



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:13 PM UTC

PDB ID : 1EA9 / pdb_00001ea9
Title : Cyclomaltodextrinase
Authors : Cho, H.-S.; Kim, M.-S.; Oh, B.-H.
Deposited on : 2001-07-12
Resolution : 3.20 Å(reported)

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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:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

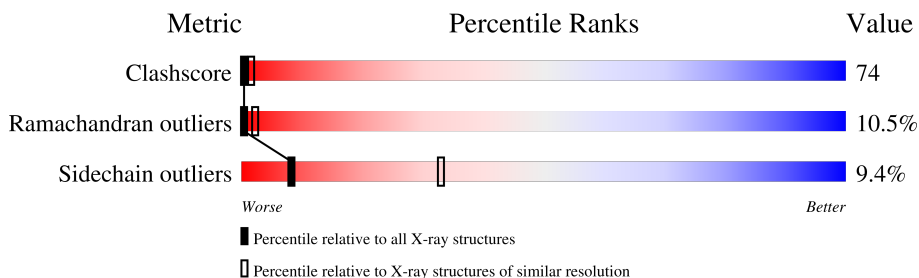
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	583	 18% 66% 14% •
1	D	583	 17% 64% 18% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9582 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CYCLOMALTODEXTRINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	583	4791	3092	804	876	19	0	0	0
1	D	583	4791	3092	804	876	19	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

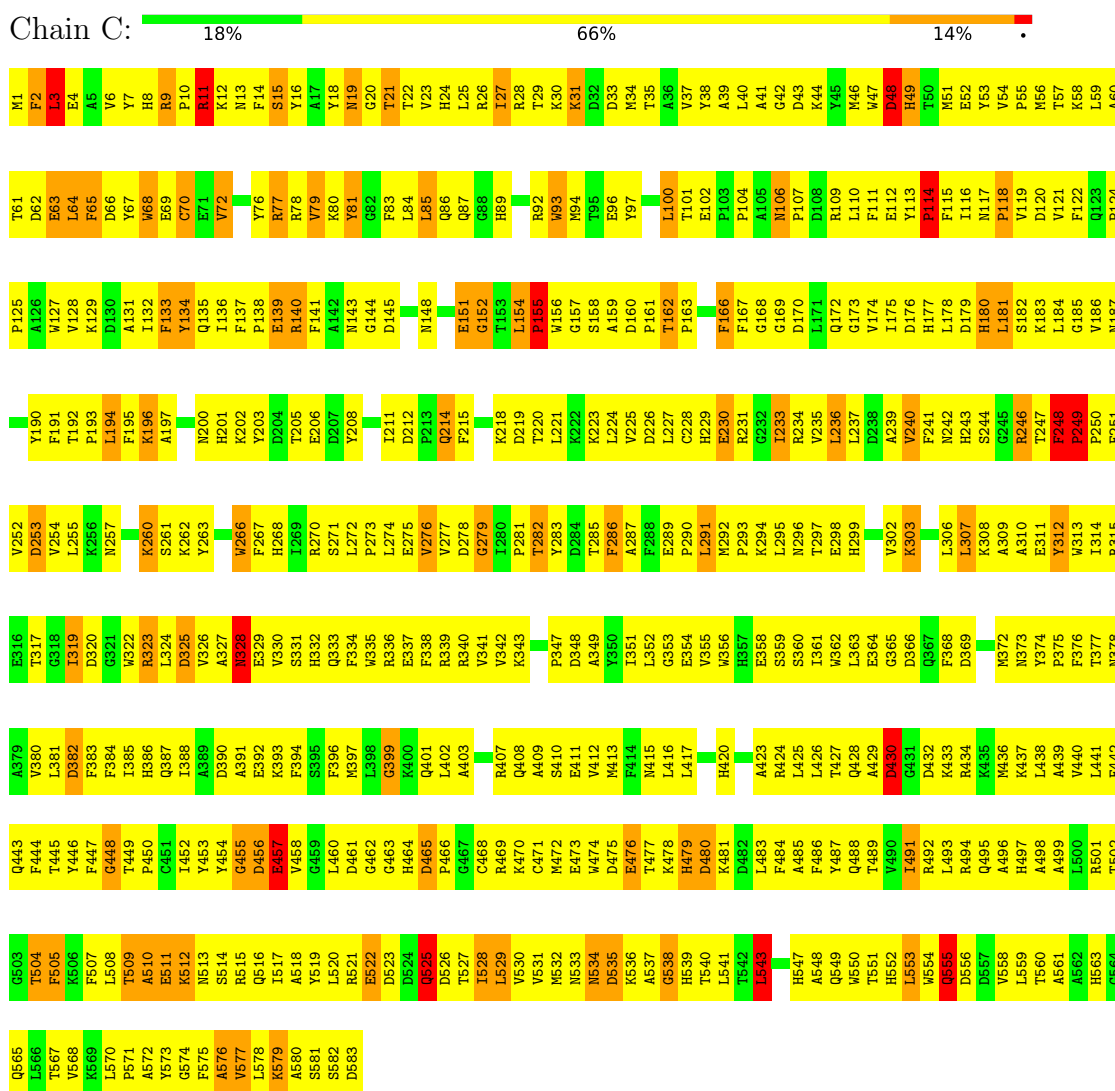
Chain	Residue	Modelled	Actual	Comment	Reference
C	14	PHE	TRP	conflict	UNP Q59226
C	105	ALA	ARG	conflict	UNP Q59226
D	14	PHE	TRP	conflict	UNP Q59226
D	105	ALA	ARG	conflict	UNP Q59226

3 Residue-property plots

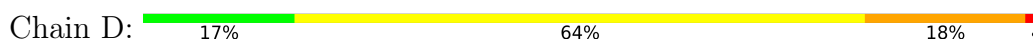
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: CYCLOMALTODEXTRINASE



- Molecule 1: CYCLOMALTODEXTRINASE



H563	H564	Q565	L566	T567	Y568	K569	L570	P571	A572	Y573	G574	F575	A576	V577	L578	K579	A580	S581	S582	D583
I590	R501	T502	G503	T504	F505	L506	L508	T509	A510	E511	K512	L513	S514	R515	Q516	A517	A518	L519	L520	E522
Q525	R526	T527	L528	L529	V530	M532	M533	M534	D535	K536	A537	G538	R539	T540	L541	L542	H543	H544	H545	H546
R434	K435	M436	K437	L438	A439	V440	L441	F442	Q443	F444	T445	Y446	F447	G448	T449	P450	C451	Y452	Y453	Y454
D455	D456	F457	C458	L459	L460	R469	K470	C471	M472	E473	W474	D475	E476	T477	K478	H479	D480	K481	D482	L483
Q649	A650	T651	L652	L653	W654	Q655	D656	D657	V658	L659	T660	A661	A662	Q663	L664	H665	F666	Y667	Y668	Y669
R670	F671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690
L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711
L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732
L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753
L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774
L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795
L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816
L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837
L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858
L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879
L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900
L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921
L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942
L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963
L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984
L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005
L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026
L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047
L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068
L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089
L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110
L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131
L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152
L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173
L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194
L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215
L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236
L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257
L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278
L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299
L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320
L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341
L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362
L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383
L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404
L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425
L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446
L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467
L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488
L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509
L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530
L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551
L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572
L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593
L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614
L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635
L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656
L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677
L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698
L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719
L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740
L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761
L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782
L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803
L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824
L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845
L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866
L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887
L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908
L1909	L1910	L1911	L1912	L1913	L1914	L191														

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	334.61Å 334.61Å 334.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	83.4 (10.00-3.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9582	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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	C	0.38	0/4940	0.94	24/6714 (0.4%)
1	D	0.37	0/4940	0.93	29/6714 (0.4%)
All	All	0.37	0/9880	0.94	53/13428 (0.4%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	VAL	N-CA-C	7.80	118.96	108.27
1	D	376	PHE	N-CA-C	-7.75	102.38	112.68
1	D	393	LYS	N-CA-C	-7.25	103.38	111.28
1	C	323	ARG	N-CA-C	-6.67	98.81	109.76
1	C	151	GLU	N-CA-C	6.58	119.02	110.53
1	D	554	TRP	N-CA-C	-6.56	102.07	110.53
1	C	369	ASP	N-CA-C	-6.39	105.37	113.43
1	C	457	GLU	N-CA-C	-6.38	104.37	111.71
1	C	166	PHE	N-CA-C	6.37	118.54	108.79
1	C	68	TRP	N-CA-C	6.34	119.48	108.76
1	C	388	ILE	N-CA-C	-6.29	107.36	113.53
1	D	289	GLU	CA-C-N	6.26	125.75	119.24
1	D	289	GLU	C-N-CA	6.26	125.75	119.24
1	D	288	PHE	N-CA-C	-6.19	103.29	113.50
1	D	543	LEU	CA-C-N	5.98	125.92	119.76
1	D	543	LEU	C-N-CA	5.98	125.92	119.76
1	C	3	LEU	N-CA-C	5.97	117.78	111.28
1	C	133	PHE	N-CA-C	5.90	118.63	109.60
1	D	399	GLY	N-CA-C	-5.89	107.03	114.16
1	C	522	GLU	N-CA-C	5.89	117.43	108.07
1	D	419	SER	N-CA-C	5.86	115.58	107.73
1	D	427	THR	N-CA-C	-5.85	104.90	112.68
1	D	81	TYR	N-CA-C	5.82	117.39	108.42
1	D	298	GLU	N-CA-C	-5.79	106.00	114.39
1	D	79	VAL	N-CA-C	5.75	115.82	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	PRO	N-CA-C	5.74	117.70	110.70
1	D	113	TYR	CA-C-N	5.66	126.91	119.84
1	D	113	TYR	C-N-CA	5.66	126.91	119.84
1	C	248	PHE	CA-C-N	5.55	126.10	120.38
1	C	248	PHE	C-N-CA	5.55	126.10	120.38
1	C	65	PHE	N-CA-C	5.51	117.64	108.99
1	C	448	GLY	N-CA-C	-5.46	103.95	111.76
1	C	543	LEU	CA-C-N	5.46	125.66	120.31
1	C	543	LEU	C-N-CA	5.46	125.66	120.31
1	D	3	LEU	N-CA-C	-5.38	106.72	113.28
1	D	287	ALA	N-CA-C	-5.36	99.39	110.80
1	D	136	ILE	N-CA-C	5.35	116.29	108.53
1	C	181	LEU	N-CA-C	-5.34	105.57	111.71
1	C	230	GLU	N-CA-C	-5.34	106.45	113.12
1	D	445	THR	N-CA-C	-5.33	105.47	111.28
1	D	113	TYR	N-CA-C	-5.28	99.65	108.94
1	C	536	LYS	N-CA-C	-5.28	106.54	112.87
1	D	154	LEU	CA-C-N	5.26	126.42	119.84
1	D	154	LEU	C-N-CA	5.26	126.42	119.84
1	D	452	ILE	N-CA-C	5.25	115.14	107.37
1	D	80	LYS	N-CA-C	-5.22	102.33	110.42
1	D	94	MET	N-CA-C	5.17	117.88	109.24
1	D	137	PHE	CA-C-N	5.11	126.22	119.84
1	D	137	PHE	C-N-CA	5.11	126.22	119.84
1	C	81	TYR	N-CA-C	5.06	115.21	108.38
1	C	89	HIS	N-CA-C	-5.05	105.83	112.94
1	D	229	HIS	N-CA-C	-5.02	105.26	111.33
1	C	72	VAL	N-CA-C	5.00	115.11	108.11

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	C	4791	0	4588	679	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4791	0	4588	715	0
All	All	9582	0	9176	1392	1

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 74.

