



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:45 AM GMT

PDB ID : 1LPQ
Title : Human DNA Topoisomerase I (70 Kda) In Non-Covalent Complex With A 22
Base Pair DNA Duplex Containing an 8-oxoG Lesion
Authors : Leshner, D.T.; Pommier, Y.; Stewart, L.; Redinbo, M.R.
Deposited on : 2002-05-08
Resolution : 3.14 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

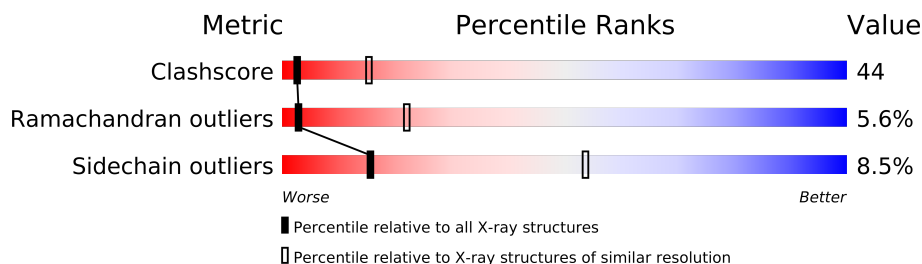
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.14 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1656 (3.20-3.08)
Ramachandran outliers	78287	1614 (3.20-3.08)
Sidechain outliers	78261	1613 (3.20-3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	22	
2	C	22	
3	A	564	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5381 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a DNA chain called 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*TP*TP*(8OG)P*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	22	Total	C	N	O	P	0	0	0
			454	219	87	127	21			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*CP*AP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			443	217	71	134	21			

- Molecule 3 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	557	Total	C	N	O	S	0	0	0
			4457	2849	784	800	24			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	723	PHE	TYR	ENGINEERED	UNP P11387

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	2	Total	O	0	0
			2	2		
4	C	3	Total	O	0	0
			3	3		

3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*TP*TP*(8OG)P*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3'

Chain B: 



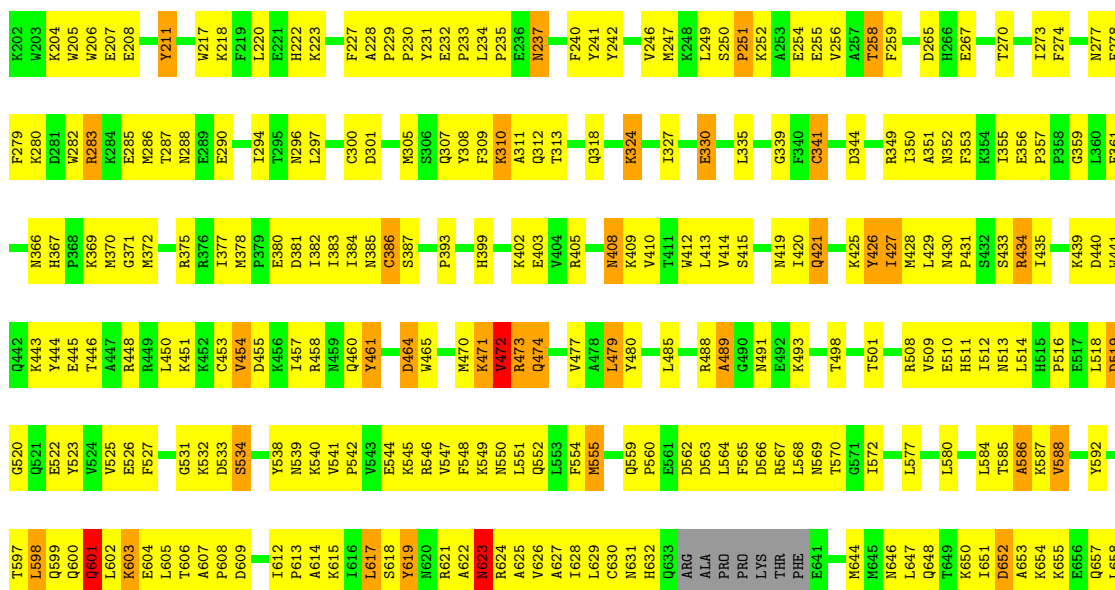
- Molecule 2: 5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*CP*AP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3'

Chain C: 



- Molecule 3: DNA topoisomerase I

Chain A: 



