434:TYR:CE1	2.54	0.43
1:A:340:GLN:OE1	1:A:412:ARG:NH2	2.52	0.43
1:A:1024:TYR:CD1	1:A:1034:VAL:HG21	2.54	0.43
1:A:2009:LEU:HG	1:A:2294:PRO:HB3	2.00	0.43
1:B:116:ALA:O	1:B:120:THR:HG23	2.19	0.43
1:B:2393:PHE:HB3	1:B:2477:ILE:O	2.18	0.43
1:C:2030:VAL:O	1:C:2034:THR:HG23	2.18	0.43
1:D:1124:ARG:NE	1:D:1142:SER:O	2.51	0.43
1:D:1124:ARG:NH2	1:D:1763:ALA:O	2.50	0.43
1:E:534:GLU:OE2	1:E:580:ASN:ND2	2.52	0.43
1:E:1178:THR:HG22	1:E:1192:THR:HG23	2.00	0.43
1:E:2416:SER:HB2	1:E:2510:HIS:HB2	2.00	0.43
1:A:1614:VAL:HG11	1:E:1166:ARG:HB2	2.01	0.43
1:B:251:LEU:HD13	1:B:446:LEU:HD13	2.01	0.43
1:D:280:GLU:OE2	1:E:1895:TYR:HB2	2.19	0.43
1:D:397:LEU:HD13	1:D:406:PHE:CZ	2.54	0.43
1:D:2207:ASP:O	1:D:2211:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:OG	1:A:948:THR:HG22	2.19	0.42
1:A:343:VAL:HG23	1:A:357:TYR:HB3	2.01	0.42
1:A:1135:LYS:HA	1:A:1135:LYS:HD3	1.81	0.42
1:B:1162:ILE:HD13	1:B:1167:LEU:HA	2.01	0.42
1:B:2337:LEU:HD23	1:B:2507:ILE:HG13	2.01	0.42
1:D:1147:ILE:HD13	1:D:1169:LEU:HD11	2.01	0.42
1:E:1773:TYR:HD2	1:E:1774:TYR:CD1	2.37	0.42
1:A:538:LEU:HB2	1:A:566:LEU:HD22	2.01	0.42
1:A:848:GLN:OE1	1:A:892:GLN:NE2	2.53	0.42
1:A:2355:GLN:HG2	1:A:2356:GLU:OE1	2.19	0.42
1:C:569:THR:HG21	1:C:587:ASN:HB3	2.01	0.42
1:D:141:ARG:NH2	1:D:1005:GLU:OE2	2.44	0.42
1:E:124:ARG:HG2	1:E:1911:ALA:HB1	2.00	0.42
1:E:538:LEU:HB2	1:E:566:LEU:HD22	2.01	0.42
1:E:2355:GLN:HG2	1:E:2356:GLU:OE1	2.19	0.42
1:A:1892:ASP:OD1	1:A:1892:ASP:N	2.50	0.42
1:A:2073:LYS:NZ	1:E:2219:ALA:HA	2.33	0.42
1:C:181:ASN:HD21	1:C:184:LYS:HG2	1.84	0.42
1:D:2130:ALA:HB2	1:E:1204:ARG:HH22	1.82	0.42
1:E:540:SER:OG	1:E:560:VAL:HA	2.20	0.42
1:E:2360:LEU:HB3	1:E:2377:PHE:HE1	1.84	0.42
1:A:1872:GLU:OE2	1:A:1875:THR:OG1	2.34	0.42
1:B:507:SER:HB3	1:B:513:SER:HB2	2.00	0.42
1:C:2018:ARG:N	1:C:2467:GLY:O	2.52	0.42
1:C:2369:GLY:HA3	1:C:2374:ASN:HA	2.01	0.42
1:D:160:SER:HA	1:D:982:LYS:HA	2.00	0.42
1:D:730:PHE:HE1	1:D:752:ILE:HG23	1.83	0.42
1:D:2009:LEU:HG	1:D:2294:PRO:HB3	2.01	0.42
1:E:273:PRO:HG3	1:E:434:TYR:CE1	2.53	0.42
1:E:340:GLN:OE1	1:E:412:ARG:NH2	2.51	0.42
1:E:1800:TRP:CZ2	1:E:1802:PRO:HG3	2.54	0.42
1:E:2372:ASN:HB2	1:E:2392:SER:HB2	2.02	0.42
1:A:1168:TYR:HD2	1:A:1200:LEU:HD11	1.85	0.42
1:A:1995:LEU:HB2	1:E:2235:GLN:HG3	2.01	0.42
1:A:2360:LEU:HB3	1:A:2377:PHE:HE1	1.85	0.42
1:C:116:ALA:O	1:C:120:THR:HG23	2.19	0.42
1:C:340:GLN:OE1	1:C:412:ARG:NH2	2.52	0.42
1:D:1146:LYS:NZ	1:D:1147:ILE:O	2.42	0.42
1:D:1800:TRP:CZ2	1:D:1802:PRO:HG3	2.54	0.42
1:E:579:LYS:HG3	1:E:581:ASN:H	1.85	0.42
1:A:124:ARG:HD3	1:A:1914:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LYS:HG3	1:A:581:ASN:H	1.84	0.42
1:A:1166:ARG:HB2	1:B:1614:VAL:HG11	2.02	0.42
1:A:2295:GLY:HA3	1:D:676:HIS:CD2	2.54	0.42
1:B:2355:GLN:HG2	1:B:2356:GLU:OE1	2.19	0.42
1:C:538:LEU:HB2	1:C:566:LEU:HD22	2.00	0.42
1:D:1056:MET:HG3	1:D:1081:TYR:CE1	2.54	0.42
1:D:2452:HIS:CE1	1:D:2456:ASP:HB2	2.54	0.42
1:E:1609:PHE:CZ	1:E:1613:LEU:HD13	2.55	0.42
1:A:569:THR:HG21	1:A:587:ASN:HB3	2.00	0.42
1:A:2448:LEU:HB2	1:A:2458:GLY:HA3	2.02	0.42
1:B:255:ILE:HG12	1:B:442:LYS:HE3	2.01	0.42
1:B:1168:TYR:HD2	1:B:1200:LEU:HD11	1.84	0.42
1:C:154:ASN:HB3	1:C:986:ILE:HG13	2.02	0.42
1:C:579:LYS:HG3	1:C:581:ASN:H	1.84	0.42
1:D:1166:ARG:HB2	1:E:1614:VAL:HG11	2.02	0.42
1:D:2355:GLN:HG2	1:D:2356:GLU:OE1	2.20	0.42
1:E:2033:LEU:CD1	1:E:2266:TYR:HA	2.50	0.42
1:E:2328:ALA:HB2	1:E:2516:LYS:HB3	2.02	0.42
1:A:2033:LEU:CD1	1:A:2266:TYR:HA	2.50	0.42
1:C:711:VAL:HG11	1:C:763:GLU:OE2	2.20	0.42
1:D:368:LEU:HG	1:D:370:ILE:CD1	2.50	0.42
1:E:397:LEU:HD13	1:E:406:PHE:CZ	2.55	0.42
1:E:1053:GLN:HE21	1:E:1057:MET:HG3	1.85	0.42
1:E:2228:LYS:HE3	1:E:2228:LYS:HB2	1.87	0.42
1:A:1239:TYR:CD1	1:A:1242:GLU:HB3	2.54	0.42
1:A:2004:GLN:N	1:A:2300:THR:HG22	2.34	0.42
1:A:2077:GLU:OE2	1:E:2216:ARG:NH2	2.52	0.42
1:A:2277:GLU:OE2	1:A:2291:PHE:HB2	2.20	0.42
1:B:1773:TYR:HD2	1:B:1774:TYR:CD1	2.37	0.42
1:B:1800:TRP:CZ2	1:B:1802:PRO:HG3	2.55	0.42
1:C:141:ARG:NH2	1:C:1005:GLU:OE2	2.43	0.42
1:C:368:LEU:HG	1:C:370:ILE:CD1	2.50	0.42
1:C:1793:ASN:O	1:C:1797:LYS:HB2	2.20	0.42
1:D:490:ILE:HD12	1:D:494:THR:HG22	2.01	0.42
1:D:579:LYS:HG3	1:D:581:ASN:H	1.85	0.42
1:D:1793:ASN:O	1:D:1797:LYS:HB2	2.20	0.42
1:A:1607:THR:HG22	1:A:1609:PHE:H	1.84	0.42
1:A:1800:TRP:CZ2	1:A:1802:PRO:HG3	2.55	0.42
1:B:2018:ARG:N	1:B:2467:GLY:O	2.50	0.42
1:C:195:SER:OG	1:C:948:THR:HG22	2.20	0.42
1:C:2355:GLN:HG2	1:C:2356:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ARG:HG2	1:D:1911:ALA:HB1	2.02	0.42
1:D:1178:THR:HG22	1:D:1192:THR:HG23	2.01	0.42
1:E:711:VAL:HG11	1:E:763:GLU:OE2	2.20	0.42
1:A:116:ALA:O	1:A:120:THR:HG23	2.20	0.41
1:A:142:ARG:HE	1:A:973:ILE:HD11	1.84	0.41
1:A:1123:TRP:NE1	1:A:1145:HIS:HB2	2.35	0.41
1:A:1162:ILE:HD13	1:A:1167:LEU:HA	2.01	0.41
1:A:2275:MET:SD	1:B:2322:LEU:HD22	2.60	0.41
1:B:493:GLU:O	1:B:497:ILE:HG12	2.20	0.41
1:B:711:VAL:HG11	1:B:763:GLU:OE2	2.20	0.41
1:B:1024:TYR:CG	1:B:1034:VAL:HG21	2.55	0.41
1:C:1676:ILE:HD12	1:C:1690:LEU:HD13	2.02	0.41
1:C:1773:TYR:HD2	1:C:1774:TYR:CD1	2.38	0.41
1:C:2275:MET:SD	1:D:2322:LEU:HD22	2.60	0.41
1:E:2452:HIS:CE1	1:E:2456:ASP:HB2	2.54	0.41
1:A:251:LEU:HD13	1:A:446:LEU:HD13	2.02	0.41
1:B:255:ILE:HD12	1:B:438:LEU:HD13	2.02	0.41
1:B:397:LEU:HD13	1:B:406:PHE:CZ	2.56	0.41
1:C:1024:TYR:O	1:C:1030:THR:OG1	2.26	0.41
1:C:1098:HIS:CE1	1:C:1100:ASN:HB3	2.55	0.41
1:C:1159:ARG:HD3	1:C:1303:ASN:ND2	2.35	0.41
1:D:195:SER:OG	1:D:948:THR:HG22	2.20	0.41
1:D:663:LEU:HD22	1:D:749:GLN:NE2	2.35	0.41
1:D:1676:ILE:HD12	1:D:1690:LEU:HD13	2.02	0.41
1:E:1123:TRP:NE1	1:E:1145:HIS:HB2	2.35	0.41
1:A:255:ILE:HG12	1:A:442:LYS:HE3	2.01	0.41
1:A:1053:GLN:HE21	1:A:1057:MET:HG3	1.86	0.41
1:A:2322:LEU:HD22	1:E:2275:MET:SD	2.60	0.41
1:B:200:TYR:CE1	1:B:941:SER:HB3	2.54	0.41
1:B:493:GLU:OE2	1:B:517:ARG:NH1	2.34	0.41
1:B:2033:LEU:CD1	1:B:2266:TYR:HA	2.50	0.41
1:B:2433:LEU:HB3	1:B:2484:LEU:HD13	2.02	0.41
1:C:283:LYS:HB2	1:C:293:LEU:HD22	2.02	0.41
1:C:784:GLU:HG3	1:C:790:THR:HA	2.02	0.41
1:C:1024:TYR:CD1	1:C:1034:VAL:HG21	2.55	0.41
1:C:1162:ILE:HD13	1:C:1167:LEU:HA	2.02	0.41
1:C:2235:GLN:HG3	1:D:1995:LEU:HB2	2.01	0.41
1:B:141:ARG:NH2	1:B:1005:GLU:OE2	2.45	0.41
1:B:368:LEU:HG	1:B:370:ILE:CD1	2.50	0.41
1:B:490:ILE:HD12	1:B:494:THR:HG22	2.01	0.41
1:B:533:ASP:HA	1:B:579:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:VAL:HG23	1:D:357:TYR:HB3	2.02	0.41
1:D:1766:LEU:O	1:D:1770:GLU:HB2	2.19	0.41
1:E:1024:TYR:CG	1:E:1034:VAL:HG21	2.55	0.41
1:E:1887:LEU:HD12	1:E:1887:LEU:HA	1.90	0.41
1:A:124:ARG:HG2	1:A:1911:ALA:HB1	2.03	0.41
1:B:579:LYS:HG3	1:B:581:ASN:H	1.84	0.41
1:B:1053:GLN:HE21	1:B:1057:MET:HG3	1.84	0.41
1:B:1120:GLU:OE2	1:E:2129:GLN:NE2	2.54	0.41
1:B:1782:ARG:HE	1:B:1782:ARG:HB3	1.76	0.41
1:C:694:PRO:HA	1:C:705:GLU:OE1	2.20	0.41
1:C:971:LEU:O	1:C:973:ILE:HG12	2.21	0.41
1:C:1053:GLN:HE21	1:C:1057:MET:HG3	1.85	0.41
1:D:694:PRO:HA	1:D:705:GLU:OE1	2.20	0.41
1:D:1024:TYR:CD1	1:D:1034:VAL:HG21	2.56	0.41
1:D:1239:TYR:HD2	1:D:1246:LEU:HD11	1.85	0.41
1:E:124:ARG:HD3	1:E:1914:THR:OG1	2.20	0.41
1:E:1113:LEU:HD11	1:E:1119:GLY:HA3	2.02	0.41
1:E:1159:ARG:HD3	1:E:1303:ASN:ND2	2.34	0.41
1:A:1617:ALA:CA	1:A:1624:ILE:HD11	2.51	0.41
1:A:2018:ARG:N	1:A:2467:GLY:O	2.52	0.41
1:A:2097:ASP:OD1	1:A:2098:SER:N	2.54	0.41
1:A:2145:PHE:CE2	1:C:1180:GLN:HG3	2.56	0.41
1:B:1609:PHE:CZ	1:B:1613:LEU:HD13	2.56	0.41
1:C:490:ILE:HD12	1:C:494:THR:HG22	2.02	0.41