All (1392) 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:C:128:VAL:HG21	1:C:412:VAL:HG13	1.27	1.10
1:D:326:VAL:H	1:D:354:GLU:HB3	1.22	1.03
1:C:132:ILE:H	1:C:187:ASN:HB2	1.22	1.03
1:C:19:ASN:HD21	1:C:22:THR:N	1.56	1.02
1:C:19:ASN:ND2	1:C:22:THR:H	1.58	1.00
1:D:175:ILE:HA	1:D:178:LEU:HD13	1.42	1.00
1:D:552:HIS:HB3	1:D:580:ALA:HB1	1.40	1.00
1:C:551:THR:HG22	1:C:552:HIS:H	1.20	1.00
1:C:157:GLY:HA3	1:C:161:PRO:HB3	1.43	1.00
1:C:37:VAL:HG12	1:C:85:LEU:HA	1.44	0.99
1:C:154:LEU:HB3	1:C:155:PRO:HD2	1.41	0.99
1:D:553:LEU:HD11	1:D:583:ASP:HB2	1.46	0.97
1:D:452:ILE:HG23	1:D:456:ASP:HB2	1.47	0.96
1:D:342:VAL:HG21	1:D:351:ILE:HD11	1.47	0.96
1:C:184:LEU:HD12	1:C:186:VAL:HG23	1.49	0.95
1:C:323:ARG:HH21	1:C:325:ASP:HA	1.30	0.95
1:D:171:LEU:HB2	1:D:215:PHE:HB3	1.45	0.95
1:C:6:VAL:HG22	1:C:29:THR:HG22	1.46	0.95
1:D:387:GLN:HE21	1:D:534:ASN:HD22	1.10	0.94
1:D:272:LEU:HD23	1:D:272:LEU:H	1.33	0.94
1:D:306:LEU:HD12	1:D:306:LEU:H	1.30	0.93
1:D:249:PRO:HG2	1:D:250:PRO:HD3	1.51	0.93
1:D:86:GLN:HG3	1:D:91:LYS:HB3	1.51	0.93
1:C:276:VAL:HG22	1:C:281:PRO:HA	1.51	0.92
1:C:424:ARG:NH1	1:C:460:LEU:HB2	1.83	0.92
1:D:25:LEU:HB2	1:D:70:CYS:HB3	1.51	0.92
1:D:307:LEU:HD22	1:D:341:VAL:HG21	1.49	0.92
1:D:442:PHE:HB2	1:D:532:MET:HE1	1.52	0.92
1:C:272:LEU:HB2	1:C:273:PRO:HD3	1.53	0.91
1:C:3:LEU:HD12	1:C:3:LEU:H	1.34	0.91
1:D:384:PHE:HA	1:D:534:ASN:HD21	1.34	0.90
1:C:249:PRO:HB2	1:C:250:PRO:HD3	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ASP:HA	1:C:51:MET:HE2	1.53	0.89
1:D:374:TYR:N	1:D:375:PRO:HD2	1.88	0.88
1:D:272:LEU:HG	1:D:273:PRO:HD3	1.55	0.88
1:C:423:ALA:HA	1:C:463:GLY:O	1.73	0.88
1:D:363:LEU:HD21	1:D:371:VAL:HG13	1.56	0.87
1:C:473:GLU:HG3	1:C:478:LYS:HG2	1.57	0.86
1:D:1:MET:HB2	1:D:92:ARG:NH2	1.89	0.86
1:D:58:LYS:HA	1:D:68:TRP:HA	1.55	0.86
1:C:355:VAL:HG11	1:C:359:SER:HB3	1.57	0.86
1:C:408:GLN:HG2	1:C:409:ALA:H	1.42	0.85
1:C:154:LEU:HB3	1:C:155:PRO:CD	2.06	0.85
1:D:275:GLU:H	1:D:282:THR:HG21	1.39	0.84
1:D:452:ILE:HG13	1:D:487:TYR:HE2	1.42	0.83
1:D:494:ARG:NH1	1:D:501:ARG:HG2	1.93	0.83
1:C:253:ASP:O	1:C:257:ASN:HB2	1.78	0.83
1:D:132:ILE:HG22	1:D:186:VAL:HG13	1.59	0.83
1:D:491:ILE:HG22	1:D:495:GLN:HE21	1.43	0.83
1:C:528:ILE:HA	1:C:581:SER:HA	1.61	0.82
1:D:80:LYS:HD2	1:D:112:GLU:HB2	1.59	0.82
1:D:377:THR:HG22	1:D:381:LEU:HD11	1.62	0.82
1:C:299:HIS:HD2	1:C:302:VAL:H	1.27	0.82
1:C:129:LYS:HD2	1:C:502:THR:HG21	1.63	0.81
1:C:162:THR:OG1	1:C:470:LYS:HA	1.80	0.81
1:C:100:LEU:HD22	1:C:102:GLU:H	1.45	0.81
1:D:47:TRP:CD1	1:D:107:PRO:HD3	2.15	0.81
1:C:563:HIS:HA	1:C:568:VAL:HG22	1.63	0.81
1:D:511:GLU:HB2	1:D:514:SER:HB3	1.61	0.81
1:D:551:THR:O	1:D:582:SER:HA	1.80	0.80
1:C:507:PHE:CE1	1:C:517:ILE:HD11	2.15	0.80
1:C:465:ASP:CG	1:C:466:PRO:HD3	2.07	0.79
1:D:324:LEU:HB2	1:D:327:ALA:HB2	1.64	0.79
1:D:234:ARG:HG2	1:D:234:ARG:HH11	1.46	0.79
1:D:48:ASP:O	1:D:51:MET:HG2	1.83	0.79
1:D:373:ASN:HD21	1:D:376:PHE:HB2	1.46	0.79
1:C:339:ARG:HG3	1:C:351:ILE:HD12	1.62	0.79
1:C:354:GLU:HA	1:C:372:MET:HG2	1.64	0.79
1:D:134:TYR:HB2	1:D:186:VAL:HG11	1.62	0.79
1:D:435:LYS:HG2	1:D:575:PHE:HE2	1.48	0.78
1:C:69:GLU:HG2	1:C:70:CYS:H	1.48	0.78
1:C:239:ALA:HB2	1:C:322:TRP:HE3	1.48	0.78
1:D:455:GLY:O	1:D:458:VAL:HG22	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:ASP:HB2	1:C:525:GLN:OE1	1.84	0.78
1:C:447:PHE:HB3	1:C:521:ARG:HH22	1.49	0.78
1:C:429:ALA:O	1:C:430:ASP:HB2	1.84	0.77
1:D:555:GLN:C	1:D:557:ASP:H	1.92	0.77
1:D:416:LEU:H	1:D:416:LEU:HD23	1.49	0.77
1:C:177:HIS:O	1:C:180:HIS:HB3	1.84	0.77
1:C:253:ASP:OD1	1:C:261:SER:HB3	1.84	0.77
1:D:236:LEU:C	1:D:237:LEU:HD12	2.09	0.77
1:D:408:GLN:HA	1:D:411:GLU:CD	2.10	0.77
1:D:424:ARG:CZ	1:D:460:LEU:HD12	2.15	0.77
1:C:59:LEU:HD12	1:C:60:ALA:N	2.00	0.77
1:C:559:LEU:HD23	1:C:560:THR:N	1.99	0.76
1:C:131:ALA:C	1:C:132:ILE:HD12	2.11	0.76
1:C:342:VAL:HG21	1:C:351:ILE:HD11	1.65	0.76
1:C:192:THR:HB	1:C:193:PRO:HD2	1.67	0.76
1:C:218:LYS:HG3	1:C:219:ASP:H	1.50	0.76
1:C:271:SER:HB3	1:C:282:THR:OG1	1.85	0.76
1:D:370:ALA:HB2	1:D:412:VAL:HG12	1.69	0.75
1:D:550:TRP:HB2	1:D:583:ASP:C	2.11	0.75
1:C:132:ILE:HD13	1:C:495:GLN:HE21	1.52	0.75
1:C:235:VAL:H	1:C:320:ASP:HB2	1.50	0.75
1:D:289:GLU:HG2	1:D:292:MET:HE3	1.68	0.75
1:D:366:ASP:O	1:D:367:GLN:HG3	1.86	0.75
1:C:132:ILE:HD13	1:C:495:GLN:NE2	2.01	0.75
1:D:406:PRO:HG2	1:D:409:ALA:HB2	1.69	0.75
1:D:43:ASP:H	1:D:50:THR:HG21	1.50	0.75
1:D:187:ASN:O	1:D:233:ILE:HG23	1.87	0.75
1:D:244:SER:HB3	1:D:295:LEU:HD21	1.69	0.75
1:D:425:LEU:HB3	1:D:436:MET:HE2	1.67	0.75
1:C:122:PHE:CD1	1:C:124:PRO:HD3	2.22	0.74
1:D:323:ARG:HD2	1:D:324:LEU:N	2.02	0.74
1:C:132:ILE:H	1:C:187:ASN:CB	2.00	0.74
1:C:324:LEU:HB2	1:C:353:GLY:HA2	1.70	0.74
1:C:412:VAL:HG12	1:C:412:VAL:O	1.88	0.74
1:C:185:GLY:O	1:C:491:ILE:HG21	1.88	0.74
1:D:382:ASP:HA	1:D:386:HIS:HB2	1.70	0.74
1:C:31:LYS:HG3	1:C:64:LEU:HA	1.70	0.73
1:D:257:ASN:HB2	1:D:261:SER:HB2	1.69	0.73
1:C:537:ALA:C	1:C:574:GLY:HA2	2.13	0.73
1:C:178:LEU:HD23	1:C:227:LEU:HD23	1.70	0.73
1:C:497:HIS:O	1:C:501:ARG:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:ILE:HG13	1:D:487:TYR:CE2	2.24	0.73
1:C:424:ARG:HH12	1:C:460:LEU:HD12	1.54	0.73
1:D:328:ASN:HD22	1:D:329:GLU:H	1.33	0.73
1:C:416:LEU:HD23	1:C:416:LEU:H	1.52	0.73
1:D:384:PHE:HD2	1:D:438:LEU:HD13	1.53	0.73
1:D:397:MET:O	1:D:401:GLN:HG2	1.88	0.73
1:C:576:ALA:C	1:C:578:LEU:H	1.94	0.73
1:D:435:LYS:HG2	1:D:575:PHE:CE2	2.24	0.73
1:D:551:THR:HG21	1:D:562:ALA:HA	1.71	0.73
1:D:511:GLU:HB2	1:D:514:SER:CB	2.19	0.72
1:C:373:ASN:ND2	1:C:415:ASN:HD21	1.87	0.72
1:D:494:ARG:CZ	1:D:501:ARG:HG2	2.18	0.72
1:D:85:LEU:O	1:D:86:GLN:HB2	1.88	0.72
1:C:8:HIS:HB2	1:C:27:ILE:HD11	1.70	0.72
1:C:56:MET:HB3	1:C:68:TRP:HB3	1.70	0.72
1:C:239:ALA:HB2	1:C:322:TRP:CE3	2.24	0.72
1:C:159:ALA:C	1:C:161:PRO:HD3	2.14	0.72
1:C:373:ASN:HD22	1:C:413:MET:HB3	1.54	0.72
1:D:43:ASP:H	1:D:50:THR:CG2	2.01	0.72
1:D:6:VAL:CG1	1:D:27:ILE:HD11	2.20	0.72
1:C:507:PHE:C	1:C:508:LEU:HD12	2.15	0.71
1:C:19:ASN:C	1:C:19:ASN:HD22	1.97	0.71
1:C:76:TYR:O	1:C:78:ARG:HG2	1.91	0.71
1:D:384:PHE:HA	1:D:534:ASN:ND2	2.03	0.71
1:D:374:TYR:H	1:D:375:PRO:HD2	1.55	0.71
1:C:520:LEU:HD22	1:C:528:ILE:O	1.91	0.71
1:C:28:ARG:HA	1:C:66:ASP:O	1.91	0.71
1:D:280:ILE:HG23	1:D:288:PHE:HD2	1.56	0.71
1:D:323:ARG:HD2	1:D:323:ARG:C	2.16	0.71
1:C:517:ILE:HD12	1:C:518:ALA:H	1.54	0.70
1:D:211:ILE:HG13	1:D:313:TRP:HH2	1.56	0.70
1:D:407:ARG:O	1:D:411:GLU:HG3	1.92	0.70
1:D:112:GLU:HG2	1:D:114:PRO:N	2.07	0.70
1:C:463:GLY:H	1:C:468:CYS:N	1.89	0.70
1:C:8:HIS:HB2	1:C:27:ILE:CD1	2.21	0.70
1:C:551:THR:HG22	1:C:552:HIS:N	2.01	0.70
1:D:59:LEU:HD13	1:D:69:GLU:HG3	1.72	0.70
1:D:374:TYR:CE1	1:D:416:LEU:HD11	2.27	0.70
1:D:508:LEU:HD13	1:D:519:TYR:HA	1.72	0.70
1:C:427:THR:HG22	1:C:461:ASP:CG	2.17	0.70
1:C:37:VAL:HG23	1:C:56:MET:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HD22	1:C:86:GLN:HB2	1.74	0.69
1:D:269:ILE:HG22	1:D:271:SER:H	1.57	0.69
1:D:374:TYR:C	1:D:376:PHE:H	2.00	0.69
1:D:342:VAL:HG23	1:D:343:LYS:N	2.07	0.69
1:C:19:ASN:HD21	1:C:22:THR:H	0.79	0.69
1:C:138:PRO:HG3	1:C:191:PHE:HD2	1.58	0.69
1:D:102:GLU:HG3	1:D:103:PRO:HD2	1.75	0.69
1:D:377:THR:HG23	1:D:417:LEU:HA	1.74	0.69
1:D:135:GLN:O	1:D:454:TYR:HB3	1.93	0.69
1:C:276:VAL:CG2	1:C:281:PRO:HA	2.23	0.69
1:D:63:GLU:HB3	1:D:64:LEU:HD23	1.74	0.69
1:D:536:LYS:HA	1:D:575:PHE:CE1	2.27	0.69
1:C:579:LYS:O	1:C:579:LYS:HD3	1.92	0.69
1:D:565:GLN:O	1:D:566:LEU:HG	1.92	0.69
1:C:274:LEU:HA	1:C:282:THR:HG21	1.75	0.68
1:D:491:ILE:CG2	1:D:495:GLN:HE21	2.05	0.68
1:C:122:PHE:HD1	1:C:124:PRO:HD3	1.59	0.68
1:C:520:LEU:HD13	1:C:521:ARG:N	2.08	0.68
1:D:528:ILE:HD13	1:D:528:ILE:C	2.17	0.68
1:C:565:GLN:C	1:C:567:THR:H	2.02	0.68
1:C:579:LYS:HZ2	1:C:579:LYS:C	2.01	0.68
1:D:374:TYR:N	1:D:375:PRO:CD	2.55	0.68
1:C:579:LYS:HZ2	1:C:580:ALA:N	1.91	0.68
1:D:140:ARG:O	1:D:471:CYS:HA	1.93	0.68
1:C:427:THR:HG21	1:C:462:GLY:O	1.93	0.68
1:C:342:VAL:CG2	1:C:351:ILE:HD11	2.24	0.67
1:D:328:ASN:HD22	1:D:329:GLU:N	1.93	0.67
1:D:310:ALA:O	1:D:314:ILE:HG12	1.94	0.67
1:D:519:TYR:CE1	1:D:530:VAL:HB	2.29	0.67
1:C:3:LEU:HD13	1:C:4:GLU:OE1	1.94	0.67
1:C:529:LEU:N	1:C:529:LEU:HD23	2.10	0.67
1:D:324:LEU:HD13	1:D:335:TRP:CH2	2.29	0.67