W722	W723	W724	W725	W726	W727	W728	W729	W730	W731	W732	W733	W734	W735	W736	W737	W738	W739	W740	W741	W742	W743	W744	W745	W746	W747	W748	W749	W750	W751	W752	W753	W754	W755	W756	W757	W758	W759	W760	W761	W762	W763	W764	W765	W766	W767	W768	W769	W770	W771	W772	W773	W774	W775	W776	W777	W778	W779	W780	W781	W782	W783	W784	W785	W786	W787	W788	W789	W790	W791	W792	W793	W794	W795	W796	W797	W798	W799	W800	W801	W802	W803	W804	W805	W806	W807	W808	W809	W810	W811	W812	W813	W814	W815	W816	W817	W818	W819	W820	W821	W822	W823	W824	W825	W826	W827	W828	W829	W830	W831	W832	W833	W834	W835	W836	W837	W838	W839	W840	W841	W842	W843	W844	W845	W846	W847	W848	W849	W850	W851	W852	W853	W854	W855	W856	W857	W858	W859	W860	W861	W862	W863	W864	W865	W866	W867	W868	W869	W870	W871	W872	W873	W874	W875	W876	W877	W878	W879	W880	W881	W882	W883	W884	W885	W886	W887	W888	W889	W890	W891	W892	W893	W894	W895	W896	W897	W898	W899	W900	W901	W902	W903	W904	W905	W906	W907	W908	W909	W910	W911	W912	W913	W914	W915	W916	W917	W918	W919	W920	W921	W922	W923	W924	W925	W926	W927	W928	W929	W930	W931	W932	W933	W934	W935	W936	W937	W938	W939	W940	W941	W942	W943	W944	W945	W946	W947	W948	W949	W950	W951	W952	W953	W954	W955	W956	W957	W958	W959	W960	W961	W962	W963	W964	W965	W966	W967	W968	W969	W970	W971	W972	W973	W974	W975	W976	W977	W978	W979	W980	W981	W982	W983	W984	W985	W986	W987	W988	W989	W990	W991	W992	W993	W994	W995	W996	W997	W998	W999	W1000	W1001	W1002	W1003	W1004	W1005	W1006	W1007	W1008	W1009	W1010	W1011	W1012	W1013	W1014	W1015	W1016	W1017	W1018	W1019	W1020	W1021	W1022	W1023	W1024	W1025	W1026	W1027	W1028	W1029	W1030	W1031	W1032	W1033	W1034	W1035	W1036	W1037	W1038	W1039	W1040	W1041	W1042	W1043	W1044	W1045	W1046	W1047	W1048	W1049	W1050	W1051	W1052	W1053	W1054	W1055	W1056	W1057	W1058	W1059	W1060	W1061	W1062	W1063	W1064	W1065	W1066	W1067	W1068	W1069	W1070	W1071	W1072	W1073	W1074	W1075	W1076	W1077	W1078	W1079	W1080	W1081	W1082	W1083	W1084	W1085	W1086	W1087	W1088	W1089	W1090	W1091	W1092	W1093	W1094	W1095	W1096	W1097	W1098	W1099	W1100	W1101	W1102	W1103	W1104	W1105	W1106	W1107	W1108	W1109	W1110	W1111	W1112	W1113	W1114	W1115	W1116	W1117	W1118	W1119	W1120	W1121	W1122	W1123	W1124	W1125	W1126	W1127	W1128	W1129	W1130	W1131	W1132	W1133	W1134	W1135	W1136	W1137	W1138	W1139	W1140	W1141	W1142	W1143	W1144	W1145	W1146	W1147	W1148	W1149	W1150	W1151	W1152	W1153	W1154	W1155	W1156	W1157	W1158	W1159	W1160	W1161	W1162	W1163	W1164	W1165	W1166	W1167	W1168	W1169	W1170	W1171	W1172	W1173	W1174	W1175	W1176	W1177	W1178	W1179	W1180	W1181	W1182	W1183	W1184	W1185	W1186	W1187	W1188	W1189	W1190	W1191	W1192	W1193	W1194	W1195	W1196	W1197	W1198	W1199	W1200	W1201	W1202	W1203	W1204	W1205	W1206	W1207	W1208	W1209	W1210	W1211	W1212	W1213	W1214	W1215	W1216	W1217	W1218	W1219	W1220	W1221	W1222	W1223	W1224	W1225	W1226	W1227	W1228	W1229	W1230	W1231	W1232	W1233	W1234	W1235	W1236	W1237	W1238	W1239	W1240	W1241	W1242	W1243	W1244	W1245	W1246	W1247	W1248	W1249	W1250	W1251	W1252	W1253	W1254	W1255	W1256	W1257	W1258	W1259	W1260	W1261	W1262	W1263	W1264	W1265	W1266	W1267	W1268	W1269	W1270	W1271	W1272	W1273	W1274	W1275	W1276	W1277	W1278	W1279	W1280	W1281	W1282	W1283	W1284	W1285	W1286	W1287	W1288	W1289	W1290	W1291	W1292	W1293	W1294	W1295	W1296	W1297	W1298	W1299	W1300	W1301	W1302	W1303	W1304	W1305	W1306	W1307	W1308	W1309	W1310	W1311	W1312	W1313	W1314	W1315	W1316	W1317	W1318	W1319	W1320	W1321	W1322	W1323	W1324	W1325	W1326	W1327	W1328	W1329	W1330	W1331	W1332	W1333	W1334	W1335	W1336	W1337	W1338	W1339	W1340	W1341	W1342	W1343	W1344	W1345	W1346	W1347	W1348	W1349	W1350	W1351	W1352	W1353	W1354	W1355	W1356	W1357	W1358	W1359	W1360	W1361	W1362	W1363	W1364	W1365	W1366	W1367	W1368	W1369	W1370	W1371	W1372	W1373	W1374	W1375	W1376	W1377	W1378	W1379	W1380	W1381	W1382	W1383	W1384	W1385	W1386	W1387	W1388	W1389	W1390	W1391	W1392	W1393	W1394	W1395	W1396	W1397	W1398	W1399	W1400	W1401	W1402	W1403	W1404	W1405	W1406	W1407	W1408	W1409	W1410	W1411	W1412	W1413	W1414	W1415	W1416	W1417	W1418	W1419	W1420	W1421	W1422	W1423	W1424	W1425	W1426	W1427	W1428	W1429	W1430	W1431	W1432	W1433	W1434	W1435	W1436	W1437	W1438	W1439	W1440	W1441	W1442	W1443	W1444	W1445	W1446	W1447	W1448	W1449	W1450	W1451	W1452	W1453	W1454	W1455	W1456	W1457	W1458	W1459	W1460	W1461	W1462	W1463	W1464	W1465	W1466	W1467	W1468	W1469	W1470	W1471	W1472	W1473	W1474	W1475	W1476	W1477	W1478	W1479	W1480	W1481	W1482	W1483	W1484	W1485	W1486	W1487	W1488	W1489	W1490	W1491	W1492	W1493	W1494	W1495	W1496	W1497	W1498	W1499	W1500	W1501	W1502	W1503	W1504	W1505	W1506	W1507	W1508	W1509	W1510	W1511	W1512	W1513	W1514	W1515	W1516	W1517	W1518	W1519	W1520	W1521	W1522	W1523	W1524	W1525	W1526	W1527	W1528	W1529	W1530	W1531	W1532	W1533	W1534	W1535	W1536	W1537	W1538	W1539	W1540	W1541	W1542	W1543	W1544	W1545	W1546	W1547	W1548	W1549	W1550	W1551	W1552	W1553	W1554	W1555	W1556	W1557	W1558	W1559	W1560	W1561	W1562	W1563	W1564	W1565	W1566	W1567	W1568	W1569	W1570	W1571	W1572	W1573	W1574	W1575	W1576	W1577	W1578	W1579	W1580	W1581	W1582	W1583	W1584	W1585	W1586	W1587	W1588	W1589	W1590	W1591	W1592	W1593	W1594	W1595	W1596	W1597	W1598	W1599	W1600	W1601	W1602	W1603	W1604	W1605	W1606	W1607	W1608	W1609	W1610	W1611	W1612	W1613	W1614	W1615	W1616	W1617	W1618	W1619	W1620	W1621	W1622	W1623	W1624	W1625	W1626	W1627	W1628	W1629	W1630	W1631	W1632	W1633	W1634	W1635	W1636	W1637	W1638	W1639	W1640	W1641	W1642	W1643	W1644	W1645	W1646	W1647	W1648	W1649	W1650	W1651	W1652	W1653	W1654	W1655	W1656	W1657	W1658	W1659	W1660	W1661	W1662	W1663	W1664	W1665	W1666	W1667	W1668	W1669	W1670	W1671	W1672	W1673	W1674	W1675	W1676	W1677	W1678	W1679	W1680	W1681	W1682	W1683	W1684	W1685	W1686	W1687	W1688	W1689	W1690	W1691	W1692	W1693	W1694	W1695	W1696	W1697	W1698	W1699	W1700	W1701	W1702	W1703	W1704	W1705	W1706	W1707	W1708	W1709	W1710	W1711	W1712	W1713	W1714	W1715	W1716	W1717	W1718	W1719	W1720	W1721	W1722	W1723	W1724	W1725	W1726	W1727	W1728	W1729	W1730	W1731	W1732	W1733	W1734	W1735	W1736	W1737	W1738	W1739	W1740	W1741	W1742	W1743	W1744	W1745	W1746	W1747	W1748	W1749	W1750	W1751	W1752	W1753	W1754	W1755	W1756	W1757	W1758	W1759	W1760	W1761	W1762	W1763	W1764	W1765	W1766	W1767	W1768	W1769	W1770	W1771	W1772	W1773	W1774	W1775	W1776	W1777	W1778	W1779	W1780	W1781	W1782	W1783	W1784	W1785	W1786	W1787	W1788	W1789	W1790	W1791	W1792	W1793	W1794	W1795	W1796	W1797	W1798	W1799	W1800	W1801	W1802	W1803	W1804	W1805	W1806	W1807	W1808	W1809	W1810	W1811	W1812	W1813	W1814	W1815	W1816	W1817	W1818	W1819	W1820	W1821	W1822	W1823	W1824	W1825	W1826	W1827	W1828	W1829	W1830	W1831	W1832	W1833	W1834	W1835	W1836	W1837	W1838	W1839	W1840	W1841	W1842	W1843	W1844	W1845	W1846	W1847	W1848	W1849	W1850	W1851	W1852	W1853	W1854	W1855	W1856	W1857	W1858	W1859	W1860	W1861	W1862	W1863	W1864	W1865	W1866	W1867	W1868	W1869	W1870	W1871	W1872	W1873	W1874	W1875	W1876	W1877	W1878	W1879	W1880	W1881	W1882	W1883	W1884	W1885	W1886	W1887	W1888	W1889	W1890	W1891	W1892	W1893	W1894	W1895	W1896	W1897	W1898	W1899	W1900	W1901	W1902	W1903	W1904	W1905	W1906	W1907	W1908	W1909	W1910	W1911	W1912	W1913	W1914	W1915	W1916	W1917	W1918	W1919	W1920	W1921	W1922	W1923	W1924	W1925	W1926	W1927	W1928	W1929	W1930	W1931	W1932	W1933	W1934	W1935	W1936	W1937	W1938	W1939	W1940	W1941	W1942	W1943	W1944	W1945	W1946	W1947	W1948	W1949	W1950	W1951	W1952	W1953	W1954	W1955	W1956	W1957	W1958	W1959	W1960	W1961	W1962	W1963	W1964	W1965	W1966	W1967	W1968	W1969	W1970	W1971	W1972	W1973	W1974	W1975	W1976	W1977	W1978	W1979	W1980	W1981	W1982	W1983	W1984	W1985	W1986	W1987</
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.20Å 122.50Å 72.00Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	19.87 – 3.14	Depositor
% Data completeness (in resolution range)	95.5 (19.87-3.14)	Depositor
R_{merge}	0.33	Depositor
R_{sym}	0.20	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.256 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5381	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 8OG