1:D:116:ALA:O	1:D:120:THR:HG23	2.20	0.41
1:E:1147:ILE:HD13	1:E:1169:LEU:HD11	2.02	0.41
1:A:200:TYR:CE1	1:A:941:SER:HB3	2.55	0.41
1:A:711:VAL:HG11	1:A:763:GLU:OE2	2.20	0.41
1:A:717:LYS:HB3	1:A:793:ALA:HB2	2.03	0.41
1:A:1124:ARG:NE	1:A:1142:SER:O	2.54	0.41
1:A:2147:PHE:HB3	1:B:2147:PHE:CD1	2.54	0.41
1:B:149:ALA:O	1:B:154:ASN:ND2	2.50	0.41
1:B:694:PRO:HA	1:B:705:GLU:OE1	2.20	0.41
1:B:938:LEU:HD23	1:B:938:LEU:HA	1.93	0.41
1:B:971:LEU:O	1:B:973:ILE:HG12	2.20	0.41
1:C:677:GLY:HA3	1:C:695:TYR:CZ	2.56	0.41
1:C:2448:LEU:HB2	1:C:2458:GLY:HA3	2.02	0.41
1:D:124:ARG:HD3	1:D:1914:THR:OG1	2.20	0.41
1:D:200:TYR:CE1	1:D:941:SER:HB3	2.56	0.41
1:D:461:VAL:HA	1:D:474:VAL:HG21	2.03	0.41
1:D:478:VAL:O	1:D:481:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ARG:HE	1:E:973:ILE:HD11	1.85	0.41
1:E:478:VAL:O	1:E:481:THR:HG22	2.21	0.41
1:E:493:GLU:O	1:E:497:ILE:HG12	2.21	0.41
1:E:784:GLU:HG3	1:E:790:THR:HA	2.02	0.41
1:E:1098:HIS:CE1	1:E:1100:ASN:HB3	2.55	0.41
1:A:125:GLU:HG3	1:A:1017:PHE:CG	2.56	0.41
1:A:397:LEU:HD13	1:A:406:PHE:CZ	2.56	0.41
1:B:253:GLU:O	1:B:442:LYS:NZ	2.29	0.41
1:B:458:GLU:HA	1:B:461:VAL:HG12	2.03	0.41
1:B:1607:THR:HG22	1:B:1609:PHE:H	1.86	0.41
1:B:1676:ILE:HD12	1:B:1690:LEU:HD13	2.01	0.41
1:C:200:TYR:CE1	1:C:941:SER:HB3	2.54	0.41
1:C:1056:MET:HG3	1:C:1081:TYR:CE1	2.56	0.41
1:C:2216:ARG:NH2	1:D:2077:GLU:OE2	2.54	0.41
1:D:125:GLU:HG3	1:D:1017:PHE:CG	2.56	0.41
1:D:193:ARG:NH2	1:D:253:GLU:OE1	2.54	0.41
1:D:273:PRO:HG3	1:D:434:TYR:CE1	2.55	0.41
1:D:569:THR:HG21	1:D:587:ASN:HB3	2.02	0.41
1:D:711:VAL:HG11	1:D:763:GLU:OE2	2.20	0.41
1:D:1162:ILE:HD13	1:D:1167:LEU:HA	2.02	0.41
1:D:2033:LEU:CD1	1:D:2266:TYR:HA	2.51	0.41
1:E:1793:ASN:O	1:E:1797:LYS:HB2	2.20	0.41
1:E:2433:LEU:HB3	1:E:2484:LEU:HD13	2.03	0.41
1:A:595:ALA:HB1	1:A:600:LEU:O	2.21	0.41
1:A:971:LEU:O	1:A:973:ILE:HG12	2.21	0.41
1:A:1098:HIS:CE1	1:A:1100:ASN:HB3	2.55	0.41
1:A:1782:ARG:HE	1:A:1782:ARG:HB3	1.76	0.41
1:A:2168:SER:HA	1:A:2171:VAL:HG12	2.03	0.41
1:A:2226:SER:HB2	1:B:2066:THR:HG21	2.03	0.41
1:B:365:ALA:HB3	1:B:384:ALA:HA	2.03	0.41
1:B:663:LEU:HD22	1:B:749:GLN:NE2	2.35	0.41
1:B:1098:HIS:CE1	1:B:1100:ASN:HB3	2.55	0.41
1:B:1239:TYR:CD1	1:B:1242:GLU:HB3	2.55	0.41
1:C:257:GLU:OE1	1:C:431:TYR:OH	2.33	0.41
1:C:397:LEU:HD13	1:C:406:PHE:CZ	2.55	0.41
1:C:733:TRP:NE1	1:C:748:THR:HB	2.36	0.41
1:C:845:LEU:HD21	1:C:881:VAL:HG13	2.03	0.41
1:C:1607:THR:HG22	1:C:1609:PHE:H	1.86	0.41
1:C:2033:LEU:CD1	1:C:2266:TYR:HA	2.50	0.41
1:D:971:LEU:O	1:D:973:ILE:HG12	2.20	0.41
1:D:1036:GLN:O	1:D:1040:TYR:N	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1805:TYR:HD2	1:D:1814:TYR:CE1	2.39	0.41
1:D:2018:ARG:N	1:D:2467:GLY:O	2.52	0.41
1:D:2372:ASN:HB2	1:D:2392:SER:HB2	2.03	0.41
1:D:2433:LEU:HB3	1:D:2484:LEU:HD13	2.03	0.41
1:E:109:VAL:HG23	1:E:155:MET:HE3	2.03	0.41
1:E:368:LEU:HG	1:E:370:ILE:CD1	2.50	0.41
1:E:500:ASN:HB2	1:E:627:LEU:HD13	2.03	0.41
1:E:595:ALA:HB1	1:E:600:LEU:O	2.21	0.41
1:E:1239:TYR:CD1	1:E:1242:GLU:HB3	2.56	0.41
1:E:2369:GLY:HA3	1:E:2374:ASN:HA	2.03	0.41
1:A:1239:TYR:HD2	1:A:1246:LEU:HD11	1.86	0.41
1:A:1607:THR:HG21	1:A:1768:PHE:CZ	2.54	0.41
1:A:1676:ILE:HD12	1:A:1690:LEU:HD13	2.03	0.41
1:B:540:SER:OG	1:B:560:VAL:HA	2.21	0.41
1:B:2275:MET:SD	1:C:2322:LEU:HD22	2.61	0.41
1:C:113:PHE:HE1	1:C:1035:SER:HG	1.67	0.41
1:C:1002:GLU:OE1	1:D:1888:HIS:NE2	2.52	0.41
1:D:142:ARG:HE	1:D:973:ILE:HD11	1.86	0.41
1:D:251:LEU:HD13	1:D:446:LEU:HD13	2.02	0.41
1:D:493:GLU:O	1:D:497:ILE:HG12	2.20	0.41
1:D:558:ASP:N	1:D:558:ASP:OD1	2.47	0.41
1:D:661:LYS:HB2	1:D:750:GLU:HB2	2.03	0.41
1:D:1113:LEU:HD11	1:D:1119:GLY:HA3	2.02	0.41
1:D:1239:TYR:CD1	1:D:1242:GLU:HB3	2.55	0.41
1:E:341:MET:HE1	1:E:410:LEU:HD22	2.02	0.41
1:E:552:LYS:NZ	1:E:558:ASP:HA	2.36	0.41
1:E:663:LEU:HD22	1:E:749:GLN:NE2	2.36	0.41
1:E:848:GLN:OE1	1:E:892:GLN:NE2	2.54	0.41
1:A:1124:ARG:NH2	1:A:1763:ALA:O	2.49	0.40
1:B:1239:TYR:HD2	1:B:1246:LEU:HD11	1.86	0.40
1:B:1793:ASN:O	1:B:1797:LYS:HB2	2.20	0.40
1:B:2369:GLY:HA3	1:B:2374:ASN:HA	2.03	0.40
1:C:478:VAL:O	1:C:481:THR:HG22	2.20	0.40
1:C:533:ASP:HA	1:C:579:LYS:NZ	2.36	0.40
1:C:1609:PHE:CZ	1:C:1613:LEU:HD13	2.56	0.40
1:C:1711:PHE:HE2	1:C:1713:LYS:HB3	1.86	0.40
1:C:1800:TRP:CZ2	1:C:1802:PRO:HG3	2.56	0.40
1:D:2097:ASP:OD1	1:D:2098:SER:N	2.54	0.40
1:E:2018:ARG:N	1:E:2467:GLY:O	2.52	0.40
1:E:2097:ASP:OD1	1:E:2098:SER:N	2.54	0.40
1:E:2448:LEU:HB2	1:E:2458:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:LEU:HD22	1:A:749:GLN:NE2	2.36	0.40
1:A:2369:GLY:HA3	1:A:2374:ASN:HA	2.03	0.40
1:B:461:VAL:HA	1:B:474:VAL:HG21	2.03	0.40
1:B:733:TRP:NE1	1:B:748:THR:HB	2.36	0.40
1:B:2168:SER:HA	1:B:2171:VAL:HG12	2.04	0.40
1:C:663:LEU:HD22	1:C:749:GLN:NE2	2.36	0.40
1:C:1048:THR:HG23	1:C:1061:LEU:HD11	2.04	0.40
1:D:1042:GLU:HA	1:D:1045:ILE:HD12	2.03	0.40
1:D:1711:PHE:HE2	1:D:1713:LYS:HB3	1.87	0.40
1:D:2124:LEU:O	1:D:2128:VAL:HG12	2.22	0.40
1:E:971:LEU:O	1:E:973:ILE:HG12	2.21	0.40
1:A:487:ARG:HE	1:A:635:ASN:HD21	1.70	0.40
1:A:1975:SER:OG	1:A:1977:ASP:OD1	2.33	0.40
1:B:371:LYS:HA	1:B:377:GLU:HA	2.04	0.40
1:B:661:LYS:HB2	1:B:750:GLU:HB2	2.04	0.40
1:B:1607:THR:HG21	1:B:1768:PHE:CZ	2.52	0.40
1:B:2097:ASP:OD1	1:B:2098:SER:N	2.54	0.40
1:C:2328:ALA:HB2	1:C:2516:LYS:HB3	2.03	0.40
1:D:540:SER:OG	1:D:560:VAL:HA	2.21	0.40
1:D:1607:THR:HG22	1:D:1609:PHE:H	1.86	0.40
1:D:1609:PHE:CZ	1:D:1613:LEU:HD13	2.57	0.40
1:D:2216:ARG:NH2	1:E:2077:GLU:OE2	2.53	0.40
1:D:2277:GLU:OE2	1:D:2291:PHE:HB2	2.21	0.40
1:D:2328:ALA:HB2	1:D:2516:LYS:HB3	2.03	0.40
1:E:116:ALA:O	1:E:120:THR:HG23	2.20	0.40
1:E:538:LEU:HD12	1:E:566:LEU:HD22	2.04	0.40
1:A:540:SER:OG	1:A:560:VAL:HA	2.22	0.40
1:A:733:TRP:NE1	1:A:748:THR:HB	2.36	0.40
1:A:2328:ALA:HB2	1:A:2516:LYS:HB3	2.04	0.40
1:B:1166:ARG:HB2	1:C:1614:VAL:HG11	2.04	0.40
1:B:1711:PHE:HE2	1:B:1713:LYS:HB3	1.87	0.40
1:B:2124:LEU:O	1:B:2128:VAL:HG12	2.22	0.40
1:B:2328:ALA:HB2	1:B:2516:LYS:HB3	2.04	0.40
1:B:2388:GLN:HA	1:B:2485:SER:HA	2.04	0.40
1:C:124:ARG:HG2	1:C:1911:ALA:HB1	2.03	0.40
1:C:456:ILE:O	1:C:460:ILE:HG13	2.21	0.40
1:C:676:HIS:CD2	1:E:2295:GLY:HA3	2.56	0.40
1:C:1094:ILE:HD11	1:C:1113:LEU:HB2	2.04	0.40
1:C:1120:GLU:HB3	1:C:1146:LYS:HE2	2.02	0.40
1:D:149:ALA:O	1:D:154:ASN:ND2	2.49	0.40
1:E:1676:ILE:HD12	1:E:1690:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2412:ILE:HD11	1:E:2477:ILE:HG12	2.02	0.40
1:A:458:GLU:HA	1:A:461:VAL:HG12	2.04	0.40
1:A:478:VAL:O	1:A:481:THR:HG22	2.21	0.40
1:B:456:ILE:O	1:B:460:ILE:HG13	2.22	0.40
1:B:569:THR:HG21	1:B:587:ASN:HB3	2.02	0.40
1:B:1050:ARG:O	1:B:1053:GLN:HB2	2.22	0.40
1:B:2295:GLY:HA3	1:E:676:HIS:CD2	2.56	0.40
1:C:500:ASN:HB2	1:C:627:LEU:HD13	2.04	0.40
1:E:283:LYS:HB2	1:E:293:LEU:HD22	2.04	0.40
1:E:1782:ARG:HE	1:E:1782:ARG:HB3	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	B	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	C	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	D	2114/2535 (83%)	2065 (98%)	49 (2%)	0	100	100
1	E	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
All	All	10570/12675 (83%)	10329 (98%)	241 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1816/2173 (84%)	1811 (100%)	5 (0%)	91	97
1	B	1816/2173 (84%)	1811 (100%)	5 (0%)	91	97
1	C	1816/2173 (84%)	1811 (100%)	5 (0%)	91	97
1	D	1816/2173 (84%)	1811 (100%)	5 (0%)	91	97
1	E	1816/2173 (84%)	1811 (100%)	5 (0%)	91	97
All	All	9080/10865 (84%)	9055 (100%)	25 (0%)	90	97