1:D:406:PRO:O	1:D:409:ALA:HB3	1.93	0.67
1:C:218:LYS:HG3	1:C:219:ASP:N	2.07	0.67
1:C:4:GLU:CD	1:C:4:GLU:H	2.03	0.67
1:D:38:TYR:CD2	1:D:55:PRO:HA	2.30	0.67
1:D:271:SER:HB3	1:D:282:THR:OG1	1.94	0.67
1:D:106:ASN:HB2	1:D:107:PRO:HD2	1.75	0.67
1:D:381:LEU:O	1:D:385:ILE:N	2.26	0.67
1:D:426:LEU:HD21	1:D:433:LYS:HD2	1.75	0.67
1:C:24:HIS:C	1:C:25:LEU:HD22	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:LEU:N	1:C:436:MET:HE3	2.09	0.67
1:D:19:ASN:C	1:D:19:ASN:HD22	2.02	0.67
1:D:551:THR:HA	1:D:563:HIS:CD2	2.29	0.67
1:C:60:ALA:HB2	1:C:402:LEU:HD23	1.76	0.67
1:C:374:TYR:N	1:C:375:PRO:HD2	2.10	0.67
1:D:442:PHE:CB	1:D:532:MET:HE1	2.24	0.67
1:D:128:VAL:O	1:D:449:THR:HG22	1.95	0.66
1:C:397:MET:O	1:C:401:GLN:HG2	1.96	0.66
1:D:48:ASP:HA	1:D:51:MET:SD	2.34	0.66
1:C:3:LEU:HD12	1:C:3:LEU:N	2.08	0.66
1:C:1:MET:HE2	1:C:87:GLN:CB	2.26	0.66
1:C:131:ALA:O	1:C:132:ILE:HD12	1.95	0.66
1:C:156:TRP:HZ2	1:C:163:PRO:HD3	1.59	0.66
1:C:442:PHE:HD1	1:C:532:MET:HE1	1.60	0.66
1:C:507:PHE:HE1	1:C:517:ILE:HD11	1.59	0.66
1:D:460:LEU:HB3	1:D:470:LYS:HD2	1.77	0.66
1:C:424:ARG:HH11	1:C:460:LEU:HB2	1.61	0.66
1:D:540:THR:HA	1:D:570:LEU:O	1.96	0.66
1:C:533:ASN:O	1:C:575:PHE:HA	1.95	0.66
1:D:246:ARG:HG3	1:D:251:PHE:HE2	1.59	0.66
1:D:195:PHE:HA	1:D:211:ILE:HA	1.77	0.66
1:D:550:TRP:HB2	1:D:583:ASP:OXT	1.96	0.66
1:C:127:TRP:CZ3	1:C:234:ARG:HG3	2.31	0.66
1:D:56:MET:SD	1:D:70:CYS:HB2	2.36	0.66
1:D:303:LYS:HD3	1:D:337:GLU:OE1	1.95	0.66
1:D:551:THR:HA	1:D:563:HIS:NE2	2.11	0.66
1:C:444:PHE:CE1	1:C:452:ILE:HD11	2.30	0.65
1:D:3:LEU:HD12	1:D:3:LEU:H	1.61	0.65
1:D:488:GLN:O	1:D:492:ARG:HG2	1.95	0.65
1:D:175:ILE:CA	1:D:178:LEU:HD13	2.23	0.65
1:D:424:ARG:HB2	1:D:427:THR:CG2	2.27	0.65
1:D:180:HIS:HA	1:D:183:LYS:HD3	1.79	0.65
1:D:452:ILE:CG2	1:D:456:ASP:HB2	2.25	0.65
1:D:508:LEU:HD11	1:D:520:LEU:HB2	1.78	0.65
1:D:218:LYS:HZ1	1:D:316:GLU:CD	2.05	0.65
1:D:536:LYS:HA	1:D:575:PHE:HE1	1.61	0.65
1:C:308:LYS:HA	1:C:311:GLU:CD	2.21	0.65
1:D:337:GLU:O	1:D:341:VAL:HG23	1.97	0.65
1:C:119:VAL:HG13	1:C:120:ASP:H	1.61	0.65
1:C:128:VAL:HG21	1:C:412:VAL:CG1	2.15	0.65
1:D:56:MET:HE1	1:D:83:PHE:CD1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ALA:HB1	1:D:236:LEU:HD11	1.78	0.65
1:D:555:GLN:C	1:D:557:ASP:N	2.55	0.65
1:D:171:LEU:HB2	1:D:215:PHE:CB	2.25	0.65
1:D:198:THR:O	1:D:199:THR:HG23	1.97	0.65
1:D:387:GLN:HE21	1:D:534:ASN:ND2	1.90	0.65
1:D:543:LEU:H	1:D:543:LEU:HD23	1.62	0.65
1:C:48:ASP:HA	1:C:51:MET:CE	2.27	0.65
1:C:424:ARG:HE	1:C:453:TYR:HE2	1.44	0.65
1:D:452:ILE:HG23	1:D:456:ASP:CB	2.24	0.65
1:C:254:VAL:HA	1:C:261:SER:OG	1.98	0.64
1:C:515:ARG:HB3	1:C:534:ASN:HB2	1.79	0.64
1:C:13:ASN:O	1:C:26:ARG:HG3	1.97	0.64
1:C:333:GLN:HE21	1:C:337:GLU:HG3	1.62	0.64
1:C:476:GLU:O	1:C:479:HIS:HB2	1.96	0.64
1:C:488:GLN:HA	1:C:491:ILE:HD12	1.79	0.64
1:D:46:MET:HG3	1:D:50:THR:OG1	1.98	0.64
1:D:84:LEU:HD23	1:D:84:LEU:O	1.97	0.64
1:D:362:TRP:HB3	1:D:368:PHE:CE2	2.32	0.64
1:C:100:LEU:HD23	1:C:101:THR:H	1.62	0.64
1:C:282:THR:HG23	1:C:283:TYR:HD1	1.61	0.64
1:D:234:ARG:HG2	1:D:234:ARG:NH1	2.13	0.64
1:D:179:ASP:O	1:D:183:LYS:HG3	1.98	0.64
1:C:139:GLU:O	1:C:169:GLY:HA3	1.97	0.64
1:C:246:ARG:HB2	1:C:291:LEU:HA	1.80	0.64
1:C:519:TYR:CE1	1:C:530:VAL:HB	2.33	0.64
1:D:24:HIS:C	1:D:25:LEU:HD22	2.21	0.64
1:D:350:TYR:HE1	1:D:412:VAL:CG1	2.09	0.64
1:C:93:TRP:CD1	1:C:100:LEU:HB3	2.32	0.64
1:C:143:ASN:OD1	1:C:148:ASN:ND2	2.30	0.64
1:D:424:ARG:HB2	1:D:427:THR:HG23	1.79	0.64
1:C:458:VAL:HG23	1:C:479:HIS:HA	1.78	0.64
1:C:180:HIS:ND1	1:C:181:LEU:HD23	2.13	0.64
1:C:1:MET:HE2	1:C:87:GLN:HB2	1.80	0.63
1:D:398:LEU:HD21	1:D:446:TYR:OH	1.98	0.63
1:D:426:LEU:HD11	1:D:431:GLY:O	1.98	0.63
1:C:507:PHE:CD1	1:C:517:ILE:HD11	2.33	0.63
1:D:196:LYS:HB2	1:D:207:ASP:HB3	1.79	0.63
1:D:212:ASP:OD1	1:D:214:GLN:HG3	1.98	0.63
1:C:122:PHE:HB3	1:C:408:GLN:HE21	1.63	0.63
1:C:450:PRO:HD3	1:C:494:ARG:HH12	1.63	0.63
1:D:504:THR:O	1:D:521:ARG:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:PRO:HD2	1:C:192:THR:OG1	1.99	0.63
1:D:194:LEU:HD23	1:D:194:LEU:H	1.63	0.63
1:C:39:ALA:HB3	1:C:54:VAL:HB	1.80	0.63
1:C:119:VAL:HG13	1:C:120:ASP:OD1	1.98	0.63
1:C:373:ASN:OD1	1:C:375:PRO:HG2	1.99	0.63
1:D:528:ILE:HG12	1:D:580:ALA:O	1.98	0.63
1:C:354:GLU:HA	1:C:372:MET:CG	2.28	0.63
1:D:46:MET:HG3	1:D:46:MET:O	1.99	0.62
1:D:160:ASP:C	1:D:162:THR:H	2.07	0.62
1:D:553:LEU:H	1:D:581:SER:H	1.46	0.62
1:D:152:GLY:HA3	1:D:167:PHE:O	1.99	0.62
1:D:224:LEU:C	1:D:224:LEU:HD23	2.24	0.62
1:D:249:PRO:CG	1:D:250:PRO:HD3	2.28	0.62
1:D:246:ARG:HG3	1:D:251:PHE:CE2	2.34	0.62
1:D:306:LEU:H	1:D:306:LEU:CD1	2.10	0.62
1:D:18:TYR:CE2	1:D:408:GLN:HB3	2.35	0.62
1:C:385:ILE:HG21	1:C:428:GLN:HB3	1.80	0.62
1:C:424:ARG:NH1	1:C:455:GLY:O	2.32	0.62
1:C:579:LYS:HZ2	1:C:579:LYS:HB2	1.65	0.62
1:D:9:ARG:HG2	1:D:9:ARG:HH11	1.64	0.62
1:C:31:LYS:CG	1:C:64:LEU:HA	2.29	0.62
1:D:251:PHE:HB2	1:D:267:PHE:CZ	2.35	0.62
1:D:308:LYS:O	1:D:312:TYR:HB2	2.00	0.62
1:D:324:LEU:HD13	1:D:335:TRP:CZ3	2.34	0.62
1:D:384:PHE:CD2	1:D:438:LEU:HB3	2.34	0.62
1:C:134:TYR:CE1	1:C:454:TYR:HA	2.35	0.62
1:D:339:ARG:O	1:D:342:VAL:HG22	1.99	0.62
1:C:83:PHE:CD2	1:C:94:MET:HE2	2.34	0.61
1:C:84:LEU:HD23	1:C:84:LEU:O	1.99	0.61
1:C:487:TYR:O	1:C:491:ILE:HG13	1.99	0.61
1:D:112:GLU:HG2	1:D:114:PRO:CD	2.30	0.61
1:D:406:PRO:HG2	1:D:409:ALA:CB	2.30	0.61
1:C:69:GLU:HG2	1:C:70:CYS:N	2.15	0.61
1:C:559:LEU:HD23	1:C:560:THR:H	1.63	0.61
1:D:518:ALA:HB1	1:D:543:LEU:HD13	1.83	0.61
1:C:162:THR:HG21	1:C:469:ARG:O	2.00	0.61
1:C:508:LEU:O	1:C:509:THR:HG23	2.00	0.61
1:C:221:LEU:O	1:C:225:VAL:HG23	2.00	0.61
1:C:373:ASN:HD22	1:C:415:ASN:HD21	1.48	0.61
1:D:225:VAL:HA	1:D:228:CYS:SG	2.41	0.61
1:C:69:GLU:O	1:C:70:CYS:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:VAL:HG23	1:C:129:LYS:N	2.14	0.61
1:C:468:CYS:SG	1:C:469:ARG:HG3	2.41	0.61
1:C:579:LYS:HB2	1:C:579:LYS:NZ	2.16	0.61
1:C:187:ASN:O	1:C:233:ILE:HA	2.00	0.61
1:C:425:LEU:O	1:C:428:GLN:HB2	2.00	0.61
1:C:157:GLY:CA	1:C:161:PRO:HB3	2.27	0.61
1:C:291:LEU:O	1:C:292:MET:HG3	2.01	0.61
1:C:298:GLU:O	1:C:303:LYS:HE3	2.01	0.61
1:D:25:LEU:HD22	1:D:25:LEU:N	2.16	0.61
1:D:328:ASN:ND2	1:D:329:GLU:N	2.49	0.61
1:C:18:TYR:HB2	1:C:24:HIS:NE2	2.15	0.61
1:C:156:TRP:CZ2	1:C:163:PRO:HD3	2.36	0.61
1:C:237:LEU:HD22	1:C:319:ILE:HD13	1.82	0.61
1:D:438:LEU:HD22	1:D:532:MET:HB3	1.83	0.61
1:C:385:ILE:HG22	1:C:386:HIS:N	2.16	0.60
1:D:13:ASN:O	1:D:26:ARG:HD2	2.01	0.60
1:D:37:VAL:HG23	1:D:56:MET:HE3	1.83	0.60
1:C:187:ASN:C	1:C:233:ILE:HG22	2.25	0.60
1:C:354:GLU:HG3	1:C:372:MET:HG3	1.83	0.60
1:D:296:ASN:C	1:D:296:ASN:HD22	2.09	0.60
1:D:362:TRP:O	1:D:363:LEU:HD23	2.00	0.60
1:C:303:LYS:O	1:C:307:LEU:HG	2.01	0.60
1:C:337:GLU:O	1:C:341:VAL:HG23	2.01	0.60
1:C:570:LEU:C	1:C:570:LEU:HD23	2.26	0.60
1:D:272:LEU:H	1:D:272:LEU:CD2	2.12	0.60
1:C:135:GLN:HG3	1:C:190:TYR:CD2	2.37	0.60
1:D:553:LEU:CD1	1:D:583:ASP:HB2	2.28	0.60
1:D:3:LEU:HD11	1:D:92:ARG:NH1	2.17	0.60
1:D:196:LYS:HZ2	1:D:196:LYS:HB3	1.65	0.60
1:D:342:VAL:HG23	1:D:343:LYS:H	1.65	0.60
1:D:393:LYS:HE2	1:D:393:LYS:HA	1.84	0.60
1:C:119:VAL:HG13	1:C:120:ASP:N	2.16	0.60
1:C:249:PRO:HB2	1:C:250:PRO:CD	2.28	0.60
1:D:355:VAL:HG11	1:D:359:SER:HB3	1.83	0.60
1:C:352:LEU:HD12	1:C:353:GLY:N	2.17	0.60
1:D:1:MET:O	1:D:1:MET:SD	2.60	0.60
1:D:83:PHE:HD2	1:D:94:MET:HE2	1.67	0.60
1:D:571:PRO:O	1:D:572:ALA:C	2.43	0.60
1:C:100:LEU:HD13	1:C:102:GLU:O	2.02	0.59
1:C:299:HIS:O	1:C:303:LYS:HG3	2.02	0.59
1:C:523:ASP:HB2	1:C:525:GLN:CD	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:LYS:HA	1:D:317:THR:HG23	1.83	0.59
1:D:296:ASN:HD21	1:D:298:GLU:HB2	1.66	0.59
1:C:19:ASN:ND2	1:C:19:ASN:C	2.58	0.59
1:C:35:THR:OG1	1:C:87:GLN:HA	2.02	0.59
1:C:550:TRP:N	1:C:583:ASP:OXT	2.36	0.59
1:D:37:VAL:C	1:D:56:MET:HE3	2.27	0.59
1:D:410:SER:O	1:D:413:MET:HB2	2.02	0.59
1:D:552:HIS:HA	1:D:581:SER:O	2.02	0.59
1:C:27:ILE:HB	1:C:56:MET:HE1	1.84	0.59
1:C:192:THR:CB	1:C:193:PRO:HD2	2.31	0.59
1:C:306:LEU:O	1:C:309:ALA:HB3	2.02	0.59
1:D:190:TYR:CE1	1:D:323:ARG:HG3	2.38	0.59
1:C:41:ALA:CB	1:C:81:TYR:HB3	2.32	0.59
1:D:326:VAL:HG12	1:D:329:GLU:HB2	1.85	0.59
1:D:529:LEU:HD21	1:D:580:ALA:HB3	1.85	0.59
1:C:411:GLU:O	1:C:448:GLY:HA2	2.02	0.59
1:D:362:TRP:HA	1:D:367:GLN:NE2	2.17	0.59