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	B	0.55	0/484	0.78	0/743
2	C	0.64	0/494	0.86	1/760 (0.1%)
3	A	0.45	0/4555	0.69	5/6142 (0.1%)
All	All	0.48	0/5533	0.71	6/7645 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	664	ASP	N-CA-C	-7.79	89.98	111.00
3	A	472	VAL	N-CA-C	-6.99	92.12	111.00
3	A	426	TYR	N-CA-C	5.43	125.66	111.00
3	A	663	ARG	N-CA-C	-5.40	96.42	111.00
3	A	723	PHE	N-CA-C	5.26	125.19	111.00
2	C	112	DC	C1'-O4'-C4'	-5.01	105.09	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	112	DC	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	454	0	251	6	0
2	C	443	0	255	16	0
3	A	4457	0	4375	433	0
4	A	22	0	0	5	0
4	B	2	0	0	0	0
4	C	3	0	0	1	0
All	All	5381	0	4881	451	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 44.

All (451) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:473:ARG:CZ	3:A:550:ASN:HB3	1.64	1.26
3:A:473:ARG:NH2	3:A:550:ASN:HB3	1.57	1.17
3:A:473:ARG:CZ	3:A:550:ASN:CB	2.37	1.01
3:A:273:ILE:HD12	3:A:273:ILE:H	1.28	0.96
3:A:267:GLU:O	3:A:270:THR:HG22	1.68	0.91
3:A:664:ASP:C	3:A:666:LYS:H	1.75	0.90
3:A:283:ARG:HB3	4:A:1018:HOH:O	1.70	0.90
3:A:421:GLN:HA	3:A:421:GLN:HE21	1.35	0.90
3:A:241:TYR:HB2	3:A:301:ASP:HB3	1.54	0.90
3:A:617:LEU:HD13	3:A:703:VAL:HG22	1.54	0.89
3:A:628:ILE:HG13	3:A:714:ILE:HG21	1.54	0.89
3:A:618:SER:HA	3:A:621:ARG:HB3	1.56	0.87
3:A:654:LYS:HA	3:A:657:GLN:HG3	1.57	0.86
3:A:472:VAL:HG12	3:A:473:ARG:H	1.39	0.86
3:A:686:SER:HA	3:A:689:LYS:HG3	1.57	0.86
3:A:433:SER:HB3	3:A:435:ILE:HG22	1.58	0.85
3:A:408:ASN:HB2	3:A:409:LYS:NZ	1.92	0.85
3:A:252:LYS:HE2	3:A:285:GLU:OE1	1.77	0.85
3:A:659:ALA:HA	3:A:662:ARG:HB2	1.58	0.84
3:A:472:VAL:O	3:A:473:ARG:C	2.16	0.84
3:A:279:PHE:CD1	3:A:297:LEU:HB2	2.14	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:523:TYR:CZ	3:A:545:LYS:HG3	2.14	0.82
3:A:508:ARG:HE	3:A:511:HIS:HE1	1.26	0.82
2:C:115:DG:H2'	2:C:116:DT:H72	1.62	0.81
3:A:585:THR:O	3:A:588:VAL:HG23	1.81	0.80
3:A:624:ARG:HD3	3:A:711:ASN:HB2	1.62	0.80
3:A:473:ARG:CZ	3:A:550:ASN:CG	2.49	0.80
3:A:627:ALA:HB1	3:A:716:LEU:HB3	1.62	0.80
3:A:408:ASN:HB2	3:A:409:LYS:HZ2	1.47	0.80
3:A:699:MET:HA	3:A:702:GLU:HG2	1.61	0.80
3:A:629:LEU:HB2	4:A:1006:HOH:O	1.81	0.79
1:B:7:DA:H2''	1:B:8:DC:H5''	1.65	0.79
3:A:598:LEU:HD21	3:A:623:ASN:HB2	1.64	0.79
3:A:655:LYS:O	3:A:658:LEU:HB3	1.83	0.78
3:A:516:PRO:O	3:A:522:GLU:HG3	1.83	0.78
3:A:601:GLN:HE21	3:A:601:GLN:HA	1.49	0.77
3:A:217:TRP:HZ3	3:A:387:SER:HB3	1.48	0.76
3:A:627:ALA:HB3	3:A:716:LEU:HD23	1.66	0.76
3:A:723:PHE:CE1	3:A:724:LEU:HG	2.21	0.76
3:A:380:GLU:O	3:A:402:LYS:HB2	1.85	0.76
3:A:470:MET:HE1	3:A:567:ARG:HG3	1.69	0.75
3:A:446:THR:HG22	3:A:588:VAL:HG11	1.68	0.75
3:A:745:ASN:ND2	3:A:748:GLN:HE21	1.84	0.75
3:A:473:ARG:NH2	3:A:550:ASN:CB	2.45	0.75
1:B:8:DC:H2'	1:B:9:DT:H72	1.69	0.74
3:A:686:SER:HA	3:A:689:LYS:HE2	1.70	0.73
3:A:426:TYR:O	3:A:427:ILE:HB	1.86	0.73
3:A:552:GLN:HA	3:A:555:MET:HG3	1.71	0.73
3:A:699:MET:HA	3:A:702:GLU:CG	2.18	0.73
3:A:444:TYR:O	3:A:448:ARG:HG3	1.89	0.72
3:A:430:ASN:OD1	3:A:431:PRO:HD2	1.89	0.72
2:C:106:DT:H2'	2:C:107:DT:H72	1.72	0.72
3:A:696:GLU:C	3:A:698:LEU:H	1.93	0.71
3:A:369:LYS:O	3:A:372:MET:HG3	1.89	0.71
3:A:235:PRO:HB2	3:A:237:ASN:ND2	2.05	0.71
3:A:617:LEU:CD1	3:A:703:VAL:HG22	2.21	0.70
3:A:621:ARG:CG	3:A:624:ARG:HH12	2.04	0.69
3:A:585:THR:H	3:A:588:VAL:CG2	2.05	0.69
3:A:719:SER:HA	3:A:723:PHE:CE2	2.27	0.69
3:A:453:CYS:O	3:A:457:ILE:HG13	1.93	0.69
3:A:297:LEU:HA	3:A:300:CYS:SG	2.33	0.69
3:A:250:SER:HB2	3:A:251:PRO:HD2	1.73	0.68
3:A:510:GLU:HB3	3:A:560:PRO:HB3	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:730:VAL:HG11	3:A:756:ILE:HA	1.74	0.68
3:A:722:ASN:O	3:A:724:LEU:N	2.27	0.68
3:A:664:ASP:O	3:A:666:LYS:N	2.26	0.68
3:A:335:LEU:HD12	3:A:339:GLY:HA3	1.76	0.68
3:A:732:TRP:O	3:A:736:TRP:HD1	1.77	0.67
3:A:222:HIS:HE1	3:A:384:ILE:HG23	1.59	0.67
3:A:414:VAL:O	3:A:426:TYR:O	2.13	0.66
3:A:433:SER:CB	3:A:435:ILE:HG22	2.25	0.66
3:A:568:LEU:HA	3:A:572:ILE:HD12	1.77	0.66
2:C:115:DG:H2'	2:C:116:DT:C7	2.26	0.66
3:A:222:HIS:CE1	3:A:384:ILE:HG23	2.31	0.66