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1049	MET
1	A	1868	TYR
1	A	1965	GLN
1	A	2399	ARG
1	A	2430	GLN
1	B	1049	MET
1	B	1868	TYR
1	B	1965	GLN
1	B	2399	ARG
1	B	2430	GLN
1	C	1049	MET
1	C	1868	TYR
1	C	1965	GLN
1	C	2399	ARG
1	C	2430	GLN
1	D	1049	MET
1	D	1868	TYR
1	D	1965	GLN
1	D	2399	ARG
1	D	2430	GLN
1	E	1049	MET
1	E	1868	TYR
1	E	1965	GLN
1	E	2399	ARG
1	E	2430	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	969	GLN
1	A	2057	GLN
1	B	852	GLN
1	B	892	GLN
1	B	969	GLN
1	B	2057	GLN
1	C	852	GLN
1	C	892	GLN
1	C	969	GLN
1	C	2057	GLN
1	D	852	GLN
1	D	892	GLN
1	D	969	GLN
1	E	852	GLN
1	E	892	GLN
1	E	969	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16791. These allow visual inspection of the internal detail of the map and identification of artifacts.

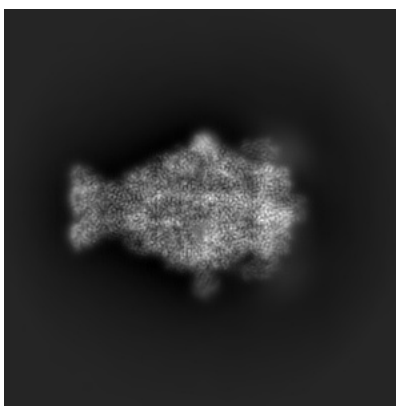
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