1:C:313:TRP:H	1:C:313:TRP:CD1	2.20	0.59
1:D:483:LEU:O	1:D:486:PHE:HB3	2.03	0.59
1:D:39:ALA:N	1:D:56:MET:HE2	2.18	0.59
1:D:43:ASP:N	1:D:50:THR:HG21	2.17	0.59
1:D:180:HIS:O	1:D:183:LYS:HB2	2.02	0.59
1:D:206:GLU:HG2	1:D:206:GLU:O	2.02	0.59
1:C:93:TRP:HD1	1:C:100:LEU:HB3	1.66	0.59
1:D:6:VAL:HG13	1:D:27:ILE:HD11	1.85	0.59
1:C:510:ALA:O	1:C:511:GLU:C	2.46	0.58
1:D:280:ILE:HG23	1:D:288:PHE:CD2	2.38	0.58
1:D:411:GLU:O	1:D:448:GLY:HA2	2.02	0.58
1:D:419:SER:HA	1:D:453:TYR:CD1	2.38	0.58
1:D:160:ASP:N	1:D:161:PRO:HD3	2.18	0.58
1:D:326:VAL:HG12	1:D:326:VAL:O	2.03	0.58
1:D:508:LEU:HB2	1:D:518:ALA:O	2.04	0.58
1:D:578:LEU:HD23	1:D:578:LEU:H	1.68	0.58
1:C:41:ALA:HB2	1:C:81:TYR:HB3	1.85	0.58
1:D:19:ASN:C	1:D:19:ASN:ND2	2.59	0.58
1:D:130:ASP:OD1	1:D:501:ARG:HD2	2.03	0.58
1:D:102:GLU:HG3	1:D:103:PRO:CD	2.33	0.58
1:D:106:ASN:C	1:D:106:ASN:HD22	2.10	0.58
1:C:274:LEU:N	1:C:274:LEU:HD22	2.18	0.58
1:D:426:LEU:HB2	1:D:436:MET:CE	2.33	0.58
1:C:3:LEU:H	1:C:3:LEU:CD1	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:PRO:O	1:C:11:ARG:HB2	2.04	0.58
1:C:86:GLN:HG2	1:C:87:GLN:N	2.17	0.58
1:D:108:ASP:C	1:D:110:LEU:H	2.11	0.58
1:D:237:LEU:HB2	1:D:322:TRP:CZ3	2.39	0.58
1:D:387:GLN:NE2	1:D:534:ASN:HD22	1.92	0.58
1:C:94:MET:HE3	1:C:111:PHE:CZ	2.39	0.58
1:C:373:ASN:C	1:C:375:PRO:HD2	2.28	0.58
1:C:289:GLU:OE2	1:C:291:LEU:HD13	2.04	0.58
1:D:9:ARG:HG2	1:D:9:ARG:NH1	2.18	0.58
1:D:167:PHE:HD1	1:D:168:GLY:N	2.02	0.58
1:D:429:ALA:O	1:D:431:GLY:N	2.37	0.58
1:C:35:THR:CB	1:C:87:GLN:HA	2.33	0.57
1:C:577:VAL:HG12	1:C:577:VAL:O	2.04	0.57
1:D:328:ASN:ND2	1:D:329:GLU:H	2.01	0.57
1:D:579:LYS:HE2	1:D:580:ALA:H	1.68	0.57
1:C:521:ARG:HB2	1:C:528:ILE:HD11	1.86	0.57
1:D:275:GLU:O	1:D:282:THR:HB	2.04	0.57
1:D:289:GLU:HG3	1:D:292:MET:HB2	1.86	0.57
1:C:408:GLN:HG2	1:C:409:ALA:N	2.16	0.57
1:C:433:LYS:O	1:C:437:LYS:HG3	2.05	0.57
1:D:398:LEU:HD23	1:D:398:LEU:O	2.03	0.57
1:D:512:LYS:NZ	1:D:512:LYS:HB3	2.19	0.57
1:C:83:PHE:HD2	1:C:94:MET:HE2	1.68	0.57
1:C:234:ARG:HA	1:C:320:ASP:OD2	2.04	0.57
1:C:308:LYS:HD3	1:C:311:GLU:OE2	2.04	0.57
1:C:425:LEU:HB3	1:C:436:MET:CE	2.34	0.57
1:D:217:ASP:OD1	1:D:219:ASP:HB2	2.04	0.57
1:D:317:THR:HB	1:D:319:ILE:HG23	1.84	0.57
1:D:545:VAL:HG21	1:D:568:VAL:HG23	1.85	0.57
1:C:184:LEU:HD12	1:C:186:VAL:CG2	2.31	0.57
1:D:520:LEU:HD23	1:D:521:ARG:N	2.19	0.57
1:C:457:GLU:HA	1:C:487:TYR:CD1	2.39	0.57
1:C:186:VAL:CG1	1:C:187:ASN:N	2.68	0.57
1:C:335:TRP:HA	1:C:335:TRP:CE3	2.40	0.57
1:C:1:MET:O	1:C:2:PHE:C	2.47	0.57
1:C:92:ARG:HG3	1:C:100:LEU:O	2.05	0.57
1:D:93:TRP:CH2	1:D:103:PRO:HG3	2.40	0.57
1:D:225:VAL:HG21	1:D:317:THR:HG22	1.86	0.57
1:C:30:LYS:HB3	1:C:33:ASP:HB3	1.86	0.57
1:C:180:HIS:CE1	1:C:181:LEU:HD23	2.40	0.57
1:C:359:SER:HB2	1:C:362:TRP:HE3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ARG:NH1	1:C:460:LEU:CB	2.65	0.56
1:D:457:GLU:CD	1:D:457:GLU:H	2.10	0.56
1:C:81:TYR:CD1	1:C:81:TYR:N	2.74	0.56
1:C:6:VAL:HA	1:C:28:ARG:O	2.05	0.56
1:C:100:LEU:HD22	1:C:102:GLU:O	2.05	0.56
1:C:138:PRO:HG3	1:C:191:PHE:CD2	2.38	0.56
1:C:246:ARG:HH11	1:C:246:ARG:HG2	1.71	0.56
1:C:291:LEU:HD12	1:C:291:LEU:N	2.21	0.56
1:C:433:LYS:HB3	1:C:437:LYS:HE3	1.87	0.56
1:D:384:PHE:CA	1:D:534:ASN:HD21	2.12	0.56
1:D:418:ASP:OD2	1:D:425:LEU:HB2	2.05	0.56
1:D:543:LEU:HD23	1:D:543:LEU:N	2.19	0.56
1:C:196:LYS:O	1:C:206:GLU:HB3	2.05	0.56
1:C:218:LYS:HD3	1:D:253:ASP:OD2	2.05	0.56
1:C:241:PHE:CD2	1:C:306:LEU:HB3	2.41	0.56
1:D:16:TYR:O	1:D:23:VAL:HG13	2.05	0.56
1:C:327:ALA:C	1:C:329:GLU:H	2.13	0.56
1:D:370:ALA:CB	1:D:412:VAL:HG12	2.35	0.56
1:C:275:GLU:O	1:C:282:THR:HG22	2.05	0.56
1:C:454:TYR:CD1	1:C:454:TYR:C	2.83	0.56
1:D:61:THR:HG23	1:D:65:PHE:O	2.03	0.56
1:D:551:THR:HG23	1:D:563:HIS:N	2.20	0.56
1:C:7:TYR:OH	1:C:9:ARG:HD2	2.06	0.56
1:C:551:THR:O	1:C:582:SER:HB2	2.06	0.56
1:D:159:ALA:C	1:D:161:PRO:HD3	2.31	0.56
1:D:211:ILE:HG13	1:D:313:TRP:CH2	2.38	0.56
1:D:422:THR:OG1	1:D:423:ALA:N	2.39	0.56
1:C:44:LYS:HE3	1:C:112:GLU:OE2	2.06	0.56
1:C:182:SER:OG	1:C:231:ARG:HD3	2.06	0.56
1:C:339:ARG:HH12	1:C:365:GLY:HA2	1.69	0.56
1:D:80:LYS:HE3	1:D:110:LEU:O	2.06	0.56
1:D:112:GLU:HG2	1:D:113:TYR:N	2.21	0.56
1:D:122:PHE:HD1	1:D:124:PRO:HD3	1.71	0.56
1:C:201:HIS:CD2	1:C:203:TYR:HB2	2.41	0.56
1:D:33:ASP:OD2	1:D:34:MET:HE2	2.06	0.56
1:D:276:VAL:HG23	1:D:280:ILE:O	2.06	0.56
1:D:283:TYR:CE2	1:D:285:THR:HG22	2.41	0.56
1:D:508:LEU:HD12	1:D:508:LEU:N	2.20	0.56
1:C:100:LEU:HD12	1:C:104:PRO:HG3	1.88	0.55
1:C:228:CYS:C	1:C:230:GLU:H	2.14	0.55
1:C:281:PRO:C	1:C:283:TYR:H	2.12	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:VAL:HG21	1:C:570:LEU:HD13	1.88	0.55
1:D:237:LEU:HD12	1:D:237:LEU:N	2.22	0.55
1:D:568:VAL:HG12	1:D:570:LEU:HG	1.87	0.55
1:C:239:ALA:HB1	1:C:241:PHE:CD1	2.42	0.55
1:C:291:LEU:HD12	1:C:291:LEU:H	1.71	0.55
1:D:46:MET:HG3	1:D:50:THR:HG1	1.71	0.55
1:D:551:THR:HG23	1:D:563:HIS:H	1.71	0.55
1:C:392:GLU:OE1	1:C:512:LYS:HG2	2.06	0.55
1:C:244:SER:O	1:C:293:PRO:HD2	2.06	0.55
1:D:138:PRO:C	1:D:140:ARG:H	2.15	0.55
1:D:209:PHE:CE1	1:D:309:ALA:HA	2.41	0.55
1:C:154:LEU:CB	1:C:155:PRO:CD	2.81	0.55
1:C:484:PHE:HD2	1:C:488:GLN:HE21	1.54	0.55
1:C:554:TRP:HB3	1:C:559:LEU:HB3	1.87	0.55
1:D:84:LEU:CD2	1:D:91:LYS:HB2	2.37	0.55
1:D:193:PRO:HD3	1:D:238:ASP:CG	2.32	0.55
1:C:297:THR:HG21	1:C:330:VAL:CG1	2.36	0.55
1:C:325:ASP:CG	1:C:326:VAL:N	2.65	0.55
1:C:33:ASP:O	1:C:34:MET:HG2	2.06	0.55
1:C:106:ASN:O	1:C:106:ASN:ND2	2.40	0.55
1:C:444:PHE:HE1	1:C:452:ILE:HD11	1.71	0.55
1:C:517:ILE:CG2	1:C:532:MET:HB2	2.37	0.55
1:D:162:THR:C	1:D:164:SER:H	2.15	0.55
1:C:194:LEU:N	1:C:194:LEU:HD23	2.22	0.55
1:C:283:TYR:OH	1:C:290:PRO:HB3	2.06	0.55
1:C:504:THR:O	1:C:505:PHE:HB2	2.07	0.55
1:D:373:ASN:HD22	1:D:415:ASN:ND2	2.04	0.55
1:D:376:PHE:O	1:D:379:ALA:HB3	2.06	0.55
1:D:385:ILE:O	1:D:387:GLN:HG3	2.06	0.55
1:D:447:PHE:N	1:D:521:ARG:HH12	2.05	0.55
1:C:53:TYR:CE2	1:C:84:LEU:HD12	2.41	0.55
1:C:136:ILE:HA	1:C:454:TYR:HD2	1.72	0.55
1:C:455:GLY:HA3	1:C:460:LEU:HD12	1.89	0.55
1:C:530:VAL:HG13	1:C:579:LYS:HB3	1.88	0.55
1:C:553:LEU:HD11	1:C:583:ASP:HB2	1.89	0.55
1:D:128:VAL:HG11	1:D:350:TYR:CD1	2.42	0.55
1:D:243:HIS:HD2	1:D:292:MET:HB3	1.72	0.55
1:C:136:ILE:O	1:C:192:THR:HG23	2.07	0.55
1:C:193:PRO:HD3	1:C:203:TYR:CE1	2.42	0.55
1:D:125:PRO:HG2	1:D:350:TYR:HA	1.89	0.55
1:D:236:LEU:HD12	1:D:236:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:MET:N	1:D:293:PRO:HD3	2.21	0.55
1:D:296:ASN:C	1:D:298:GLU:H	2.15	0.55
1:D:335:TRP:CE3	1:D:335:TRP:HA	2.42	0.55
1:C:554:TRP:HE3	1:C:559:LEU:HD22	1.72	0.54
1:D:203:TYR:C	1:D:205:THR:H	2.14	0.54
1:D:264:LYS:C	1:D:266:TRP:H	2.15	0.54
1:D:418:ASP:OD1	1:D:453:TYR:HB2	2.07	0.54
1:D:194:LEU:HD23	1:D:194:LEU:N	2.22	0.54
1:C:134:TYR:CZ	1:C:454:TYR:HA	2.42	0.54
1:C:465:ASP:OD2	1:C:466:PRO:HD3	2.08	0.54
1:C:483:LEU:O	1:C:486:PHE:HB3	2.08	0.54
1:D:385:ILE:N	1:D:385:ILE:HD12	2.22	0.54
1:D:508:LEU:H	1:D:508:LEU:CD1	2.21	0.54
1:D:555:GLN:O	1:D:557:ASP:N	2.41	0.54
1:C:192:THR:O	1:C:194:LEU:HD22	2.06	0.54
1:C:297:THR:HG21	1:C:330:VAL:HG13	1.87	0.54
1:C:543:LEU:N	1:C:543:LEU:HD23	2.22	0.54
1:C:553:LEU:N	1:C:553:LEU:HD12	2.22	0.54
1:C:38:TYR:CD1	1:C:84:LEU:HD13	2.43	0.54
1:C:442:PHE:CD1	1:C:532:MET:HE1	2.42	0.54
1:D:241:PHE:HB3	1:D:306:LEU:HD23	1.90	0.54
1:D:432:ASP:OD1	1:D:434:ARG:HB2	2.07	0.54
1:C:4:GLU:CD	1:C:4:GLU:N	2.65	0.54
1:C:29:THR:O	1:C:65:PHE:HA	2.08	0.54
1:C:383:PHE:O	1:C:387:GLN:HA	2.07	0.54
1:D:264:LYS:O	1:D:266:TRP:N	2.40	0.54
1:D:289:GLU:HG2	1:D:292:MET:CE	2.37	0.54
1:C:37:VAL:HG23	1:C:37:VAL:O	2.07	0.54
1:C:244:SER:HB3	1:C:295:LEU:HD21	1.90	0.54
1:D:60:ALA:O	1:D:66:ASP:O	2.25	0.54
1:D:377:THR:HG22	1:D:381:LEU:CD1	2.35	0.54
1:D:386:HIS:HB3	1:D:388:ILE:HG12	1.90	0.54
1:D:393:LYS:O	1:D:397:MET:HG2	2.08	0.54
1:D:438:LEU:HD23	1:D:577:VAL:HG12	1.90	0.54
1:C:219:ASP:O	1:C:223:LYS:N	2.32	0.54
1:C:565:GLN:C	1:C:567:THR:N	2.66	0.54
1:C:143:ASN:CG	1:C:168:GLY:O	2.51	0.54
1:C:158:SER:N	1:C:161:PRO:HG3	2.23	0.54
1:C:323:ARG:HD2	1:C:324:LEU:N	2.22	0.54
1:C:517:ILE:HG21	1:C:532:MET:HE3	1.89	0.54
1:C:390:ASP:OD1	1:C:392:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:THR:HG22	1:D:110:LEU:HD23	1.88	0.54
1:D:554:TRP:NE1	1:D:578:LEU:HA	2.23	0.54