3:A:470:MET:CE	3:A:567:ARG:HG3	2.26	0.65
3:A:451:LYS:HA	3:A:592:TYR:CE1	2.31	0.65
3:A:421:GLN:CA	3:A:421:GLN:HE21	2.08	0.65
3:A:211:TYR:OH	3:A:218:LYS:HB2	1.97	0.65
3:A:552:GLN:O	3:A:555:MET:HB2	1.97	0.65
3:A:421:GLN:HA	3:A:421:GLN:NE2	2.10	0.65
3:A:448:ARG:HG2	3:A:765:PHE:CD1	2.31	0.65
2:C:109:DT:OP1	3:A:746:LYS:HD2	1.96	0.64
3:A:473:ARG:NE	3:A:550:ASN:CG	2.51	0.64
3:A:461:TYR:HA	3:A:464:ASP:CG	2.17	0.64
3:A:665:LEU:HA	3:A:687:LYS:HG3	1.79	0.64
3:A:600:GLN:HA	3:A:603:LYS:HE2	1.80	0.64
3:A:688:LYS:HA	3:A:691:VAL:HB	1.77	0.64
3:A:546:ARG:O	3:A:550:ASN:HB2	1.98	0.64
3:A:310:LYS:HG3	3:A:311:ALA:N	2.12	0.64
3:A:473:ARG:NH1	3:A:550:ASN:HB3	2.11	0.64
3:A:448:ARG:HG2	3:A:765:PHE:CE1	2.33	0.64
3:A:408:ASN:HD22	3:A:408:ASN:N	1.93	0.64
3:A:255:GLU:O	3:A:258:THR:CG2	2.46	0.64
3:A:664:ASP:C	3:A:666:LYS:N	2.47	0.64
3:A:460:GLN:O	3:A:464:ASP:OD1	2.16	0.64
3:A:621:ARG:NE	3:A:706:THR:HG21	2.13	0.63
3:A:696:GLU:O	3:A:700:LYS:N	2.24	0.63
3:A:489:ALA:HB1	3:A:570:THR:HG22	1.80	0.63
3:A:723:PHE:CD1	3:A:724:LEU:HG	2.34	0.63
3:A:599:GLN:HE22	3:A:765:PHE:H	1.47	0.63
3:A:448:ARG:HD2	3:A:727:ARG:NH2	2.13	0.63
3:A:493:LYS:NZ	3:A:501:THR:OG1	2.31	0.63
3:A:277:ASN:HA	3:A:280:LYS:NZ	2.13	0.63
3:A:351:ALA:HB2	3:A:429:LEU:O	1.99	0.63
3:A:754:TRP:O	3:A:758:MET:HG3	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:283:ARG:HA	3:A:286:MET:CE	2.29	0.62
3:A:598:LEU:CD2	3:A:623:ASN:HB2	2.29	0.62
2:C:106:DT:H2"	2:C:107:DT:C6	2.35	0.62
3:A:651:ILE:O	3:A:655:LYS:HB2	1.99	0.62
3:A:601:GLN:O	3:A:604:GLU:HB3	1.99	0.62
3:A:601:GLN:HB3	3:A:622:ALA:HB1	1.81	0.62
3:A:255:GLU:O	3:A:258:THR:HG23	1.99	0.62
3:A:566:ASP:O	3:A:567:ARG:HB2	2.00	0.61
3:A:509:VAL:CG2	3:A:560:PRO:HA	2.31	0.61
3:A:471:LYS:O	3:A:472:VAL:HB	2.01	0.61
3:A:523:TYR:OH	3:A:545:LYS:HG3	2.01	0.60
3:A:273:ILE:H	3:A:273:ILE:CD1	2.05	0.60
3:A:696:GLU:CB	3:A:700:LYS:HE3	2.31	0.60
3:A:327:ILE:HA	3:A:330:GLU:HB2	1.83	0.60
3:A:247:MET:HE1	3:A:294:ILE:HD11	1.83	0.60
3:A:696:GLU:O	3:A:698:LEU:N	2.34	0.60
3:A:619:TYR:HD2	3:A:619:TYR:C	2.05	0.60
3:A:473:ARG:NH2	3:A:550:ASN:C	2.54	0.60
3:A:282:TRP:O	3:A:286:MET:HG3	2.01	0.60
3:A:429:LEU:HD12	3:A:435:ILE:HG21	1.83	0.60
3:A:508:ARG:HE	3:A:511:HIS:CE1	2.15	0.60
3:A:678:ALA:O	3:A:682:LYS:HG2	2.01	0.60
3:A:450:LEU:O	3:A:454:VAL:HG12	2.02	0.60
3:A:472:VAL:HG12	3:A:473:ARG:N	2.14	0.60
3:A:663:ARG:O	3:A:664:ASP:CB	2.48	0.60
3:A:431:PRO:HB3	3:A:751:LYS:HG3	1.83	0.60
3:A:568:LEU:HD13	3:A:568:LEU:C	2.22	0.60
3:A:533:ASP:O	3:A:534:SER:HB2	2.02	0.60
3:A:659:ALA:CA	3:A:662:ARG:HB2	2.31	0.59
3:A:434:ARG:HG2	3:A:434:ARG:O	2.02	0.59
3:A:658:LEU:HD21	4:A:1038:HOH:O	2.02	0.59
3:A:555:MET:HA	3:A:555:MET:HE3	1.84	0.59
3:A:454:VAL:HG22	3:A:455:ASP:N	2.16	0.59
3:A:433:SER:C	3:A:435:ILE:H	2.05	0.59
3:A:602:LEU:C	3:A:604:GLU:H	2.04	0.59
3:A:696:GLU:C	3:A:698:LEU:N	2.55	0.59
3:A:222:HIS:HB3	3:A:341:CYS:HB2	1.84	0.59
3:A:356:GLU:OE2	3:A:425:LYS:NZ	2.36	0.59
3:A:477:VAL:O	3:A:480:TYR:HB3	2.03	0.59
3:A:465:TRP:O	3:A:473:ARG:HD3	2.03	0.59
3:A:617:LEU:HG	3:A:618:SER:N	2.18	0.58
3:A:621:ARG:HA	3:A:624:ARG:NH2	2.19	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:414:VAL:CG1	3:A:415:SER:N	2.65	0.58
3:A:220:LEU:HB3	3:A:386:CYS:HA	1.84	0.58
3:A:619:TYR:C	3:A:619:TYR:CD2	2.76	0.58
3:A:217:TRP:CZ3	3:A:387:SER:HB3	2.33	0.58
3:A:628:ILE:HA	3:A:714:ILE:HG21	1.85	0.58
3:A:351:ALA:HB3	3:A:428:MET:O	2.04	0.58
1:B:8:DC:H2'	1:B:9:DT:C7	2.33	0.57
3:A:691:VAL:O	3:A:695:GLU:HG3	2.05	0.57
3:A:621:ARG:HG3	3:A:624:ARG:HH12	1.67	0.57
3:A:694:LEU:HA	3:A:697:GLN:HB2	1.87	0.57
3:A:429:LEU:HB3	3:A:433:SER:OG	2.04	0.57
3:A:414:VAL:HG12	3:A:415:SER:N	2.19	0.57
3:A:614:ALA:O	3:A:617:LEU:HB3	2.04	0.57
3:A:665:LEU:HA	3:A:687:LYS:HD2	1.87	0.57
3:A:628:ILE:HG13	3:A:714:ILE:HG13	1.86	0.57
3:A:685:GLU:HG2	3:A:686:SER:N	2.16	0.57
3:A:668:ALA:HB1	3:A:684:VAL:HG22	1.87	0.56
3:A:508:ARG:HB2	3:A:511:HIS:CE1	2.40	0.56
3:A:568:LEU:HD13	3:A:569:ASN:N	2.20	0.56
3:A:231:TYR:CE2	3:A:233:PRO:HA	2.41	0.56
3:A:671:ASP:C	3:A:673:LYS:H	2.08	0.56
3:A:283:ARG:HA	3:A:286:MET:HE3	1.87	0.56