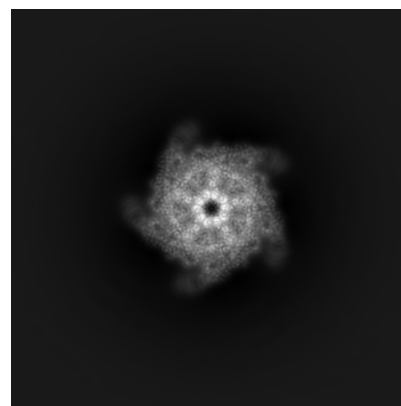
6.1.1 Primary map



X

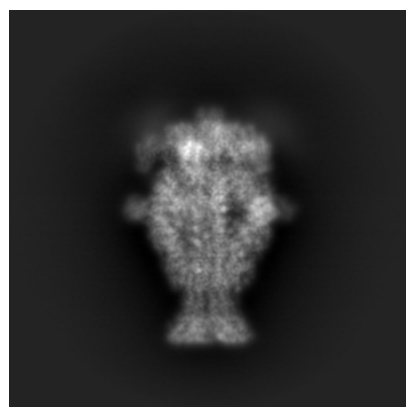


Y

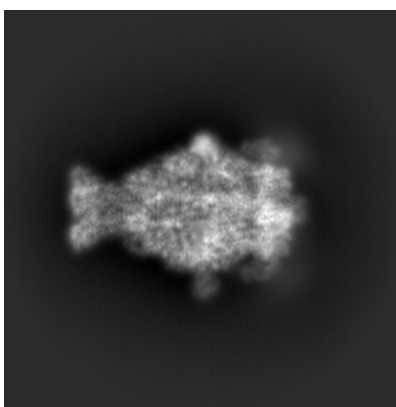


Z

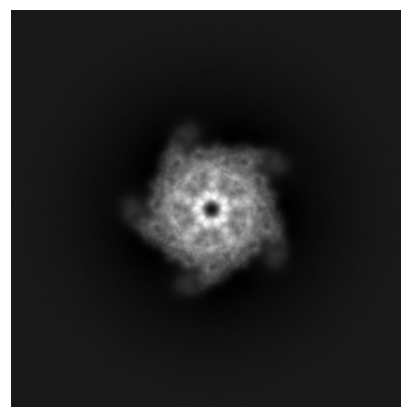
6.1.2 Raw map



X



Y



Z

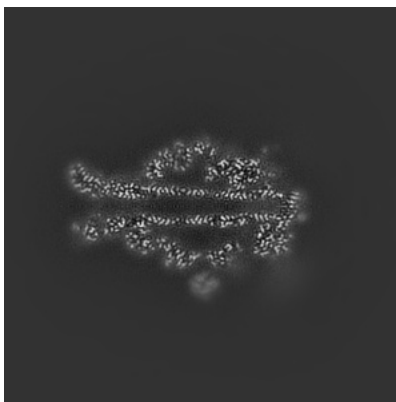
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