1:D:515:ARG:H	1:D:516:GLN:NE2	2.06	0.53
1:C:572:ALA:CB	1:C:576:ALA:HB2	2.38	0.53
1:C:576:ALA:C	1:C:578:LEU:N	2.63	0.53
1:D:37:VAL:HG23	1:D:56:MET:SD	2.48	0.53
1:D:162:THR:HG21	1:D:469:ARG:HB2	1.89	0.53
1:D:498:ALA:O	1:D:501:ARG:N	2.31	0.53
1:C:23:VAL:N	1:C:72:VAL:O	2.40	0.53
1:C:392:GLU:HG3	1:C:393:LYS:N	2.23	0.53
1:C:429:ALA:O	1:C:430:ASP:CB	2.56	0.53
1:C:438:LEU:HD11	1:C:575:PHE:CA	2.38	0.53
1:C:489:THR:O	1:C:493:LEU:HB2	2.09	0.53
1:D:343:LYS:HA	1:D:346:ASN:O	2.09	0.53
1:D:529:LEU:HG	1:D:529:LEU:O	2.08	0.53
1:D:14:PHE:O	1:D:25:LEU:HA	2.09	0.53
1:D:241:PHE:CG	1:D:306:LEU:HD23	2.44	0.53
1:D:516:GLN:HG3	1:D:533:ASN:HB2	1.90	0.53
1:C:38:TYR:H	1:C:84:LEU:HB3	1.72	0.53
1:C:224:LEU:HD23	1:C:224:LEU:O	2.08	0.53
1:C:324:LEU:HD13	1:C:335:TRP:CH2	2.43	0.53
1:D:3:LEU:HD12	1:D:3:LEU:N	2.23	0.53
1:D:374:TYR:C	1:D:376:PHE:N	2.64	0.53
1:D:551:THR:HA	1:D:563:HIS:CE1	2.43	0.53
1:C:77:ARG:N	1:C:77:ARG:HD2	2.23	0.53
1:C:186:VAL:HG12	1:C:187:ASN:N	2.23	0.53
1:C:197:ALA:HB3	1:C:202:LYS:HD2	1.90	0.53
1:C:247:THR:O	1:C:248:PHE:C	2.51	0.53
1:C:332:HIS:O	1:C:336:ARG:HG2	2.08	0.53
1:C:352:LEU:HD12	1:C:353:GLY:H	1.74	0.53
1:D:351:ILE:HG22	1:D:368:PHE:HA	1.90	0.53
1:C:377:THR:HG23	1:C:417:LEU:HA	1.90	0.53
1:C:425:LEU:HB3	1:C:436:MET:HE3	1.91	0.53
1:C:454:TYR:O	1:C:455:GLY:O	2.27	0.53
1:C:479:HIS:O	1:C:481:LYS:N	2.42	0.53
1:D:37:VAL:HG22	1:D:68:TRP:CD1	2.44	0.53
1:D:206:GLU:HG3	1:D:247:THR:O	2.09	0.53
1:D:578:LEU:HD23	1:D:578:LEU:N	2.22	0.53
1:C:14:PHE:O	1:C:15:SER:HB2	2.08	0.53
1:C:392:GLU:HG3	1:C:393:LYS:H	1.73	0.53
1:C:445:THR:HG21	1:C:519:TYR:OH	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:ALA:HB1	1:C:576:ALA:HB2	1.89	0.53
1:D:188:ALA:HA	1:D:234:ARG:O	2.09	0.53
1:C:7:TYR:CE2	1:C:9:ARG:HB2	2.44	0.53
1:C:25:LEU:HD22	1:C:25:LEU:N	2.24	0.53
1:C:392:GLU:HG2	1:C:512:LYS:HA	1.89	0.53
1:C:424:ARG:HH12	1:C:460:LEU:HB2	1.70	0.53
1:D:75:PRO:HB2	1:D:76:TYR:CD2	2.44	0.53
1:C:324:LEU:HG	1:C:352:LEU:O	2.09	0.52
1:C:377:THR:HG22	1:C:381:LEU:HD12	1.91	0.52
1:C:535:ASP:HB2	1:C:537:ALA:O	2.09	0.52
1:C:582:SER:O	1:C:583:ASP:C	2.52	0.52
1:D:127:TRP:CZ3	1:D:234:ARG:HD3	2.44	0.52
1:D:209:PHE:HE1	1:D:309:ALA:HA	1.73	0.52
1:D:392:GLU:HA	1:D:395:SER:OG	2.09	0.52
1:D:441:LEU:HD23	1:D:577:VAL:HB	1.90	0.52
1:C:52:GLU:O	1:C:52:GLU:HG3	2.09	0.52
1:D:378:ASN:O	1:D:382:ASP:HB2	2.10	0.52
1:D:426:LEU:HB2	1:D:436:MET:HE3	1.91	0.52
1:C:224:LEU:HD23	1:C:224:LEU:C	2.34	0.52
1:D:143:ASN:ND2	1:D:170:ASP:CG	2.68	0.52
1:D:221:LEU:HG	1:D:317:THR:HG21	1.92	0.52
1:D:254:VAL:C	1:D:256:LYS:H	2.18	0.52
1:D:442:PHE:O	1:D:446:TYR:HB2	2.10	0.52
1:C:579:LYS:HD3	1:C:579:LYS:C	2.34	0.52
1:C:299:HIS:CD2	1:C:302:VAL:HG23	2.45	0.52
1:C:416:LEU:H	1:C:416:LEU:CD2	2.18	0.52
1:D:8:HIS:CE1	1:D:14:PHE:HB3	2.44	0.52
1:D:11:ARG:HA	1:D:15:SER:O	2.10	0.52
1:D:241:PHE:CD1	1:D:306:LEU:HD23	2.44	0.52
1:D:440:VAL:O	1:D:443:GLN:HB3	2.10	0.52
1:D:118:PRO:HA	1:D:121:VAL:HG23	1.90	0.52
1:D:206:GLU:HG3	1:D:247:THR:HG22	1.92	0.52
1:D:275:GLU:N	1:D:282:THR:HG21	2.16	0.52
1:C:143:ASN:HA	1:C:170:ASP:OD2	2.10	0.52
1:D:190:TYR:CZ	1:D:323:ARG:HG3	2.45	0.52
1:D:272:LEU:CG	1:D:273:PRO:HD3	2.35	0.52
1:C:18:TYR:CE1	1:C:407:ARG:HB3	2.44	0.52
1:C:29:THR:HG23	1:C:68:TRP:HZ3	1.75	0.52
1:C:270:ARG:HB2	1:C:282:THR:O	2.09	0.52
1:D:20:GLY:O	1:D:21:THR:HB	2.10	0.52
1:D:28:ARG:O	1:D:29:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ASN:HB3	1:D:170:ASP:OD2	2.10	0.52
1:D:186:VAL:HG12	1:D:187:ASN:N	2.24	0.52
1:D:204:ASP:O	1:D:205:THR:C	2.53	0.52
1:C:538:GLY:HA2	1:C:572:ALA:O	2.09	0.52
1:D:373:ASN:ND2	1:D:415:ASN:ND2	2.58	0.52
1:C:356:TRP:N	1:C:356:TRP:CD1	2.78	0.52
1:D:112:GLU:CG	1:D:113:TYR:N	2.73	0.52
1:D:476:GLU:HA	1:D:479:HIS:CG	2.45	0.52
1:D:43:ASP:C	1:D:45:TYR:H	2.16	0.51
1:D:268:HIS:CE1	1:D:296:ASN:HA	2.44	0.51
1:D:529:LEU:H	1:D:529:LEU:HD23	1.74	0.51
1:C:106:ASN:HD22	1:C:106:ASN:H	1.58	0.51
1:C:193:PRO:HB2	1:C:202:LYS:HB2	1.91	0.51
1:C:555:GLN:OE1	1:C:555:GLN:HA	2.10	0.51
1:D:193:PRO:N	1:D:238:ASP:HB3	2.25	0.51
1:C:505:PHE:HA	1:C:520:LEU:O	2.09	0.51
1:C:508:LEU:HD12	1:C:508:LEU:N	2.26	0.51
1:D:62:ASP:CB	1:D:400:LYS:HD3	2.40	0.51
1:D:100:LEU:HD12	1:D:104:PRO:HG3	1.91	0.51
1:C:8:HIS:CE1	1:C:14:PHE:O	2.64	0.51
1:C:35:THR:HB	1:C:87:GLN:HA	1.92	0.51
1:C:290:PRO:C	1:C:292:MET:H	2.18	0.51
1:D:148:ASN:H	1:D:148:ASN:HD22	1.58	0.51
1:D:164:SER:O	1:D:200:ASN:ND2	2.43	0.51
1:C:480:ASP:HB3	1:C:483:LEU:HB3	1.92	0.51
1:C:579:LYS:HZ2	1:C:579:LYS:CB	2.24	0.51
1:D:14:PHE:HD1	1:D:26:ARG:O	1.93	0.51
1:C:440:VAL:O	1:C:443:GLN:HB3	2.10	0.51
1:D:522:GLU:OE1	1:D:522:GLU:N	2.43	0.51
1:D:539:HIS:O	1:D:540:THR:CB	2.59	0.51
1:C:457:GLU:CD	1:C:457:GLU:H	2.17	0.51
1:C:522:GLU:HB3	1:C:527:THR:HA	1.92	0.51
1:D:72:VAL:HG22	1:D:74:PRO:HD3	1.93	0.51
1:D:111:PHE:O	1:D:112:GLU:HB2	2.11	0.51
1:C:333:GLN:NE2	1:C:337:GLU:HG3	2.26	0.51
1:C:399:GLY:HA2	1:C:402:LEU:HB3	1.93	0.51
1:D:272:LEU:HD23	1:D:272:LEU:N	2.14	0.51
1:D:37:VAL:O	1:D:38:TYR:HD2	1.94	0.51
1:D:192:THR:O	1:D:194:LEU:HD22	2.10	0.51
1:D:385:ILE:HG22	1:D:386:HIS:N	2.25	0.51
1:C:296:ASN:HD22	1:C:296:ASN:C	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ALA:O	1:C:312:TYR:HB3	2.11	0.51
1:D:53:TYR:HE2	1:D:93:TRP:CZ3	2.29	0.51
1:D:122:PHE:HE1	1:D:124:PRO:HB3	1.76	0.51
1:C:282:THR:HG23	1:C:283:TYR:CD1	2.45	0.50
1:C:341:VAL:C	1:C:343:LYS:H	2.18	0.50
1:D:38:TYR:C	1:D:56:MET:HE2	2.36	0.50
1:D:167:PHE:CD1	1:D:168:GLY:N	2.78	0.50
1:D:306:LEU:O	1:D:309:ALA:HB3	2.11	0.50
1:D:434:ARG:H	1:D:434:ARG:HE	1.58	0.50
1:D:530:VAL:HA	1:D:579:LYS:HB3	1.93	0.50
1:D:564:GLY:O	1:D:565:GLN:C	2.53	0.50
1:C:480:ASP:O	1:C:483:LEU:HB3	2.11	0.50
1:D:48:ASP:C	1:D:50:THR:H	2.19	0.50
1:D:106:ASN:HB2	1:D:107:PRO:CD	2.39	0.50
1:D:112:GLU:HG2	1:D:114:PRO:HD3	1.93	0.50
1:D:241:PHE:CB	1:D:306:LEU:HD23	2.41	0.50
1:C:9:ARG:O	1:C:14:PHE:HB2	2.11	0.50
1:C:286:PHE:CG	1:C:287:ALA:N	2.74	0.50
1:D:390:ASP:OD2	1:D:512:LYS:O	2.29	0.50
1:C:310:ALA:O	1:C:314:ILE:HG13	2.10	0.50
1:D:227:LEU:O	1:D:230:GLU:HB3	2.10	0.50
1:D:572:ALA:HB1	1:D:576:ALA:HB3	1.93	0.50
1:C:155:PRO:HG3	1:C:471:CYS:CB	2.42	0.50
1:D:122:PHE:CD1	1:D:124:PRO:HD3	2.46	0.50
1:D:125:PRO:HB3	1:D:127:TRP:NE1	2.26	0.50
1:D:225:VAL:CG2	1:D:317:THR:HG22	2.41	0.50
1:D:420:HIS:ND1	1:D:421:ASP:N	2.53	0.50
1:C:174:VAL:HB	1:C:224:LEU:HD11	1.92	0.50
1:C:201:HIS:O	1:C:201:HIS:CG	2.65	0.50
1:D:38:TYR:CE2	1:D:55:PRO:HA	2.46	0.50
1:D:193:PRO:O	1:D:202:LYS:HB2	2.10	0.50
1:D:489:THR:O	1:D:490:VAL:C	2.54	0.50
1:C:241:PHE:CE2	1:C:306:LEU:HB3	2.47	0.50
1:C:324:LEU:HD13	1:C:335:TRP:CZ3	2.46	0.50
1:C:262:LYS:NZ	1:D:315:ARG:HG2	2.26	0.50
1:C:313:TRP:O	1:C:317:THR:N	2.45	0.50
1:C:325:ASP:CG	1:C:326:VAL:H	2.19	0.50
1:C:456:ASP:N	1:C:457:GLU:OE1	2.45	0.50
1:D:53:TYR:HE2	1:D:93:TRP:CH2	2.29	0.50
1:D:97:TYR:CD1	1:D:109:ARG:HB3	2.47	0.50
1:D:140:ARG:C	1:D:471:CYS:HA	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:PRO:O	1:D:254:VAL:HG23	2.11	0.50
1:D:335:TRP:HA	1:D:335:TRP:HE3	1.76	0.50
1:D:517:ILE:HG23	1:D:518:ALA:N	2.26	0.50
1:D:553:LEU:HD23	1:D:558:VAL:HG13	1.93	0.50
1:C:80:LYS:HG2	1:C:110:LEU:HB2	1.93	0.50
1:C:184:LEU:C	1:C:184:LEU:HD13	2.37	0.50
1:C:312:TYR:O	1:C:315:ARG:HB3	2.12	0.50
1:C:410:SER:O	1:C:413:MET:HG2	2.11	0.50
1:D:84:LEU:O	1:D:92:ARG:O	2.29	0.50
1:D:370:ALA:HB2	1:D:412:VAL:CG1	2.40	0.50
1:C:553:LEU:O	1:C:580:ALA:HB1	2.12	0.49
1:D:95:THR:HB	1:D:109:ARG:O	2.11	0.49
1:D:351:ILE:CG2	1:D:368:PHE:HA	2.41	0.49
1:D:516:GLN:HE21	1:D:535:ASP:HB2	1.77	0.49
1:C:16:TYR:O	1:C:23:VAL:HG13	2.13	0.49
1:C:29:THR:O	1:C:66:ASP:N	2.39	0.49
1:C:46:MET:HG3	1:C:46:MET:O	2.11	0.49
1:C:214:GLN:HG3	1:C:215:PHE:N	2.27	0.49
1:C:324:LEU:O	1:C:325:ASP:C	2.55	0.49
1:C:361:ILE:N	1:C:361:ILE:HD12	2.27	0.49
1:D:172:GLN:O	1:D:173:GLY:C	2.54	0.49
1:D:328:ASN:HD22	1:D:328:ASN:N	2.09	0.49
1:D:370:ALA:HB1	1:D:413:MET:HA	1.94	0.49
1:D:416:LEU:HD23	1:D:416:LEU:N	2.24	0.49
1:D:445:THR:O	1:D:521:ARG:NH1	2.44	0.49
1:C:96:GLU:HG2	1:C:111:PHE:HA	1.93	0.49
1:D:178:LEU:O	1:D:179:ASP:C	2.55	0.49
1:D:263:TYR:O	1:D:266:TRP:HB2	2.12	0.49
1:D:441:LEU:HD12	1:D:445:THR:HG23	1.94	0.49
1:C:23:VAL:O	1:C:72:VAL:HG12	2.13	0.49
1:C:48:ASP:CA	1:C:51:MET:HE2	2.36	0.49