3:A:296:ASN:O	3:A:297:LEU:HB3	2.05	0.56
3:A:461:TYR:O	3:A:464:ASP:HB2	2.05	0.56
3:A:662:ARG:O	3:A:664:ASP:O	2.23	0.56
3:A:231:TYR:O	3:A:233:PRO:HD3	2.05	0.55
3:A:473:ARG:NE	3:A:550:ASN:OD1	2.38	0.55
3:A:369:LYS:HE3	3:A:421:GLN:HE22	1.70	0.55
3:A:597:THR:O	3:A:601:GLN:HG2	2.05	0.55
3:A:488:ARG:O	3:A:489:ALA:C	2.44	0.55
3:A:223:LYS:HA	3:A:393:PRO:HB3	1.89	0.55
3:A:648:GLN:O	3:A:652:ASP:HB2	2.07	0.55
3:A:665:LEU:HD12	3:A:687:LYS:HB3	1.89	0.55
3:A:217:TRP:CH2	3:A:408:ASN:ND2	2.74	0.55
3:A:367:HIS:HD2	3:A:369:LYS:H	1.54	0.54
3:A:508:ARG:HB2	3:A:511:HIS:ND1	2.21	0.54
3:A:509:VAL:HG22	3:A:560:PRO:HA	1.89	0.54
3:A:231:TYR:CD1	3:A:255:GLU:HG3	2.43	0.54
3:A:606:THR:O	3:A:606:THR:HG22	2.06	0.54
3:A:686:SER:HA	3:A:689:LYS:CG	2.34	0.54
3:A:674:VAL:O	3:A:676:LYS:HG3	2.07	0.54
3:A:485:LEU:HD11	3:A:541:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:380:GLU:OE1	3:A:399:HIS:HD2	1.90	0.54
3:A:647:LEU:O	3:A:651:ILE:N	2.34	0.54
3:A:382:ILE:HG23	3:A:414:VAL:HG13	1.89	0.54
3:A:471:LYS:C	3:A:472:VAL:O	2.37	0.54
3:A:745:ASN:CG	3:A:748:GLN:HE21	2.11	0.54
3:A:234:LEU:HG	3:A:254:GLU:OE2	2.08	0.54
3:A:547:VAL:O	3:A:551:LEU:HB2	2.06	0.54
3:A:356:GLU:CD	3:A:425:LYS:HZ2	2.11	0.53
3:A:612:ILE:HB	3:A:613:PRO:HD3	1.89	0.53
3:A:665:LEU:HA	3:A:687:LYS:CG	2.37	0.53
3:A:629:LEU:HD21	4:A:1008:HOH:O	2.08	0.53
3:A:231:TYR:HE2	3:A:233:PRO:HA	1.74	0.53
1:B:11:8OG:H2"	1:B:11:8OG:O8	2.07	0.53
3:A:628:ILE:CG1	3:A:714:ILE:HG21	2.35	0.53
3:A:683:VAL:O	3:A:687:LYS:HG2	2.09	0.53
3:A:367:HIS:CD2	3:A:369:LYS:H	2.26	0.53
3:A:686:SER:CA	3:A:689:LYS:HG3	2.35	0.53
3:A:532:LYS:C	3:A:534:SER:H	2.11	0.53
3:A:693:ARG:HD3	3:A:694:LEU:HG	1.91	0.53
3:A:600:GLN:O	3:A:602:LEU:N	2.42	0.53
3:A:254:GLU:O	3:A:258:THR:HG22	2.09	0.52
3:A:733:CYS:SG	3:A:743:ILE:HD11	2.49	0.52
3:A:585:THR:O	3:A:586:ALA:C	2.47	0.52
3:A:205:TRP:CG	3:A:434:ARG:HB2	2.44	0.52
3:A:431:PRO:HB3	3:A:751:LYS:CD	2.40	0.52
3:A:508:ARG:NE	3:A:511:HIS:HE1	2.01	0.52
3:A:240:PHE:CD2	3:A:249:LEU:HD11	2.43	0.52
3:A:703:VAL:O	3:A:705:ALA:N	2.43	0.52
3:A:273:ILE:HG22	3:A:277:ASN:ND2	2.25	0.52
2:C:115:DG:P	3:A:493:LYS:NZ	2.83	0.52
3:A:451:LYS:HA	3:A:592:TYR:HE1	1.74	0.52
3:A:615:LYS:C	3:A:617:LEU:H	2.13	0.51
3:A:559:GLN:N	3:A:562:ASP:OD2	2.39	0.51
3:A:479:LEU:O	3:A:479:LEU:HD12	2.09	0.51
3:A:725:ASP:OD1	3:A:727:ARG:HG3	2.11	0.51
3:A:408:ASN:ND2	3:A:408:ASN:N	2.57	0.51
3:A:622:ALA:C	3:A:624:ARG:H	2.14	0.51
3:A:259:PHE:CD2	3:A:359:GLY:HA2	2.45	0.51
3:A:746:LYS:O	3:A:750:GLU:HG3	2.10	0.51
3:A:361:PHE:HB2	3:A:420:ILE:CD1	2.40	0.51
3:A:382:ILE:HG22	3:A:383:ILE:N	2.25	0.51
3:A:726:PRO:HG2	3:A:755:ALA:CB	2.40	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:615:LYS:C	3:A:617:LEU:N	2.62	0.51
3:A:510:GLU:HB3	3:A:560:PRO:CB	2.40	0.51
3:A:686:SER:CA	3:A:689:LYS:HE2	2.39	0.51
3:A:722:ASN:H	3:A:722:ASN:HD22	1.58	0.51
3:A:664:ASP:O	3:A:665:LEU:HB3	2.11	0.51
3:A:242:TYR:CZ	3:A:294:ILE:HA	2.46	0.51
2:C:115:DG:H8	2:C:115:DG:H5'	1.75	0.50
3:A:457:ILE:HG12	3:A:580:LEU:HD13	1.92	0.50
3:A:353:PHE:HD2	3:A:353:PHE:H	1.58	0.50
3:A:698:LEU:O	3:A:702:GLU:HG2	2.11	0.50
3:A:726:PRO:O	3:A:730:VAL:HG23	2.11	0.50
3:A:413:LEU:HD23	3:A:413:LEU:N	2.26	0.50
3:A:501:THR:HB	3:A:531:GLY:O	2.12	0.50
3:A:597:THR:O	3:A:600:GLN:HB3	2.12	0.50
3:A:691:VAL:O	3:A:695:GLU:CG	2.60	0.50
3:A:513:ASN:O	3:A:514:LEU:HG	2.11	0.50
3:A:665:LEU:CA	3:A:687:LYS:HD2	2.41	0.50
3:A:703:VAL:C	3:A:705:ALA:N	2.63	0.50
3:A:686:SER:CB	3:A:689:LYS:HE2	2.42	0.50
3:A:727:ARG:HD3	3:A:754:TRP:HZ3	1.77	0.50
3:A:237:ASN:HD22	3:A:237:ASN:C	2.13	0.50
3:A:324:LYS:O	3:A:327:ILE:HG12	2.12	0.50
3:A:624:ARG:CD	3:A:711:ASN:HB2	2.39	0.49
3:A:703:VAL:O	3:A:706:THR:N	2.45	0.49
3:A:733:CYS:SG	3:A:743:ILE:CD1	3.00	0.49
3:A:309:PHE:O	3:A:312:GLN:HB3	2.12	0.49
3:A:663:ARG:C	3:A:664:ASP:O	2.45	0.49
3:A:622:ALA:O	3:A:624:ARG:N	2.45	0.49
1:B:8:DC:H2''	1:B:9:DT:C6	2.48	0.49
3:A:632:HIS:O	3:A:715:ALA:N	2.45	0.49
3:A:621:ARG:HA	3:A:624:ARG:CZ	2.43	0.49
3:A:628:ILE:HG13	3:A:714:ILE:CG2	2.35	0.49
3:A:430:ASN:O	3:A:433:SER:OG	2.23	0.49