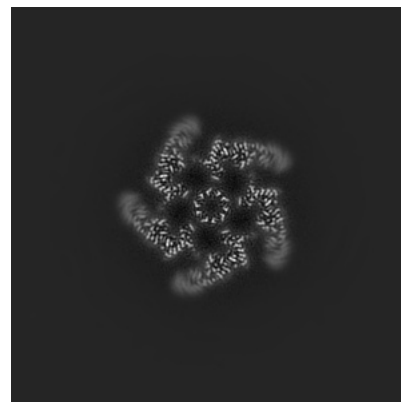
6.2.1 Primary map



X Index: 176

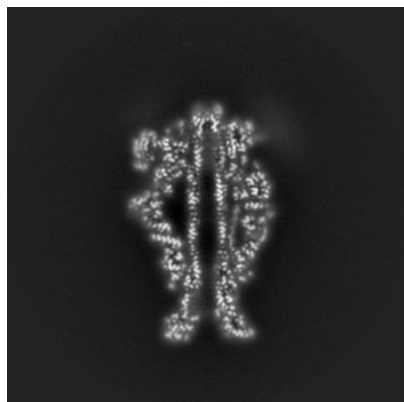


Y Index: 176

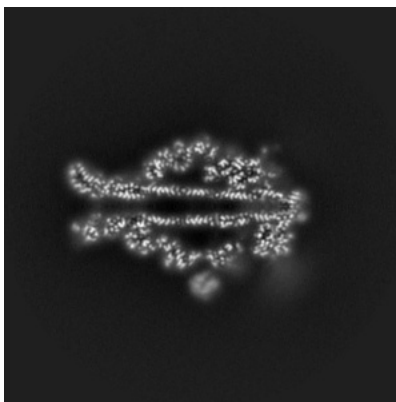


Z Index: 176

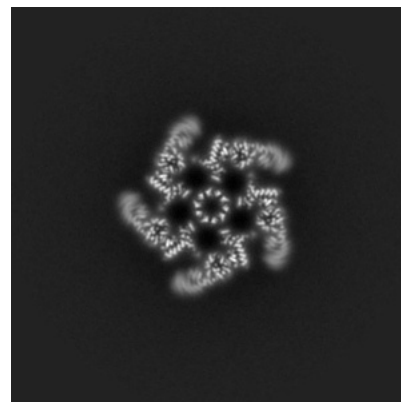
6.2.2 Raw map



X Index: 176



Y Index: 176

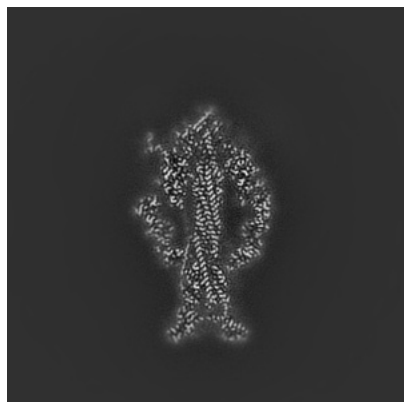


Z Index: 176

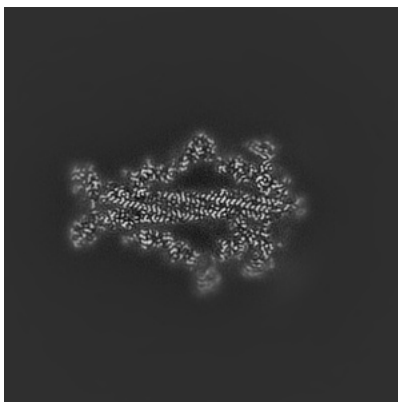
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

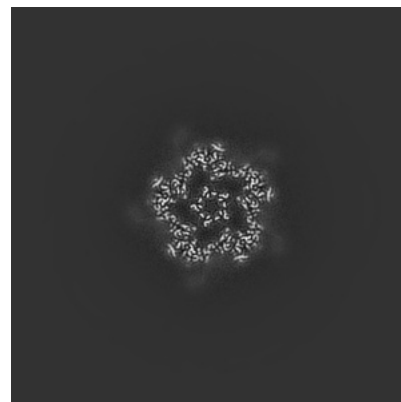
6.3.1 Primary map



X Index: 187

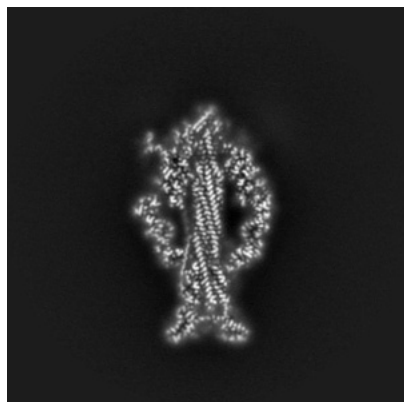


Y Index: 166

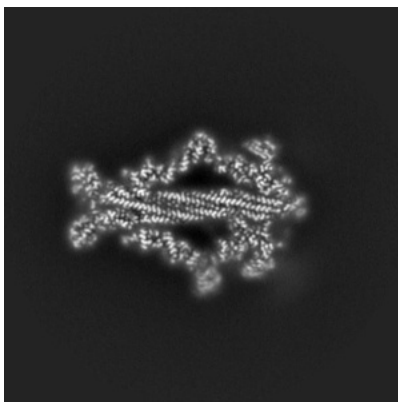


Z Index: 192

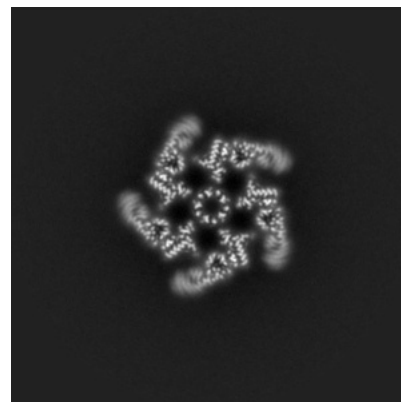
6.3.2 Raw map



X Index: 187



Y Index: 166

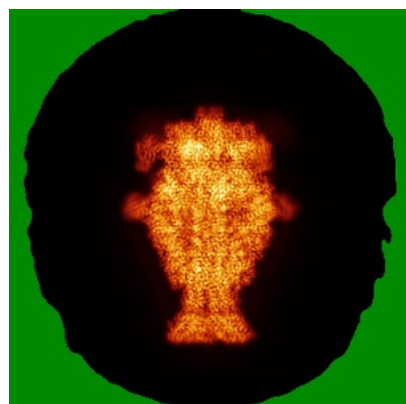


Z Index: 177

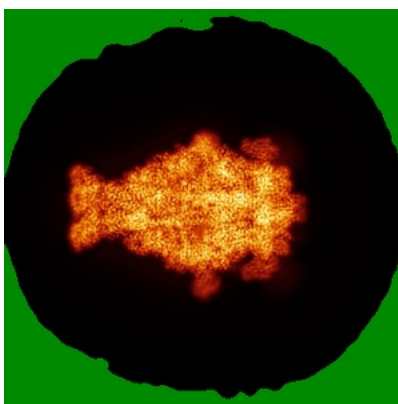
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

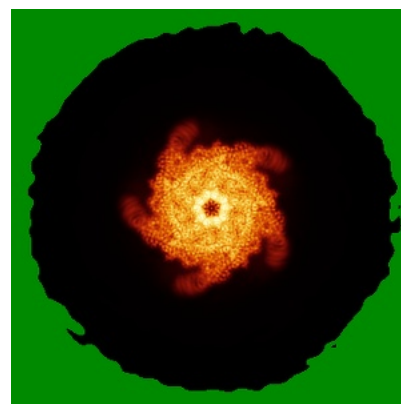
6.4.1 Primary map



X



Y

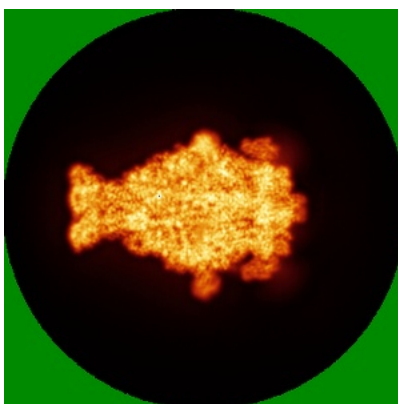


Z

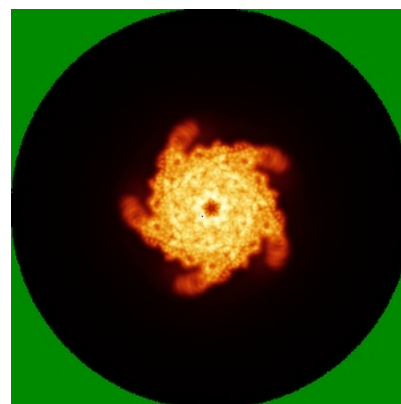
6.4.2 Raw map



X



Y

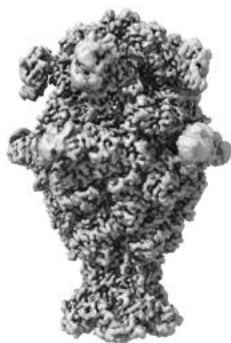


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

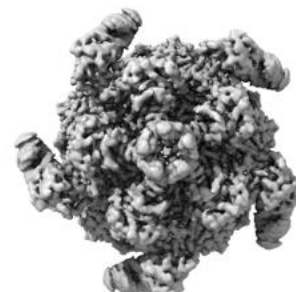
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

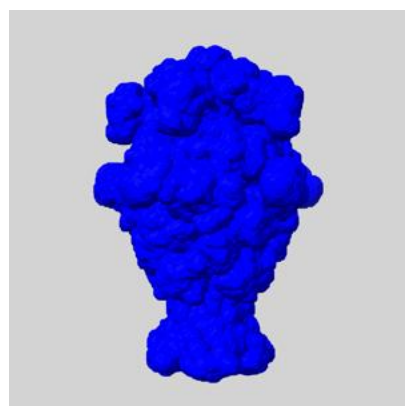
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