1:C:246:ARG:HG2	1:C:246:ARG:NH1	2.27	0.49
1:D:43:ASP:C	1:D:45:TYR:N	2.70	0.49
1:D:78:ARG:HB2	1:D:114:PRO:O	2.12	0.49
1:D:125:PRO:C	1:D:127:TRP:H	2.20	0.49
1:C:16:TYR:CE1	1:C:24:HIS:HD2	2.31	0.49
1:C:155:PRO:HG2	1:C:472:MET:O	2.12	0.49
1:D:204:ASP:O	1:D:245:GLY:HA3	2.12	0.49
1:D:283:TYR:O	1:D:285:THR:HG23	2.12	0.49
1:D:351:ILE:N	1:D:369:ASP:OD2	2.44	0.49
1:C:155:PRO:HG3	1:C:471:CYS:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:GLY:HA3	1:C:161:PRO:CB	2.31	0.49
1:C:339:ARG:HG3	1:C:351:ILE:CD1	2.36	0.49
1:D:179:ASP:C	1:D:183:LYS:HG3	2.37	0.49
1:D:553:LEU:N	1:D:553:LEU:HD12	2.28	0.49
1:C:31:LYS:HG2	1:C:63:GLU:O	2.12	0.49
1:D:31:LYS:HG2	1:D:64:LEU:HA	1.95	0.49
1:D:43:ASP:H	1:D:50:THR:CB	2.25	0.49
1:D:357:HIS:HD1	1:D:357:HIS:C	2.20	0.49
1:D:430:ASP:O	1:D:432:ASP:N	2.39	0.49
1:D:556:ASP:O	1:D:557:ASP:HB2	2.12	0.49
1:C:11:ARG:H	1:C:15:SER:HB3	1.76	0.49
1:C:26:ARG:HA	1:C:68:TRP:O	2.12	0.49
1:C:100:LEU:CD2	1:C:101:THR:H	2.25	0.49
1:C:378:ASN:O	1:C:382:ASP:HB2	2.12	0.49
1:D:30:LYS:O	1:D:31:LYS:C	2.56	0.49
1:D:373:ASN:ND2	1:D:376:PHE:HB2	2.22	0.49
1:C:144:GLY:HA3	1:C:176:ASP:OD2	2.13	0.49
1:C:248:PHE:CE2	1:C:250:PRO:HD2	2.48	0.49
1:C:517:ILE:HG22	1:C:532:MET:HB2	1.95	0.49
1:C:528:ILE:O	1:C:528:ILE:HD13	2.11	0.49
1:C:563:HIS:HA	1:C:568:VAL:CG2	2.41	0.49
1:D:498:ALA:HA	1:D:501:ARG:HH21	1.77	0.49
1:C:187:ASN:HD21	1:C:495:GLN:NE2	2.11	0.48
1:C:579:LYS:NZ	1:C:580:ALA:N	2.60	0.48
1:D:207:ASP:CG	1:D:210:GLN:HB3	2.37	0.48
1:D:237:LEU:O	1:D:322:TRP:HE3	1.95	0.48
1:C:228:CYS:C	1:C:230:GLU:N	2.70	0.48
1:C:308:LYS:HD3	1:C:311:GLU:CD	2.37	0.48
1:D:139:GLU:O	1:D:140:ARG:HD3	2.13	0.48
1:D:184:LEU:HB3	1:D:186:VAL:HG23	1.95	0.48
1:C:41:ALA:HB1	1:C:79:VAL:HG23	1.95	0.48
1:C:483:LEU:O	1:C:487:TYR:HD1	1.96	0.48
1:D:141:PHE:CE1	1:D:472:MET:HG2	2.49	0.48
1:D:342:VAL:CG2	1:D:343:LYS:N	2.74	0.48
1:C:47:TRP:O	1:C:51:MET:HG3	2.13	0.48
1:C:515:ARG:HB3	1:C:534:ASN:CB	2.44	0.48
1:D:15:SER:HA	1:D:24:HIS:O	2.13	0.48
1:D:37:VAL:HG22	1:D:68:TRP:CG	2.48	0.48
1:C:80:LYS:HG3	1:C:111:PHE:O	2.13	0.48
1:C:374:TYR:N	1:C:375:PRO:CD	2.77	0.48
1:C:243:HIS:CD2	1:C:292:MET:HE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:TYR:C	1:C:312:TYR:CD2	2.88	0.48
1:C:336:ARG:HD3	1:C:366:ASP:O	2.14	0.48
1:D:337:GLU:O	1:D:338:PHE:C	2.56	0.48
1:D:436:MET:O	1:D:437:LYS:C	2.56	0.48
1:C:297:THR:HG22	1:C:334:PHE:HB2	1.94	0.48
1:C:314:ILE:CG1	1:C:322:TRP:HE1	2.27	0.48
1:D:8:HIS:ND1	1:D:14:PHE:HB3	2.29	0.48
1:D:224:LEU:O	1:D:227:LEU:HB2	2.13	0.48
1:D:342:VAL:CG2	1:D:343:LYS:H	2.26	0.48
1:D:362:TRP:HB3	1:D:368:PHE:CD2	2.49	0.48
1:D:439:ALA:O	1:D:443:GLN:N	2.38	0.48
1:D:39:ALA:HA	1:D:82:GLY:O	2.14	0.48
1:D:134:TYR:O	1:D:189:VAL:HA	2.13	0.48
1:D:376:PHE:O	1:D:380:VAL:HG23	2.13	0.48
1:C:84:LEU:HD23	1:C:84:LEU:C	2.38	0.48
1:C:143:ASN:ND2	1:C:145:ASP:O	2.46	0.48
1:C:553:LEU:HD12	1:C:553:LEU:H	1.79	0.48
1:D:237:LEU:HD11	1:D:319:ILE:CG2	2.43	0.48
1:D:383:PHE:CZ	1:D:517:ILE:HD13	2.49	0.48
1:C:492:ARG:O	1:C:496:ALA:N	2.34	0.48
1:D:76:TYR:HB3	1:D:78:ARG:NH1	2.28	0.48
1:D:148:ASN:N	1:D:148:ASN:ND2	2.61	0.48
1:D:171:LEU:HD23	1:D:171:LEU:C	2.39	0.48
1:D:398:LEU:HD23	1:D:398:LEU:C	2.39	0.48
1:D:456:ASP:C	1:D:458:VAL:H	2.22	0.48
1:C:135:GLN:HG3	1:C:190:TYR:HD2	1.78	0.47
1:C:139:GLU:HG3	1:C:200:ASN:HB2	1.96	0.47
1:C:487:TYR:O	1:C:488:GLN:C	2.57	0.47
1:D:37:VAL:HG23	1:D:56:MET:CE	2.44	0.47
1:D:286:PHE:HB3	1:D:289:GLU:HB3	1.95	0.47
1:D:508:LEU:N	1:D:508:LEU:CD1	2.76	0.47
1:C:472:MET:SD	1:C:473:GLU:N	2.87	0.47
1:C:520:LEU:HD13	1:C:520:LEU:C	2.39	0.47
1:C:534:ASN:O	1:C:535:ASP:C	2.55	0.47
1:D:133:PHE:HB2	1:D:451:CYS:HB2	1.96	0.47
1:C:214:GLN:HG3	1:C:215:PHE:H	1.79	0.47
1:C:339:ARG:HA	1:C:351:ILE:HD11	1.96	0.47
1:D:1:MET:H1	1:D:92:ARG:HH22	1.61	0.47
1:D:271:SER:OG	1:D:273:PRO:HD2	2.15	0.47
1:D:352:LEU:O	1:D:352:LEU:HD23	2.15	0.47
1:C:283:TYR:O	1:C:285:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:LYS:HB3	1:D:68:TRP:CD2	2.49	0.47
1:C:139:GLU:HB3	1:C:140:ARG:HD2	1.95	0.47
1:C:160:ASP:N	1:C:161:PRO:HD3	2.29	0.47
1:C:338:PHE:CZ	1:C:342:VAL:HG11	2.48	0.47
1:C:393:LYS:O	1:C:396:PHE:HB2	2.14	0.47
1:C:535:ASP:OD2	1:C:539:HIS:HD2	1.98	0.47
1:D:194:LEU:N	1:D:194:LEU:CD2	2.77	0.47
1:D:352:LEU:HD23	1:D:352:LEU:H	1.79	0.47
1:D:430:ASP:C	1:D:432:ASP:H	2.21	0.47
1:D:551:THR:HG22	1:D:552:HIS:H	1.79	0.47
1:D:576:ALA:HB1	1:D:578:LEU:HG	1.96	0.47
1:C:197:ALA:HB3	1:C:202:LYS:CD	2.45	0.47
1:C:299:HIS:CD2	1:C:302:VAL:H	2.19	0.47
1:C:516:GLN:NE2	1:C:535:ASP:OD1	2.47	0.47
1:D:254:VAL:O	1:D:258:GLY:HA2	2.15	0.47
1:D:339:ARG:HD2	1:D:367:GLN:N	2.29	0.47
1:D:528:ILE:C	1:D:528:ILE:CD1	2.84	0.47
1:C:107:PRO:HA	1:C:110:LEU:CD1	2.45	0.47
1:C:195:PHE:O	1:C:196:LYS:C	2.57	0.47
1:C:240:VAL:HG12	1:C:243:HIS:O	2.15	0.47
1:C:339:ARG:O	1:C:340:ARG:C	2.57	0.47
1:C:412:VAL:O	1:C:412:VAL:CG1	2.60	0.47
1:D:2:PHE:N	1:D:2:PHE:CD1	2.82	0.47
1:D:62:ASP:HB3	1:D:400:LYS:HD3	1.97	0.47
1:D:64:LEU:HD23	1:D:64:LEU:N	2.29	0.47
1:D:171:LEU:O	1:D:172:GLN:C	2.58	0.47
1:D:291:LEU:O	1:D:292:MET:HG3	2.14	0.47
1:D:475:ASP:C	1:D:477:THR:H	2.23	0.47
1:D:534:ASN:O	1:D:535:ASP:C	2.57	0.47
1:C:200:ASN:OD1	1:C:201:HIS:N	2.47	0.47
1:D:148:ASN:ND2	1:D:149:ASP:H	2.12	0.47
1:D:390:ASP:O	1:D:391:ALA:C	2.58	0.47
1:D:398:LEU:HD11	1:D:442:PHE:HZ	1.79	0.47
1:D:553:LEU:O	1:D:580:ALA:HA	2.15	0.47
1:C:221:LEU:O	1:C:224:LEU:HB3	2.15	0.47
1:C:268:HIS:CE1	1:C:296:ASN:HA	2.49	0.47
1:C:529:LEU:HD11	1:C:552:HIS:CE1	2.50	0.47
1:D:57:THR:O	1:D:69:GLU:HB2	2.15	0.47
1:C:13:ASN:O	1:C:26:ARG:CG	2.63	0.47
1:C:140:ARG:NH1	1:C:200:ASN:HB2	2.30	0.47
1:C:173:GLY:HA2	1:C:176:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:PRO:C	1:C:202:LYS:HB2	2.40	0.47
1:C:324:LEU:N	1:C:352:LEU:O	2.48	0.47
1:C:364:GLU:HB3	1:C:366:ASP:OD1	2.15	0.47
1:D:167:PHE:CD1	1:D:167:PHE:C	2.92	0.47
1:D:195:PHE:O	1:D:212:ASP:HB2	2.15	0.47
1:C:425:LEU:HD23	1:C:436:MET:HG3	1.95	0.46
1:C:512:LYS:O	1:C:514:SER:N	2.47	0.46
1:D:22:THR:OG1	1:D:73:THR:HG22	2.15	0.46
1:D:247:THR:O	1:D:247:THR:HG22	2.16	0.46
1:D:427:THR:CG2	1:D:462:GLY:H	2.28	0.46
1:C:334:PHE:CD1	1:C:334:PHE:C	2.94	0.46
1:C:391:ALA:HB3	1:C:510:ALA:O	2.15	0.46
1:D:222:LYS:HD3	1:D:222:LYS:C	2.40	0.46
1:D:424:ARG:HG3	1:D:460:LEU:O	2.15	0.46
1:C:408:GLN:O	1:C:411:GLU:N	2.48	0.46
1:C:517:ILE:HD12	1:C:518:ALA:N	2.25	0.46
1:C:529:LEU:N	1:C:529:LEU:CD2	2.77	0.46
1:D:302:VAL:O	1:D:305:TYR:HB3	2.16	0.46
1:D:330:VAL:HB	1:D:335:TRP:NE1	2.30	0.46
1:D:427:THR:HG21	1:D:462:GLY:C	2.41	0.46
1:D:520:LEU:HD21	1:D:527:THR:HG23	1.98	0.46
1:C:27:ILE:O	1:C:67:TYR:HA	2.14	0.46
1:C:380:VAL:HA	1:C:394:PHE:HE1	1.80	0.46
1:D:45:TYR:HB2	1:D:78:ARG:HH21	1.80	0.46
1:D:93:TRP:CD1	1:D:93:TRP:N	2.84	0.46
1:D:244:SER:O	1:D:293:PRO:HD2	2.15	0.46
1:D:299:HIS:CD2	1:D:301:ASP:HB2	2.50	0.46
1:D:338:PHE:O	1:D:342:VAL:HG13	2.15	0.46
1:D:350:TYR:CE2	1:D:352:LEU:HD13	2.50	0.46
1:C:311:GLU:O	1:C:312:TYR:C	2.59	0.46
1:C:385:ILE:HG23	1:C:428:GLN:O	2.15	0.46
1:D:59:LEU:HD13	1:D:69:GLU:CG	2.41	0.46
1:D:245:GLY:C	1:D:293:PRO:HD2	2.40	0.46
1:D:394:PHE:O	1:D:395:SER:C	2.58	0.46
1:D:504:THR:HG22	1:D:505:PHE:N	2.30	0.46
1:D:508:LEU:HD11	1:D:520:LEU:CB	2.44	0.46
1:C:218:LYS:O	1:C:221:LEU:HB3	2.16	0.46
1:C:268:HIS:HE1	1:C:296:ASN:HA	1.80	0.46
1:C:323:ARG:HD2	1:C:324:LEU:H	1.80	0.46
1:C:559:LEU:CD2	1:C:560:THR:H	2.27	0.46
1:D:30:LYS:HB3	1:D:33:ASP:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:ASP:HA	1:D:323:ARG:HB3	1.98	0.46
1:D:254:VAL:C	1:D:256:LYS:N	2.73	0.46
1:D:565:GLN:HG3	1:D:566:LEU:N	2.31	0.46
1:C:62:ASP:OD2	1:C:65:PHE:HB2	2.16	0.46
1:C:234:ARG:HB3	1:C:320:ASP:CB	2.45	0.46
1:C:330:VAL:O	1:C:331:SER:C	2.59	0.46
1:C:347:PRO:C	1:C:349:ALA:H	2.23	0.46
1:C:446:TYR:O	1:C:494:ARG:NH2	2.48	0.46
1:D:107:PRO:C	1:D:108:ASP:OD1	2.59	0.46
1:D:135:GLN:HG3	1:D:190:TYR:CD2	2.51	0.46
1:D:539:HIS:O	1:D:540:THR:HB	2.15	0.46
1:C:117:ASN:C	1:C:119:VAL:H	2.24	0.46
1:C:122:PHE:HE2	1:C:363:LEU:C	2.23	0.46
1:C:128:VAL:CG2	1:C:129:LYS:N	2.79	0.46
1:C:219:ASP:O	1:C:220:THR:C	2.57	0.46
1:C:281:PRO:O	1:C:283:TYR:N	2.49	0.46
1:C:358:GLU:OE2	1:C:360:SER:HB3	2.15	0.46
1:D:194:LEU:O	1:D:211:ILE:HG23	2.16	0.46
1:D:538:GLY:H	1:D:574:GLY:HA2	1.80	0.46
1:C:176:ASP:C	1:C:178:LEU:H	2.23	0.46