3:A:445:GLU:OE1	3:A:448:ARG:HD3	2.12	0.49
3:A:255:GLU:O	3:A:258:THR:HG22	2.12	0.49
3:A:711:ASN:HD21	3:A:716:LEU:HD11	1.77	0.49
2:C:115:DG:P	3:A:493:LYS:HZ3	2.36	0.49
3:A:512:ILE:HD11	3:A:564:LEU:CD2	2.42	0.49
3:A:686:SER:O	3:A:689:LYS:HB2	2.13	0.48
3:A:665:LEU:HA	3:A:687:LYS:CD	2.42	0.48
3:A:431:PRO:HB3	3:A:751:LYS:CG	2.43	0.48
3:A:287:THR:HG23	3:A:290:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:277:ASN:HA	3:A:280:LYS:HZ2	1.77	0.48
3:A:375:ARG:HG3	3:A:419:ASN:ND2	2.28	0.48
2:C:103:DA:H2"	2:C:104:DA:OP2	2.12	0.48
3:A:471:LYS:O	3:A:472:VAL:C	2.47	0.48
3:A:654:LYS:O	3:A:657:GLN:HB2	2.13	0.48
3:A:624:ARG:HD3	3:A:710:GLU:O	2.13	0.48
3:A:622:ALA:C	3:A:624:ARG:N	2.66	0.48
3:A:522:GLU:HG2	3:A:523:TYR:CD1	2.49	0.48
3:A:458:ARG:C	3:A:460:GLN:N	2.66	0.48
3:A:465:TRP:O	3:A:473:ARG:CD	2.61	0.48
3:A:440:ASP:O	3:A:443:LYS:HB3	2.14	0.48
2:C:106:DT:H2'	2:C:107:DT:C7	2.41	0.48
3:A:648:GLN:C	3:A:650:LYS:H	2.17	0.48
3:A:665:LEU:O	3:A:668:ALA:HB3	2.14	0.47
3:A:621:ARG:HA	3:A:624:ARG:NH1	2.29	0.47
3:A:685:GLU:O	3:A:689:LYS:HG3	2.14	0.47
3:A:335:LEU:HD12	3:A:335:LEU:O	2.15	0.47
3:A:310:LYS:O	3:A:313:THR:N	2.47	0.47
3:A:518:LEU:O	3:A:520:GLY:N	2.47	0.47
3:A:274:PHE:CE1	3:A:371:GLY:HA2	2.48	0.47
3:A:658:LEU:HD11	3:A:662:ARG:NH1	2.30	0.47
3:A:654:LYS:CA	3:A:657:GLN:HG3	2.38	0.47
3:A:695:GLU:O	3:A:698:LEU:HB3	2.14	0.47
3:A:509:VAL:HB	3:A:555:MET:HE1	1.96	0.47
3:A:410:VAL:HB	3:A:412:TRP:CD1	2.50	0.47
3:A:241:TYR:CE2	3:A:246:VAL:HG22	2.50	0.47
3:A:686:SER:HA	3:A:689:LYS:CE	2.44	0.47
3:A:527:PHE:O	3:A:538:TYR:HA	2.15	0.47
3:A:663:ARG:O	3:A:664:ASP:HB2	2.15	0.47
3:A:703:VAL:C	3:A:705:ALA:H	2.18	0.47
3:A:533:ASP:O	3:A:534:SER:CB	2.62	0.47
3:A:585:THR:H	3:A:588:VAL:HG23	1.79	0.47
3:A:699:MET:HA	3:A:702:GLU:HG3	1.96	0.47
3:A:720:LYS:HB2	3:A:720:LYS:HE3	1.61	0.47
3:A:682:LYS:HA	3:A:685:GLU:OE1	2.14	0.47
3:A:601:GLN:O	3:A:605:LEU:HD12	2.16	0.46
3:A:297:LEU:HD13	3:A:297:LEU:O	2.15	0.46
3:A:235:PRO:HB2	3:A:237:ASN:HD21	1.78	0.46
3:A:650:LYS:O	3:A:653:ALA:HB3	2.15	0.46
3:A:585:THR:O	3:A:587:LYS:N	2.48	0.46
3:A:723:PHE:CD1	3:A:723:PHE:C	2.88	0.46
3:A:220:LEU:O	3:A:386:CYS:HB2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:632:HIS:CE1	3:A:718:THR:HG1	2.34	0.46
3:A:604:GLU:HB3	3:A:605:LEU:HD12	1.98	0.46
3:A:632:HIS:CE1	3:A:718:THR:OG1	2.68	0.46
3:A:246:VAL:HG12	3:A:247:MET:N	2.30	0.46
3:A:699:MET:CA	3:A:702:GLU:HG2	2.40	0.46
3:A:651:ILE:O	3:A:655:LYS:CB	2.63	0.46
3:A:283:ARG:O	3:A:286:MET:HB2	2.15	0.46
3:A:555:MET:HA	3:A:555:MET:CE	2.44	0.46
3:A:619:TYR:OH	3:A:729:THR:CG2	2.64	0.46
3:A:473:ARG:HH21	3:A:550:ASN:C	2.19	0.45
3:A:621:ARG:HA	3:A:624:ARG:HH22	1.80	0.45
3:A:548:PHE:C	3:A:548:PHE:CD2	2.89	0.45
3:A:434:ARG:O	3:A:434:ARG:CG	2.63	0.45
3:A:615:LYS:O	3:A:617:LEU:N	2.49	0.45
3:A:565:PHE:O	3:A:568:LEU:HB3	2.16	0.45
3:A:429:LEU:HD12	3:A:435:ILE:CG2	2.45	0.45
3:A:644:MET:C	3:A:646:ASN:H	2.20	0.45
3:A:485:LEU:CD1	3:A:541:VAL:HG21	2.47	0.45
3:A:680:THR:C	3:A:682:LYS:H	2.18	0.45
3:A:512:ILE:HD11	3:A:564:LEU:HD22	1.97	0.45
3:A:470:MET:O	3:A:473:ARG:O	2.35	0.45
3:A:600:GLN:O	3:A:601:GLN:C	2.55	0.45
3:A:673:LYS:HB3	3:A:674:VAL:H	1.48	0.45
3:A:665:LEU:CD1	3:A:687:LYS:HB3	2.47	0.45
3:A:369:LYS:O	3:A:370:MET:C	2.55	0.45
3:A:247:MET:CE	3:A:294:ILE:HD11	2.46	0.45
3:A:217:TRP:O	3:A:408:ASN:HB3	2.17	0.45
3:A:457:ILE:HG23	3:A:580:LEU:CD1	2.47	0.45
3:A:385:ASN:HD21	3:A:410:VAL:CG2	2.28	0.45
3:A:667:SER:O	3:A:671:ASP:HB2	2.17	0.45
2:C:113:DA:H2"	2:C:114:DA:H8	1.82	0.45
3:A:545:LYS:HD3	3:A:549:LYS:HZ1	1.81	0.45
3:A:668:ALA:HB2	3:A:687:LYS:HG3	1.98	0.44
3:A:231:TYR:CE1	3:A:255:GLU:HA	2.53	0.44
3:A:514:LEU:CD2	3:A:525:VAL:HG22	2.47	0.44
3:A:677:ASP:CG	3:A:678:ALA:H	2.21	0.44
3:A:378:MET:C	3:A:380:GLU:N	2.71	0.44
3:A:310:LYS:O	3:A:310:LYS:HE3	2.17	0.44
3:A:628:ILE:C	3:A:630:CYS:H	2.21	0.44
3:A:431:PRO:CB	3:A:751:LYS:HG3	2.48	0.44
3:A:732:TRP:O	3:A:736:TRP:CD1	2.65	0.44
3:A:355:ILE:CG2	3:A:356:GLU:N	2.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:669:LYS:HD2	3:A:669:LYS:N	2.32	0.44