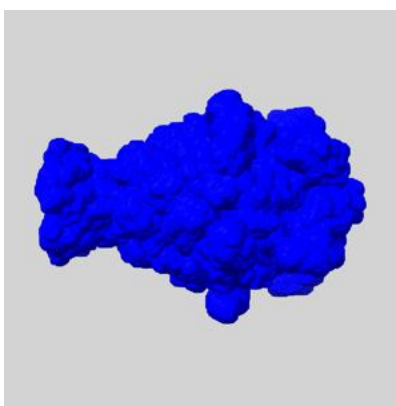
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

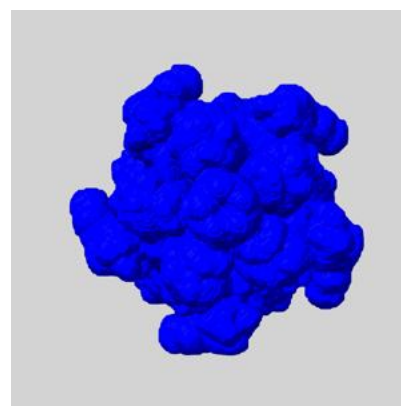
6.6.1 emd_16791_msk_1.map [i](#)



X



Y

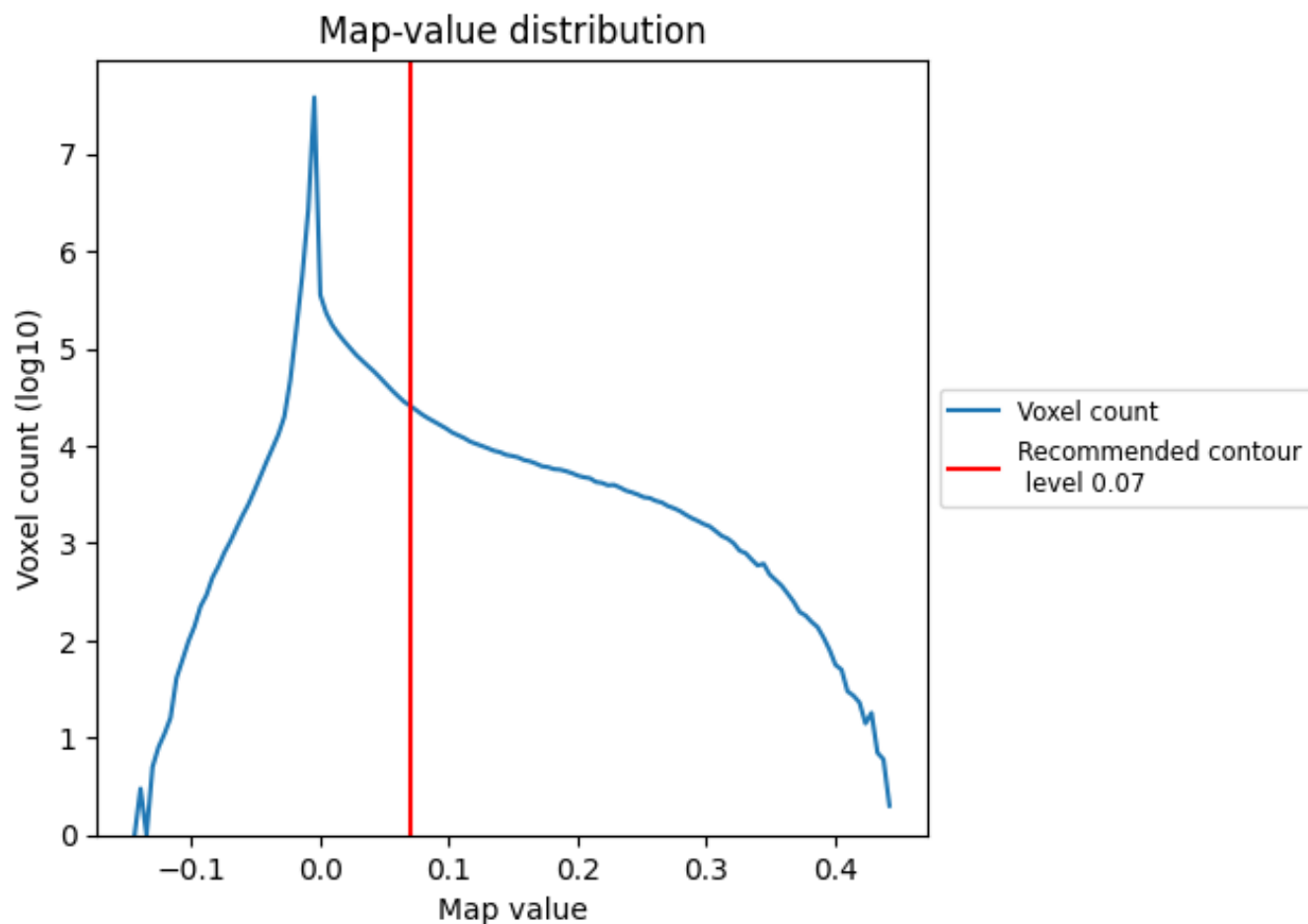


Z

7 Map analysis [i](#)

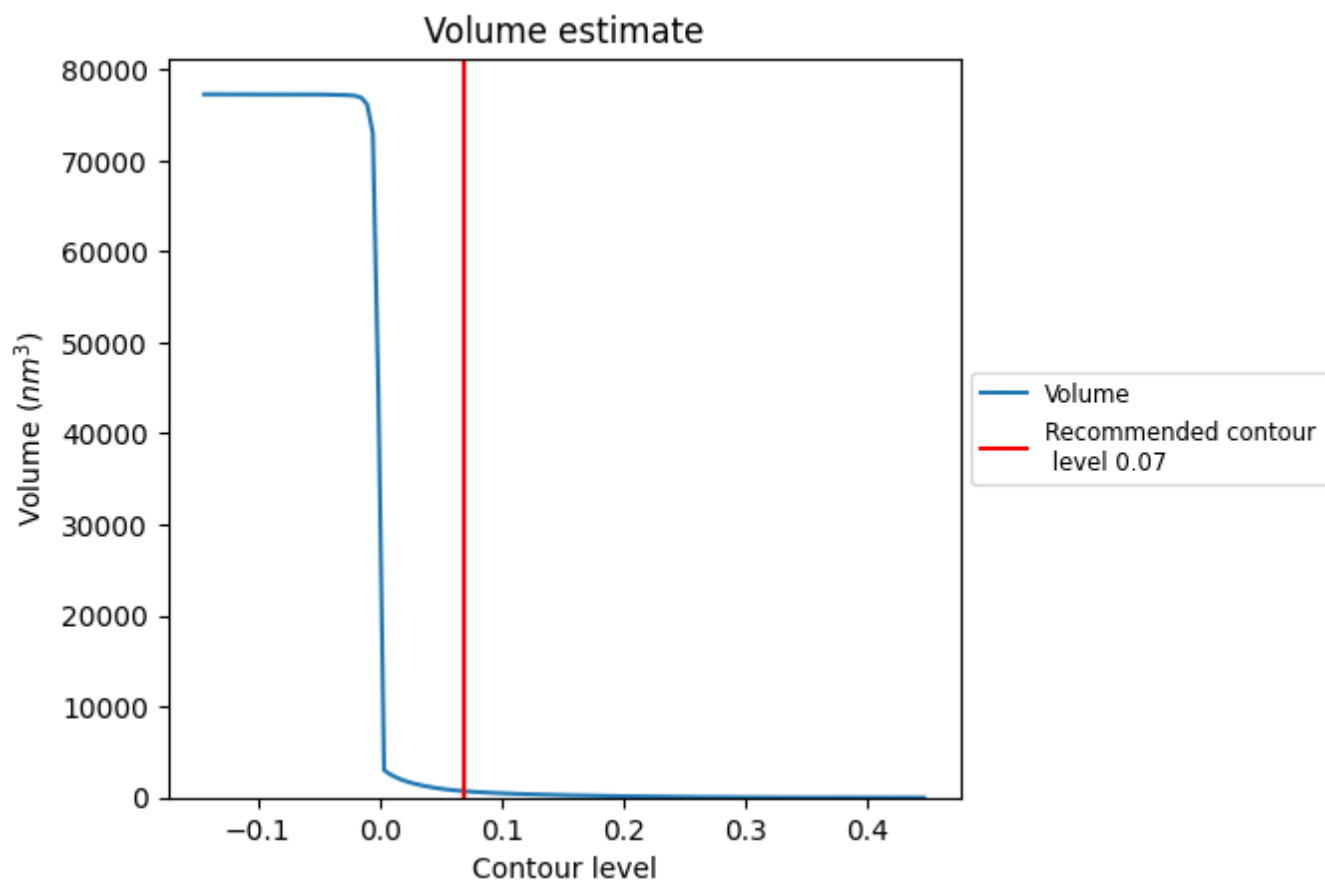
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