1:C:243:HIS:HA	1:C:293:PRO:O	2.16	0.46
1:C:283:TYR:CE2	1:C:293:PRO:HG3	2.51	0.46
1:C:330:VAL:HB	1:C:335:TRP:CZ2	2.51	0.46
1:D:47:TRP:CG	1:D:107:PRO:HD3	2.50	0.46
1:D:251:PHE:HB2	1:D:267:PHE:CE2	2.50	0.46
1:D:551:THR:HG22	1:D:552:HIS:N	2.30	0.46
1:C:23:VAL:HB	1:C:72:VAL:HG13	1.98	0.46
1:C:214:GLN:C	1:C:214:GLN:OE1	2.59	0.46
1:C:310:ALA:HA	1:C:322:TRP:CZ2	2.51	0.46
1:C:336:ARG:HG3	1:C:336:ARG:HH11	1.81	0.46
1:D:112:GLU:C	1:D:114:PRO:HD3	2.41	0.46
1:D:113:TYR:HE2	1:D:116:ILE:HA	1.80	0.46
1:D:184:LEU:HD11	1:D:457:GLU:HG2	1.98	0.46
1:D:350:TYR:HE1	1:D:412:VAL:HG13	1.78	0.46
1:D:380:VAL:O	1:D:381:LEU:C	2.59	0.46
1:D:438:LEU:O	1:D:439:ALA:C	2.58	0.46
1:C:100:LEU:HD22	1:C:102:GLU:N	2.23	0.45
1:C:106:ASN:ND2	1:C:106:ASN:H	2.14	0.45
1:C:308:LYS:O	1:C:311:GLU:HG2	2.16	0.45
1:C:438:LEU:HD12	1:C:575:PHE:HD2	1.81	0.45
1:C:535:ASP:C	1:C:537:ALA:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:GLN:HE22	1:C:581:SER:HB3	1.80	0.45
1:D:1:MET:C	1:D:2:PHE:HD1	2.24	0.45
1:D:132:ILE:H	1:D:187:ASN:HD22	1.64	0.45
1:D:132:ILE:N	1:D:132:ILE:HD12	2.31	0.45
1:D:175:ILE:HD13	1:D:227:LEU:HD12	1.98	0.45
1:C:8:HIS:CB	1:C:94:MET:HE1	2.46	0.45
1:C:314:ILE:HG13	1:C:322:TRP:HE1	1.81	0.45
1:C:434:ARG:NH1	1:C:434:ARG:HB2	2.30	0.45
1:C:447:PHE:HB3	1:C:521:ARG:NH2	2.25	0.45
1:D:128:VAL:HG21	1:D:412:VAL:HG13	1.99	0.45
1:D:205:THR:CG2	1:D:244:SER:HA	2.45	0.45
1:C:373:ASN:CB	1:C:415:ASN:ND2	2.79	0.45
1:C:543:LEU:N	1:C:543:LEU:CD2	2.80	0.45
1:D:40:LEU:HD21	1:D:53:TYR:CE2	2.51	0.45
1:D:330:VAL:HB	1:D:335:TRP:CE2	2.52	0.45
1:D:374:TYR:O	1:D:376:PHE:N	2.48	0.45
1:C:42:GLY:O	1:C:79:VAL:HA	2.17	0.45
1:C:106:ASN:HD22	1:C:106:ASN:N	2.13	0.45
1:C:136:ILE:HD11	1:C:141:PHE:CD2	2.51	0.45
1:C:464:HIS:O	1:C:465:ASP:C	2.58	0.45
1:D:139:GLU:O	1:D:167:PHE:HB3	2.17	0.45
1:D:237:LEU:O	1:D:322:TRP:CE3	2.69	0.45
1:D:425:LEU:HD23	1:D:436:MET:HG3	1.97	0.45
1:D:438:LEU:CD2	1:D:532:MET:HB3	2.47	0.45
1:D:452:ILE:HG22	1:D:452:ILE:O	2.16	0.45
1:D:520:LEU:HA	1:D:529:LEU:HA	1.99	0.45
1:C:314:ILE:HA	1:C:319:ILE:HG12	1.97	0.45
1:C:339:ARG:HA	1:C:342:VAL:HG22	1.97	0.45
1:C:341:VAL:C	1:C:343:LYS:N	2.72	0.45
1:C:529:LEU:HD23	1:C:529:LEU:H	1.82	0.45
1:C:540:THR:O	1:C:541:LEU:HD23	2.17	0.45
1:D:69:GLU:OE2	1:D:70:CYS:N	2.49	0.45
1:D:109:ARG:H	1:D:109:ARG:HD2	1.82	0.45
1:D:540:THR:HA	1:D:571:PRO:HA	1.99	0.45
1:C:66:ASP:HB3	1:C:68:TRP:CH2	2.52	0.45
1:C:184:LEU:HD23	1:C:484:PHE:CE1	2.51	0.45
1:C:474:TRP:CE3	1:C:474:TRP:HA	2.51	0.45
1:D:42:GLY:HA2	1:D:50:THR:HG22	1.97	0.45
1:D:125:PRO:O	1:D:128:VAL:HG22	2.16	0.45
1:D:148:ASN:HD22	1:D:148:ASN:N	2.12	0.45
1:D:192:THR:HB	1:D:193:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:LYS:HZ1	1:D:214:GLN:CD	2.24	0.45
1:D:234:ARG:NH1	1:D:234:ARG:CG	2.80	0.45
1:D:339:ARG:O	1:D:340:ARG:C	2.58	0.45
1:D:529:LEU:O	1:D:529:LEU:CG	2.64	0.45
1:D:552:HIS:ND1	1:D:582:SER:N	2.64	0.45
1:C:547:HIS:O	1:C:548:ALA:C	2.59	0.45
1:D:9:ARG:O	1:D:10:PRO:C	2.60	0.45
1:D:283:TYR:OH	1:D:290:PRO:O	2.34	0.45
1:D:442:PHE:HD1	1:D:519:TYR:OH	2.00	0.45
1:C:281:PRO:C	1:C:283:TYR:N	2.75	0.45
1:C:535:ASP:C	1:C:537:ALA:H	2.25	0.45
1:D:40:LEU:O	1:D:81:TYR:HA	2.17	0.45
1:D:383:PHE:HE1	1:D:391:ALA:H	1.63	0.45
1:D:530:VAL:HA	1:D:579:LYS:CB	2.47	0.45
1:C:178:LEU:HD23	1:C:227:LEU:CD2	2.44	0.45
1:C:251:PHE:O	1:C:252:VAL:C	2.59	0.45
1:C:522:GLU:HB3	1:C:527:THR:HG23	1.99	0.45
1:D:1:MET:HB2	1:D:92:ARG:CZ	2.46	0.45
1:D:16:TYR:CD2	1:D:406:PRO:HB3	2.52	0.45
1:D:242:ASN:OD1	1:D:329:GLU:HB3	2.17	0.45
1:D:373:ASN:HD21	1:D:376:PHE:CB	2.23	0.45
1:D:385:ILE:N	1:D:385:ILE:CD1	2.80	0.45
1:D:424:ARG:O	1:D:428:GLN:HG3	2.17	0.45
1:C:76:TYR:C	1:C:77:ARG:HD2	2.42	0.45
1:C:135:GLN:OE1	1:C:420:HIS:CD2	2.70	0.45
1:C:137:PHE:HA	1:C:192:THR:CG2	2.47	0.45
1:D:108:ASP:C	1:D:110:LEU:N	2.75	0.45
1:D:195:PHE:N	1:D:195:PHE:CD2	2.83	0.45
1:D:373:ASN:O	1:D:373:ASN:CG	2.59	0.45
1:D:381:LEU:HA	1:D:385:ILE:HD13	1.98	0.45
1:C:11:ARG:HA	1:C:15:SER:O	2.17	0.44
1:C:237:LEU:HD22	1:C:319:ILE:HG21	2.00	0.44
1:C:241:PHE:CD1	1:C:241:PHE:N	2.85	0.44
1:D:56:MET:HE1	1:D:83:PHE:HD1	1.77	0.44
1:D:306:LEU:HD12	1:D:306:LEU:N	2.14	0.44
1:C:139:GLU:O	1:C:169:GLY:CA	2.64	0.44
1:C:283:TYR:CD1	1:C:283:TYR:N	2.84	0.44
1:C:324:LEU:CB	1:C:353:GLY:HA2	2.44	0.44
1:D:148:ASN:ND2	1:D:149:ASP:N	2.66	0.44
1:D:361:ILE:HD11	1:D:362:TRP:CH2	2.52	0.44
1:D:380:VAL:HG13	1:D:384:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:LYS:O	1:D:436:MET:HB3	2.15	0.44
1:C:6:VAL:HG12	1:C:7:TYR:N	2.32	0.44
1:C:69:GLU:O	1:C:70:CYS:CB	2.65	0.44
1:C:205:THR:HG23	1:C:244:SER:HA	1.98	0.44
1:C:323:ARG:NH1	1:C:372:MET:HE1	2.32	0.44
1:C:416:LEU:HD23	1:C:416:LEU:N	2.26	0.44
1:D:89:HIS:O	1:D:90:GLU:C	2.60	0.44
1:D:160:ASP:O	1:D:162:THR:N	2.49	0.44
1:C:47:TRP:HA	1:C:47:TRP:CE3	2.53	0.44
1:C:59:LEU:HD12	1:C:59:LEU:C	2.42	0.44
1:D:43:ASP:O	1:D:45:TYR:N	2.50	0.44
1:D:56:MET:HG2	1:D:70:CYS:SG	2.58	0.44
1:D:196:LYS:CB	1:D:207:ASP:HB3	2.47	0.44
1:D:222:LYS:O	1:D:223:LYS:C	2.60	0.44
1:D:485:ALA:HA	1:D:488:GLN:OE1	2.18	0.44
1:D:508:LEU:HD12	1:D:508:LEU:H	1.81	0.44
1:D:511:GLU:HB2	1:D:514:SER:HB2	1.99	0.44
1:C:38:TYR:HB2	1:C:53:TYR:HD2	1.82	0.44
1:C:335:TRP:HA	1:C:335:TRP:HE3	1.83	0.44
1:C:416:LEU:HA	1:C:443:GLN:HE21	1.83	0.44
1:C:438:LEU:HD11	1:C:575:PHE:CB	2.47	0.44
1:C:438:LEU:HD23	1:C:577:VAL:HG22	1.99	0.44
1:C:441:LEU:O	1:C:442:PHE:C	2.60	0.44
1:D:303:LYS:HG2	1:D:307:LEU:CD1	2.47	0.44
1:D:313:TRP:HB2	1:D:322:TRP:HZ2	1.83	0.44
1:D:392:GLU:OE2	1:D:512:LYS:HG2	2.17	0.44
1:D:475:ASP:O	1:D:477:THR:N	2.51	0.44
1:D:480:ASP:O	1:D:481:LYS:C	2.60	0.44
1:C:54:VAL:HB	1:C:70:CYS:SG	2.58	0.44
1:C:57:THR:HG22	1:C:58:LYS:N	2.32	0.44
1:C:438:LEU:HD11	1:C:575:PHE:HB3	1.98	0.44
1:D:17:ALA:HB2	1:D:113:TYR:CZ	2.51	0.44
1:D:237:LEU:N	1:D:237:LEU:CD1	2.81	0.44
1:D:281:PRO:HG2	1:D:288:PHE:HA	1.98	0.44
1:D:531:VAL:CG1	1:D:541:LEU:HD12	2.48	0.44
1:C:113:TYR:O	1:C:114:PRO:C	2.61	0.44
1:C:172:GLN:O	1:C:175:ILE:HB	2.18	0.44
1:C:205:THR:HG21	1:C:208:TYR:CZ	2.52	0.44
1:C:457:GLU:HA	1:C:487:TYR:CE1	2.52	0.44
1:D:175:ILE:O	1:D:178:LEU:HB2	2.17	0.44
1:D:323:ARG:HH21	1:D:325:ASP:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ASN:O	1:D:443:GLN:NE2	2.51	0.44
1:D:508:LEU:HD13	1:D:519:TYR:CA	2.46	0.44
1:D:579:LYS:O	1:D:580:ALA:HB2	2.17	0.44
1:C:328:ASN:N	1:C:328:ASN:HD22	2.16	0.44
1:C:332:HIS:HE1	1:C:362:TRP:CZ2	2.36	0.44
1:C:362:TRP:HB3	1:C:368:PHE:CD2	2.53	0.44
1:C:497:HIS:HD2	1:C:526:ASP:OD2	2.00	0.44
1:D:42:GLY:C	1:D:79:VAL:HG23	2.43	0.44
1:D:79:VAL:HG22	1:D:80:LYS:O	2.18	0.44
1:D:222:LYS:C	1:D:222:LYS:CD	2.91	0.44
1:D:391:ALA:O	1:D:510:ALA:C	2.60	0.44
1:D:544:PRO:HA	1:D:567:THR:HG22	1.99	0.44
1:C:11:ARG:NH2	1:C:114:PRO:HD2	2.33	0.44
1:C:515:ARG:O	1:C:534:ASN:HB2	2.17	0.44
1:C:534:ASN:HD22	1:C:534:ASN:HA	1.60	0.44
1:D:173:GLY:O	1:D:174:VAL:C	2.61	0.44
1:C:18:TYR:HB2	1:C:24:HIS:CD2	2.52	0.43
1:C:432:ASP:O	1:C:433:LYS:C	2.61	0.43
1:D:12:LYS:HA	1:D:364:GLU:OE1	2.17	0.43
1:D:142:ALA:O	1:D:169:GLY:HA2	2.18	0.43
1:D:296:ASN:ND2	1:D:298:GLU:HB2	2.32	0.43
1:C:23:VAL:HB	1:C:72:VAL:CG1	2.48	0.43
1:C:136:ILE:O	1:C:138:PRO:HD3	2.18	0.43
1:C:242:ASN:OD1	1:C:294:LYS:HG3	2.17	0.43
1:C:242:ASN:OD1	1:C:294:LYS:HE2	2.18	0.43
1:C:281:PRO:HG3	1:C:290:PRO:HG3	2.01	0.43
1:C:424:ARG:NE	1:C:453:TYR:CE2	2.85	0.43
1:D:75:PRO:HB2	1:D:76:TYR:CE2	2.53	0.43
1:D:237:LEU:CD1	1:D:319:ILE:HG21	2.49	0.43
1:C:263:TYR:N	1:C:263:TYR:CD1	2.86	0.43
1:C:267:PHE:C	1:C:268:HIS:ND1	2.76	0.43
1:C:333:GLN:O	1:C:336:ARG:N	2.50	0.43
1:C:552:HIS:HB2	1:C:561:ALA:O	2.17	0.43
1:C:554:TRP:CB	1:C:559:LEU:HB3	2.47	0.43
1:D:153:THR:OG1	1:D:154:LEU:N	2.48	0.43
1:D:177:HIS:HB3	1:D:474:TRP:CH2	2.53	0.43
1:D:260:LYS:O	1:D:261:SER:C	2.61	0.43
1:D:446:TYR:C	1:D:521:ARG:HH12	2.27	0.43
1:D:529:LEU:HD23	1:D:580:ALA:O	2.19	0.43
1:D:84:LEU:HD21	1:D:91:LYS:HB2	2.00	0.43
1:C:139:GLU:O	1:C:139:GLU:OE1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:LEU:C	1:C:237:LEU:HD12	2.43	0.43
1:C:323:ARG:NH2	1:C:325:ASP:HA	2.14	0.43
1:C:327:ALA:O	1:C:329:GLU:N	2.47	0.43
1:C:393:LYS:O	1:C:397:MET:HG3	2.18	0.43
1:C:439:ALA:O	1:C:440:VAL:C	2.62	0.43
1:D:75:PRO:C	1:D:77:ARG:N	2.75	0.43
1:D:156:TRP:CH2	1:D:163:PRO:HD3	2.54	0.43