3:A:283:ARG:HG3	3:A:286:MET:HE3	1.99	0.44
3:A:523:TYR:O	3:A:542:PRO:HA	2.17	0.44
3:A:378:MET:O	3:A:380:GLU:N	2.50	0.44
3:A:441:TRP:CD2	4:A:1005:HOH:O	2.69	0.44
3:A:687:LYS:HD3	3:A:687:LYS:HA	1.70	0.44
3:A:256:VAL:HG21	3:A:285:GLU:HG3	1.99	0.44
3:A:355:ILE:HG22	3:A:356:GLU:N	2.32	0.44
3:A:597:THR:HA	3:A:600:GLN:HB3	2.00	0.44
3:A:523:TYR:HD2	3:A:548:PHE:CG	2.36	0.44
3:A:446:THR:HG22	3:A:588:VAL:CG1	2.43	0.44
3:A:513:ASN:HB3	3:A:526:GLU:HB3	1.99	0.44
3:A:403:GLU:OE1	3:A:405:ARG:HB3	2.18	0.44
3:A:544:GLU:HB2	3:A:547:VAL:HG23	1.99	0.43
3:A:246:VAL:CG1	3:A:247:MET:N	2.80	0.43
3:A:237:ASN:ND2	3:A:237:ASN:C	2.72	0.43
3:A:433:SER:C	3:A:435:ILE:N	2.70	0.43
3:A:349:ARG:HG3	3:A:430:ASN:HB2	1.99	0.43
3:A:694:LEU:O	3:A:697:GLN:N	2.51	0.43
3:A:722:ASN:ND2	3:A:722:ASN:H	2.17	0.43
3:A:448:ARG:O	3:A:451:LYS:HB3	2.18	0.43
3:A:205:TRP:O	3:A:208:GLU:HB2	2.18	0.43
4:C:1003:HOH:O	3:A:352:ASN:HB2	2.18	0.43
3:A:577:LEU:HB3	3:A:584:LEU:HD23	2.00	0.43
2:C:115:DG:H2"	2:C:116:DT:C6	2.53	0.43
3:A:458:ARG:C	3:A:460:GLN:H	2.22	0.43
1:B:21:DT:H5"	3:A:650:LYS:HE2	2.00	0.43
3:A:625:ALA:HA	3:A:628:ILE:HG22	2.01	0.43
3:A:356:GLU:HA	3:A:357:PRO:HD3	1.93	0.43
3:A:472:VAL:O	3:A:474:GLN:N	2.52	0.43
3:A:597:THR:HG21	3:A:626:VAL:HG22	2.01	0.43
3:A:351:ALA:CB	3:A:428:MET:O	2.66	0.43
3:A:732:TRP:CE3	3:A:733:CYS:HA	2.54	0.43
3:A:628:ILE:C	3:A:630:CYS:N	2.72	0.43
3:A:367:HIS:CE1	3:A:498:THR:HA	2.54	0.42
3:A:518:LEU:O	3:A:519:ASP:C	2.57	0.42
3:A:339:GLY:O	3:A:349:ARG:HD3	2.19	0.42
3:A:736:TRP:N	3:A:736:TRP:CD1	2.88	0.42
2:C:113:DA:H2"	2:C:114:DA:C8	2.53	0.42
3:A:662:ARG:C	3:A:663:ARG:O	2.54	0.42
3:A:451:LYS:HG2	3:A:592:TYR:HE1	1.84	0.42
3:A:621:ARG:O	3:A:624:ARG:CB	2.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:353:PHE:CD2	3:A:353:PHE:N	2.86	0.42
3:A:305:MET:O	3:A:308:TYR:HB3	2.19	0.42
3:A:282:TRP:CZ3	3:A:297:LEU:HD23	2.54	0.42
3:A:427:ILE:HG22	3:A:427:ILE:O	2.17	0.42
3:A:617:LEU:CG	3:A:618:SER:N	2.82	0.42
3:A:532:LYS:O	3:A:533:ASP:HB2	2.19	0.42
3:A:628:ILE:CD1	3:A:714:ILE:HG13	2.50	0.42
3:A:682:LYS:O	3:A:685:GLU:OE1	2.37	0.42
3:A:408:ASN:HB2	3:A:409:LYS:HZ3	1.81	0.42
3:A:629:LEU:C	3:A:629:LEU:HD12	2.40	0.42
3:A:526:GLU:HA	3:A:540:LYS:HA	2.01	0.42
3:A:204:LYS:HG2	3:A:206:TRP:CZ2	2.54	0.42
3:A:602:LEU:C	3:A:604:GLU:N	2.71	0.42
2:C:109:DT:H2"	2:C:110:DT:OP2	2.19	0.42
3:A:229:PRO:HA	3:A:230:PRO:HD3	1.89	0.42
3:A:607:ALA:HA	3:A:608:PRO:HD3	1.92	0.42
3:A:662:ARG:O	3:A:665:LEU:HB3	2.20	0.42
3:A:644:MET:C	3:A:646:ASN:N	2.71	0.42
3:A:204:LYS:HB3	3:A:207:GLU:HG3	2.02	0.42
3:A:282:TRP:HZ3	3:A:297:LEU:HD23	1.84	0.41
3:A:719:SER:HA	3:A:723:PHE:CZ	2.55	0.41
3:A:491:ASN:ND2	3:A:570:THR:HG21	2.35	0.41
3:A:722:ASN:N	3:A:722:ASN:ND2	2.68	0.41
3:A:568:LEU:HA	3:A:572:ILE:CD1	2.48	0.41
3:A:659:ALA:HA	3:A:662:ARG:CB	2.41	0.41
3:A:668:ALA:HB1	3:A:684:VAL:HG13	2.01	0.41
3:A:598:LEU:HD22	3:A:598:LEU:HA	1.95	0.41
3:A:518:LEU:HG	3:A:519:ASP:N	2.35	0.41
3:A:744:TYR:HB3	3:A:748:GLN:HB2	2.01	0.41
3:A:277:ASN:HA	3:A:280:LYS:HZ3	1.86	0.41
3:A:350:ILE:HG21	3:A:353:PHE:HB3	2.03	0.41
3:A:760:ASP:C	3:A:762:ASP:N	2.72	0.41
3:A:443:LYS:HE2	3:A:444:TYR:CZ	2.55	0.41
3:A:369:LYS:HE3	3:A:421:GLN:NE2	2.35	0.41
3:A:730:VAL:HG11	3:A:755:ALA:O	2.21	0.41
3:A:532:LYS:C	3:A:534:SER:N	2.72	0.41
3:A:664:ASP:CG	3:A:687:LYS:HZ1	2.22	0.41
3:A:627:ALA:CB	3:A:716:LEU:HB3	2.40	0.41
3:A:445:GLU:O	3:A:448:ARG:N	2.53	0.41
3:A:256:VAL:HG12	3:A:278:PHE:CE1	2.56	0.41
3:A:488:ARG:HG3	3:A:488:ARG:HH11	1.86	0.41
3:A:621:ARG:O	3:A:624:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:711:ASN:HD21	3:A:716:LEU:CD1	2.34	0.40
3:A:686:SER:HB2	3:A:689:LYS:HE2	2.03	0.40
3:A:745:ASN:OD1	3:A:745:ASN:C	2.59	0.40
3:A:732:TRP:CE3	3:A:733:CYS:N	2.90	0.40
2:C:108:DT:H1'	2:C:109:DT:H5'	2.03	0.40
3:A:228:ALA:HB1	3:A:229:PRO:HD2	2.02	0.40
3:A:377:ILE:HG23	3:A:381:ASP:HB2	2.04	0.40
3:A:240:PHE:CG	3:A:241:TYR:N	2.89	0.40
3:A:612:ILE:HD13	3:A:612:ILE:HA	1.99	0.40
2:C:119:DT:H2'	2:C:120:DT:H72	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	553/564 (98%)	412 (74%)	110 (20%)	31 (6%)	3 22