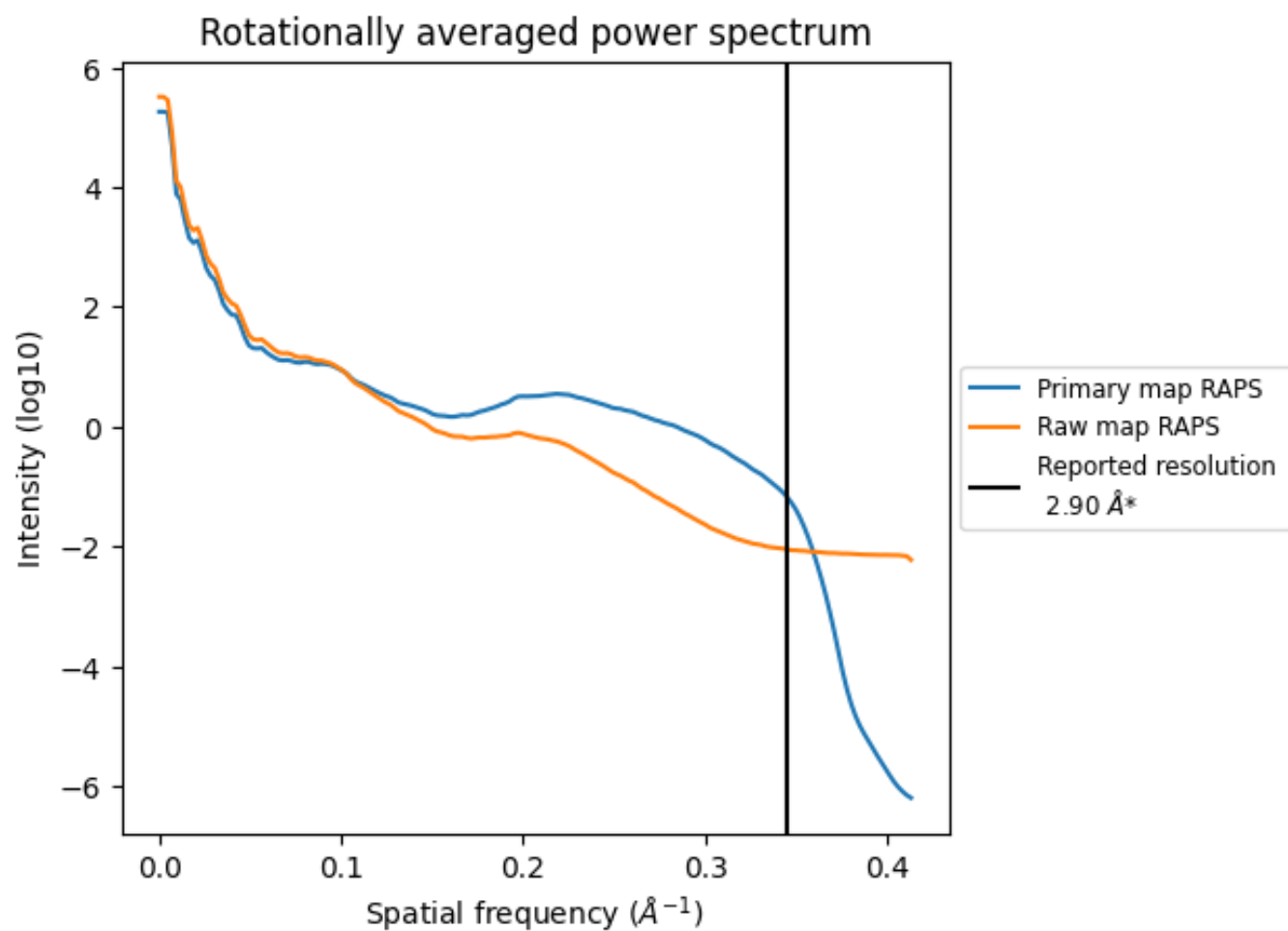
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 702 nm³; this corresponds to an approximate mass of 634 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

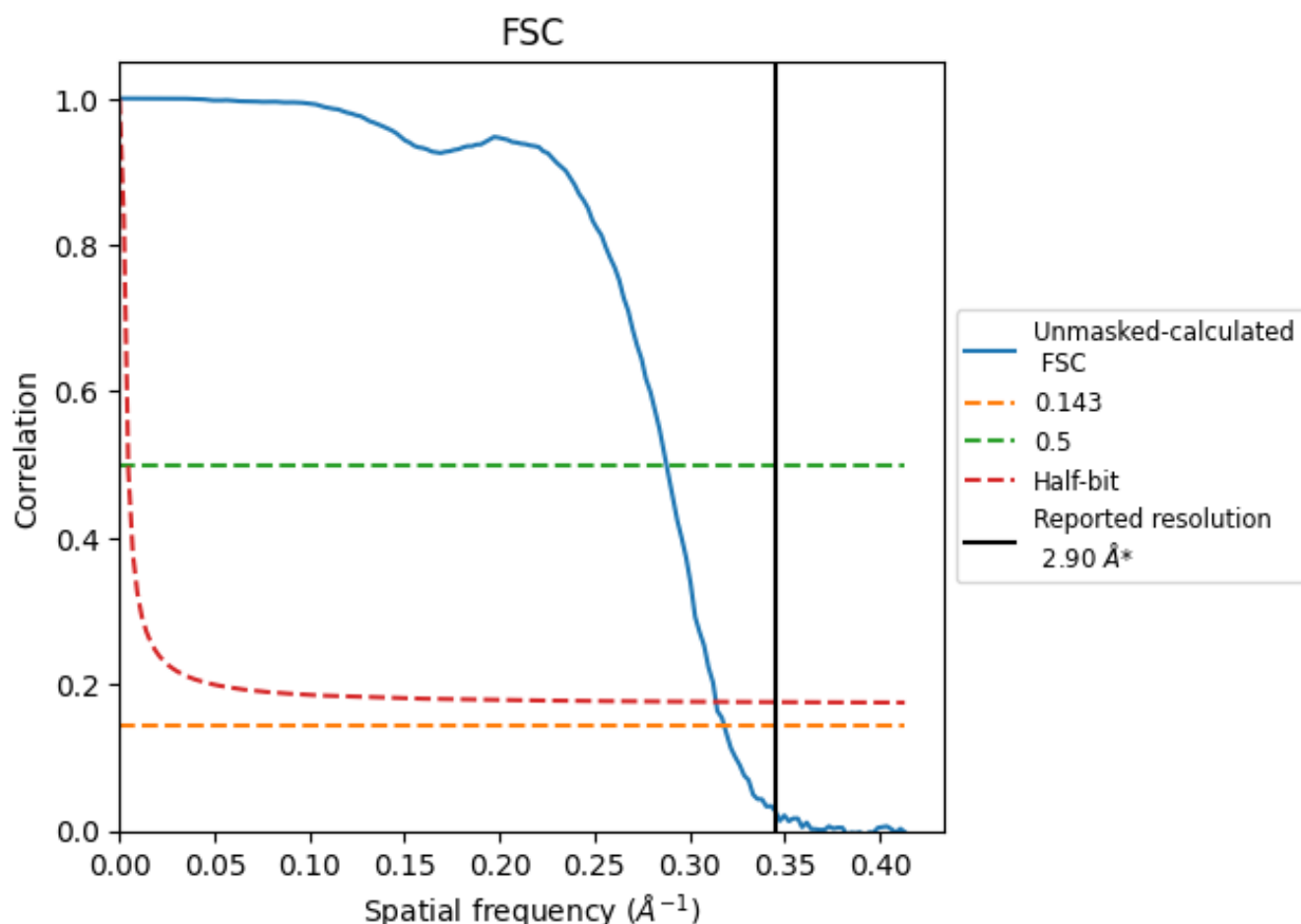


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

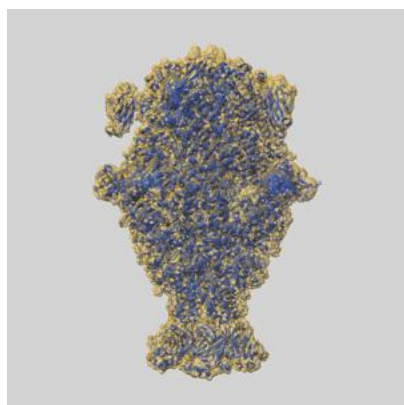
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.47	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