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	386	CYS
3	A	473	ARG
3	A	519	ASP
3	A	673	LYS
3	A	723	PHE
3	A	427	ILE
3	A	472	VAL
3	A	474	GLN
3	A	586	ALA
3	A	601	GLN
3	A	609	ASP
3	A	617	LEU
3	A	678	ALA

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Mol	Chain	Res	Type
3	A	697	GLN
3	A	318	GLN
3	A	344	ASP
3	A	489	ALA
3	A	539	ASN
3	A	603	LYS
3	A	623	ASN
3	A	681	LYS
3	A	704	GLN
3	A	366	ASN
3	A	534	SER
3	A	672	ALA
3	A	712	LYS
3	A	720	LYS
3	A	227	PHE
3	A	324	LYS
3	A	251	PRO
3	A	471	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	457/508 (90%)	418 (92%)	39 (8%)	15	54

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	211	TYR
3	A	232	GLU
3	A	237	ASN
3	A	258	THR
3	A	265	ASP
3	A	283	ARG
3	A	288	ASN
3	A	307	GLN
3	A	310	LYS
3	A	330	GLU

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Mol	Chain	Res	Type
3	A	341	CYS
3	A	408	ASN
3	A	421	GLN
3	A	434	ARG
3	A	439	LYS
3	A	454	VAL
3	A	461	TYR
3	A	464	ASP
3	A	479	LEU
3	A	554	PHE
3	A	555	MET
3	A	563	ASP
3	A	588	VAL
3	A	598	LEU
3	A	601	GLN
3	A	619	TYR
3	A	623	ASN
3	A	631	ASN
3	A	652	ASP
3	A	662	ARG
3	A	671	ASP
3	A	685	GLU
3	A	693	ARG
3	A	699	MET
3	A	716	LEU
3	A	722	ASN
3	A	723	PHE
3	A	761	GLU
3	A	762	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	237	ASN
3	A	288	ASN
3	A	307	GLN
3	A	346	HIS
3	A	367	HIS
3	A	385	ASN
3	A	399	HIS
3	A	406	HIS
3	A	408	ASN

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Mol	Chain	Res	Type
3	A	421	GLN
3	A	474	GLN
3	A	511	HIS
3	A	599	GLN
3	A	601	GLN
3	A	632	HIS
3	A	697	GLN
3	A	722	ASN
3	A	748	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	8OG	B	11	1,2	23,25,26	0.83	1 (4%)	27,37,40	1.91	5 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	8OG	B	11	1,2	-	0/6/21/22	0/1/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	8OG	P-OP1	2.79	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	11	8OG	C4-C5-N7	5.78	110.97	106.14
1	B	11	8OG	C8-N9-C1'	4.80	127.83	125.17
1	B	11	8OG	C8-N7-C5	-3.73	103.70	107.48
1	B	11	8OG	C6-N1-C2	3.13	124.98	119.51
1	B	11	8OG	C2-N3-C4	-2.38	111.74	115.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.