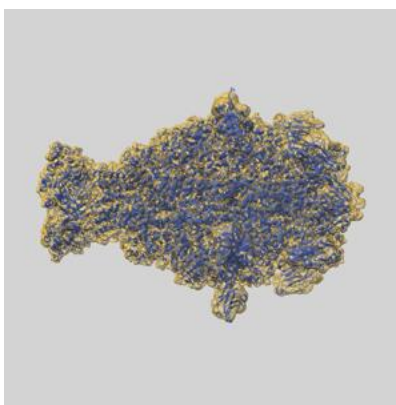
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16791 and PDB model 8CPZ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

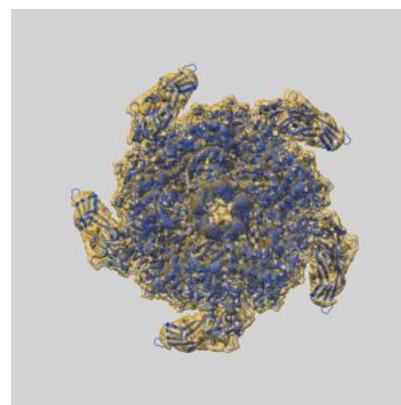
9.1 Map-model overlay [i](#)



X



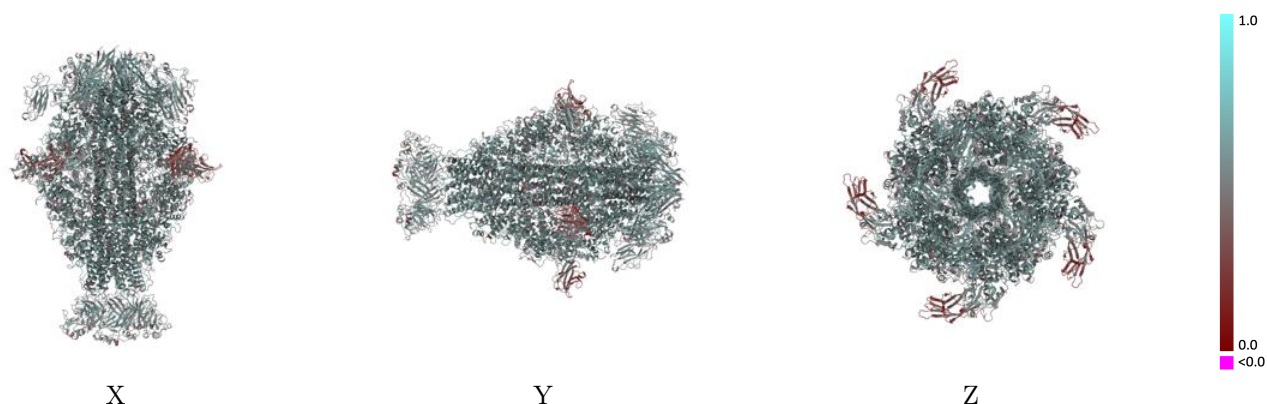
Y



Z

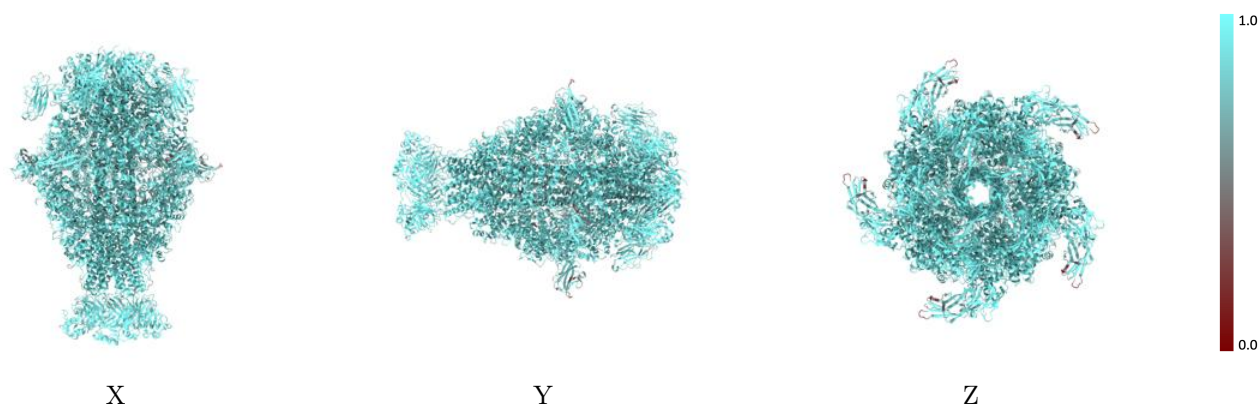
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



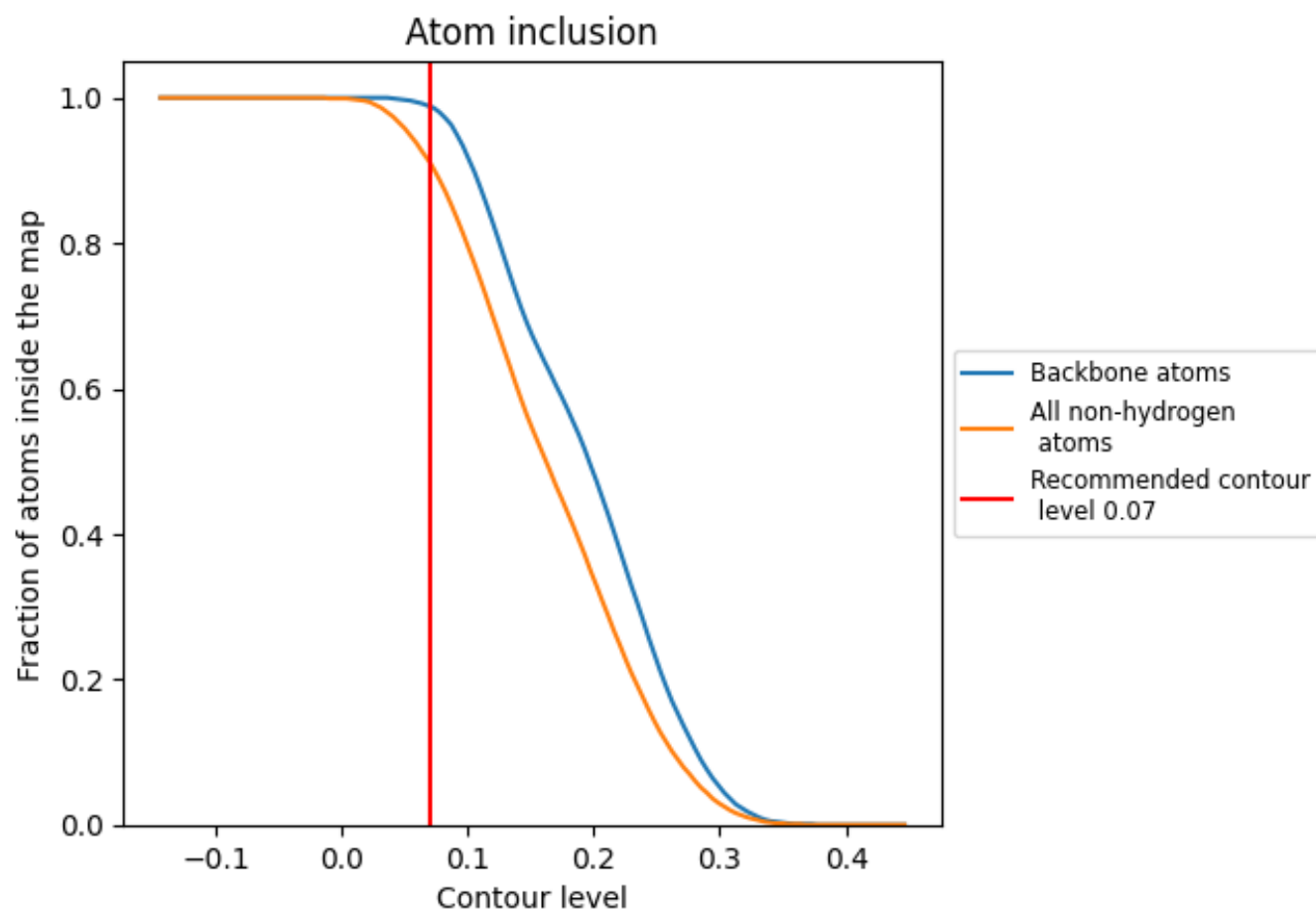
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9110	<div><div></div></div> 0.5260
A	<div><div></div></div> 0.9100	<div><div></div></div> 0.5260
B	<div><div></div></div> 0.9110	<div><div></div></div> 0.5270
C	<div><div></div></div> 0.9100	<div><div></div></div> 0.5270
D	<div><div></div></div> 0.9110	<div><div></div></div> 0.5260
E	<div><div></div></div> 0.9110	<div><div></div></div> 0.5260