1:D:241:PHE:HB3	1:D:306:LEU:CD2	2.48	0.43
1:D:493:LEU:HD12	1:D:493:LEU:N	2.34	0.43
1:C:206:GLU:CD	1:C:247:THR:HG21	2.43	0.43
1:C:211:ILE:O	1:C:212:ASP:C	2.59	0.43
1:C:327:ALA:HB1	1:C:368:PHE:HZ	1.84	0.43
1:C:332:HIS:O	1:C:335:TRP:HB2	2.18	0.43
1:C:519:TYR:OH	1:C:532:MET:HE2	2.19	0.43
1:D:40:LEU:HD23	1:D:40:LEU:HA	1.89	0.43
1:D:138:PRO:O	1:D:140:ARG:N	2.51	0.43
1:D:296:ASN:C	1:D:296:ASN:ND2	2.76	0.43
1:D:427:THR:HG21	1:D:462:GLY:H	1.84	0.43
1:D:546:ARG:HB2	1:D:549:GLN:NE2	2.33	0.43
1:C:13:ASN:ND2	1:C:403:ALA:O	2.51	0.43
1:C:19:ASN:HD21	1:C:22:THR:CA	2.26	0.43
1:C:214:GLN:CG	1:C:215:PHE:N	2.82	0.43
1:C:444:PHE:C	1:C:494:ARG:HD3	2.43	0.43
1:C:578:LEU:N	1:C:578:LEU:HD12	2.33	0.43
1:D:471:CYS:O	1:D:472:MET:C	2.61	0.43
1:D:498:ALA:O	1:D:499:ALA:C	2.60	0.43
1:D:552:HIS:C	1:D:553:LEU:HD12	2.44	0.43
1:C:58:LYS:HD2	1:C:61:THR:OG1	2.19	0.43
1:C:139:GLU:HG3	1:C:200:ASN:CA	2.49	0.43
1:C:250:PRO:HG2	1:C:266:TRP:CZ3	2.53	0.43
1:C:373:ASN:ND2	1:C:415:ASN:ND2	2.61	0.43
1:D:203:TYR:C	1:D:205:THR:N	2.77	0.43
1:D:248:PHE:O	1:D:252:VAL:HG23	2.18	0.43
1:D:332:HIS:O	1:D:336:ARG:HG3	2.18	0.43
1:D:551:THR:O	1:D:552:HIS:CG	2.72	0.43
1:C:180:HIS:O	1:C:183:LYS:HB3	2.19	0.43
1:C:494:ARG:HG2	1:C:494:ARG:HH11	1.84	0.43
1:C:530:VAL:HG22	1:C:579:LYS:HB2	2.01	0.43
1:C:555:GLN:O	1:C:556:ASP:C	2.61	0.43
1:D:168:GLY:O	1:D:169:GLY:C	2.62	0.43
1:D:219:ASP:O	1:D:220:THR:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:PHE:O	1:D:242:ASN:C	2.60	0.43
1:C:60:ALA:CB	1:C:402:LEU:HD23	2.46	0.43
1:C:96:GLU:C	1:C:97:TYR:CD2	2.96	0.43
1:C:380:VAL:HA	1:C:394:PHE:CE1	2.54	0.43
1:C:475:ASP:O	1:C:477:THR:N	2.52	0.43
1:D:28:ARG:HD2	1:D:65:PHE:CG	2.54	0.43
1:D:143:ASN:HD21	1:D:170:ASP:CG	2.26	0.43
1:D:160:ASP:C	1:D:162:THR:N	2.72	0.43
1:D:239:ALA:HB2	1:D:322:TRP:CE3	2.54	0.43
1:D:357:HIS:C	1:D:357:HIS:ND1	2.76	0.43
1:C:373:ASN:CB	1:C:415:ASN:HD22	2.31	0.42
1:C:552:HIS:O	1:C:561:ALA:N	2.48	0.42
1:C:558:VAL:HG12	1:C:558:VAL:O	2.18	0.42
1:D:212:ASP:C	1:D:214:GLN:H	2.27	0.42
1:D:491:ILE:C	1:D:493:LEU:N	2.77	0.42
1:C:81:TYR:O	1:C:111:PHE:N	2.53	0.42
1:C:408:GLN:O	1:C:409:ALA:C	2.61	0.42
1:D:81:TYR:CE1	1:D:111:PHE:HB2	2.54	0.42
1:D:86:GLN:HG3	1:D:91:LYS:CB	2.36	0.42
1:D:137:PHE:CE1	1:D:140:ARG:HG2	2.54	0.42
1:D:167:PHE:CE2	1:D:471:CYS:HB2	2.54	0.42
1:C:144:GLY:HA3	1:C:172:GLN:OE1	2.18	0.42
1:C:179:ASP:HA	1:C:182:SER:OG	2.19	0.42
1:C:446:TYR:C	1:C:521:ARG:HH12	2.28	0.42
1:C:499:ALA:HB3	1:C:528:ILE:HD12	2.01	0.42
1:D:3:LEU:HA	1:D:6:VAL:HG23	2.00	0.42
1:D:148:ASN:H	1:D:148:ASN:ND2	2.17	0.42
1:D:174:VAL:O	1:D:175:ILE:C	2.61	0.42
1:D:208:TYR:HD1	1:D:305:TYR:HH	1.67	0.42
1:D:244:SER:O	1:D:292:MET:HA	2.19	0.42
1:D:322:TRP:CE3	1:D:322:TRP:HA	2.54	0.42
1:D:426:LEU:HB2	1:D:436:MET:HE1	2.00	0.42
1:C:27:ILE:CB	1:C:56:MET:HE1	2.49	0.42
1:C:41:ALA:HB1	1:C:79:VAL:CG2	2.50	0.42
1:C:373:ASN:O	1:C:376:PHE:HB3	2.19	0.42
1:C:384:PHE:O	1:C:387:GLN:HG3	2.20	0.42
1:D:123:GLN:HE21	1:D:123:GLN:HB3	1.55	0.42
1:D:137:PHE:CZ	1:D:469:ARG:NE	2.87	0.42
1:D:246:ARG:HA	1:D:251:PHE:CD2	2.54	0.42
1:D:441:LEU:CD2	1:D:577:VAL:HB	2.49	0.42
1:C:226:ASP:O	1:C:230:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:CYS:HA	1:D:200:ASN:HB3	2.01	0.42
1:C:194:LEU:HD23	1:C:194:LEU:H	1.84	0.42
1:C:251:PHE:CZ	1:C:255:LEU:HD21	2.55	0.42
1:C:323:ARG:HG2	1:C:352:LEU:HD23	2.00	0.42
1:C:456:ASP:C	1:C:458:VAL:N	2.73	0.42
1:D:133:PHE:CE1	1:D:449:THR:HB	2.54	0.42
1:C:96:GLU:C	1:C:97:TYR:HD2	2.28	0.42
1:C:107:PRO:HA	1:C:110:LEU:HG	2.01	0.42
1:C:122:PHE:CD2	1:C:365:GLY:N	2.87	0.42
1:C:274:LEU:CA	1:C:282:THR:HG21	2.44	0.42
1:D:128:VAL:C	1:D:130:ASP:N	2.76	0.42
1:D:192:THR:O	1:D:193:PRO:C	2.63	0.42
1:C:29:THR:HG21	1:C:34:MET:HG3	2.02	0.42
1:C:97:TYR:CD2	1:C:97:TYR:N	2.85	0.42
1:C:184:LEU:HD13	1:C:491:ILE:HD13	2.01	0.42
1:C:570:LEU:HA	1:C:571:PRO:HD3	1.76	0.42
1:D:239:ALA:N	1:D:323:ARG:O	2.40	0.42
1:D:459:GLY:O	1:D:460:LEU:HD23	2.20	0.42
1:D:550:TRP:HA	1:D:550:TRP:CE3	2.55	0.42
1:C:24:HIS:CE1	1:C:407:ARG:HH11	2.37	0.42
1:C:37:VAL:O	1:C:56:MET:HB2	2.20	0.42
1:C:81:TYR:O	1:C:110:LEU:HB3	2.20	0.42
1:C:151:GLU:O	1:C:152:GLY:O	2.37	0.42
1:C:574:GLY:O	1:C:575:PHE:CD1	2.73	0.42
1:D:37:VAL:O	1:D:56:MET:HB2	2.20	0.42
1:D:122:PHE:CD1	1:D:122:PHE:C	2.97	0.42
1:D:534:ASN:O	1:D:575:PHE:CZ	2.73	0.42
1:C:117:ASN:O	1:C:119:VAL:N	2.53	0.42
1:C:228:CYS:CA	1:C:233:ILE:HG13	2.50	0.42
1:C:246:ARG:HD3	1:C:251:PHE:HE2	1.85	0.42
1:C:430:ASP:C	1:C:432:ASP:H	2.27	0.42
1:C:438:LEU:HD21	1:C:575:PHE:O	2.20	0.42
1:D:125:PRO:C	1:D:127:TRP:N	2.77	0.42
1:D:189:VAL:CG1	1:D:191:PHE:HE2	2.32	0.42
1:D:410:SER:O	1:D:411:GLU:C	2.63	0.42
1:D:578:LEU:H	1:D:578:LEU:CD2	2.31	0.42
1:C:12:LYS:HD3	1:C:360:SER:OG	2.20	0.41
1:C:254:VAL:HA	1:C:261:SER:CB	2.50	0.41
1:D:1:MET:C	1:D:2:PHE:CD1	2.98	0.41
1:D:236:LEU:CG	1:D:321:GLY:HA3	2.50	0.41
1:D:412:VAL:O	1:D:413:MET:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:TRP:C	1:C:127:TRP:CE3	2.98	0.41
1:C:271:SER:O	1:C:272:LEU:C	2.64	0.41
1:D:134:TYR:O	1:D:190:TYR:N	2.53	0.41
1:D:538:GLY:O	1:D:539:HIS:HB2	2.20	0.41
1:C:225:VAL:O	1:C:228:CYS:HB2	2.19	0.41
1:C:249:PRO:O	1:C:250:PRO:C	2.61	0.41
1:C:510:ALA:O	1:C:511:GLU:O	2.37	0.41
1:C:518:ALA:CB	1:C:531:VAL:HG22	2.51	0.41
1:D:106:ASN:C	1:D:106:ASN:ND2	2.77	0.41
1:C:1:MET:SD	1:C:34:MET:HE1	2.60	0.41
1:C:2:PHE:HB2	1:C:33:ASP:OD2	2.20	0.41
1:C:127:TRP:HE3	1:C:127:TRP:O	2.03	0.41
1:C:137:PHE:HB3	1:C:454:TYR:HE2	1.85	0.41
1:C:179:ASP:OD1	1:C:231:ARG:NH1	2.51	0.41
1:C:324:LEU:HB2	1:C:353:GLY:CA	2.47	0.41
1:C:481:LYS:C	1:C:483:LEU:N	2.78	0.41
1:C:537:ALA:O	1:C:574:GLY:HA2	2.20	0.41
1:D:74:PRO:HA	1:D:75:PRO:HD3	1.80	0.41
1:D:224:LEU:C	1:D:224:LEU:CD2	2.93	0.41
1:D:237:LEU:HD11	1:D:319:ILE:HG21	2.01	0.41
1:D:248:PHE:HD2	1:D:267:PHE:HZ	1.67	0.41
1:D:332:HIS:O	1:D:333:GLN:C	2.64	0.41
1:C:8:HIS:CE1	1:C:83:PHE:HZ	2.38	0.41
1:C:128:VAL:HG23	1:C:129:LYS:H	1.85	0.41
1:C:430:ASP:C	1:C:432:ASP:N	2.79	0.41
1:D:248:PHE:CD2	1:D:250:PRO:HD2	2.55	0.41
1:D:248:PHE:C	1:D:252:VAL:HG23	2.46	0.41
1:D:386:HIS:CB	1:D:388:ILE:HG12	2.49	0.41
1:D:577:VAL:O	1:D:578:LEU:C	2.63	0.41
1:C:140:ARG:NH2	1:C:167:PHE:CD2	2.89	0.41
1:C:241:PHE:N	1:C:241:PHE:HD1	2.18	0.41
1:C:303:LYS:C	1:C:307:LEU:HG	2.46	0.41
1:C:485:ALA:O	1:C:486:PHE:C	2.64	0.41
1:D:23:VAL:HG23	1:D:116:ILE:HD11	2.03	0.41
1:D:31:LYS:O	1:D:66:ASP:CG	2.64	0.41
1:D:390:ASP:N	1:D:390:ASP:OD1	2.53	0.41
1:D:416:LEU:H	1:D:416:LEU:CD2	2.25	0.41
1:D:446:TYR:C	1:D:521:ARG:NH1	2.78	0.41
1:D:486:PHE:O	1:D:490:VAL:HG23	2.21	0.41
1:D:491:ILE:O	1:D:493:LEU:N	2.53	0.41
1:D:516:GLN:CD	1:D:516:GLN:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LYS:HD3	1:C:33:ASP:HB2	2.03	0.41
1:C:137:PHE:HA	1:C:192:THR:HG23	2.03	0.41
1:C:194:LEU:N	1:C:194:LEU:CD2	2.82	0.41
1:C:354:GLU:HG2	1:C:356:TRP:HE1	1.86	0.41
1:C:413:MET:HB3	1:C:415:ASN:ND2	2.36	0.41
1:C:517:ILE:O	1:C:531:VAL:HA	2.21	0.41
1:C:554:TRP:N	1:C:559:LEU:O	2.53	0.41
1:D:62:ASP:HB3	1:D:400:LYS:HB2	2.01	0.41
1:D:243:HIS:C	1:D:295:LEU:CD2	2.93	0.41
1:D:246:ARG:HH11	1:D:255:LEU:CD1	2.33	0.41
1:D:274:LEU:HA	1:D:282:THR:HG21	2.02	0.41
1:D:352:LEU:HA	1:D:370:ALA:O	2.20	0.41
1:D:383:PHE:HD2	1:D:384:PHE:CZ	2.38	0.41
1:D:490:VAL:O	1:D:493:LEU:HB2	2.20	0.41
1:D:531:VAL:H	1:D:579:LYS:HB3	1.85	0.41
1:D:533:ASN:O	1:D:533:ASN:CG	2.63	0.41
1:C:100:LEU:CD1	1:C:104:PRO:HG3	2.49	0.41
1:C:118:PRO:HA	1:C:121:VAL:CG2	2.51	0.41
1:D:156:TRP:CH2	1:D:161:PRO:HA	2.55	0.41
1:D:302:VAL:O	1:D:306:LEU:HD12	2.20	0.41
1:D:498:ALA:HB1	1:D:502:THR:OG1	2.21	0.41
1:D:512:LYS:HB3	1:D:512:LYS:HZ2	1.85	0.41
1:C:201:HIS:HD2	1:C:203:TYR:HB2	1.85	0.41
1:C:283:TYR:HE2	1:C:293:PRO:HG3	1.85	0.41
1:C:291:LEU:H	1:C:291:LEU:CD1	2.34	0.41
1:C:339:ARG:O	1:C:343:LYS:HG2	2.21	0.41
1:C:498:ALA:O	1:C:501:ARG:HB2	2.21	0.41
1:D:62:ASP:OD1	1:D:400:LYS:HD3	2.21	0.41
1:D:111:PHE:CD2	1:D:111:PHE:N	2.88	0.41
1:D:516:GLN:O	1:D:517:ILE:HD12	2.20	0.41
1:D:540:THR:O	1:D:540:THR:HG22	2.20	0.41
1:D:554:TRP:CD1	1:D:579:LYS:H	2.39	0.41
1:C:29:THR:OG1	1:C:68:TRP:CH2	2.73	0.41
1:C:230:GLU:OE1	1:C:230:GLU:HA	2.21	0.41
1:C:260:LYS:O	1:C:261:SER:C	2.64	0.41
1:C:278:ASP:O	1:C:279:GLY:O	2.38	0.41
1:C:308:LYS:HA	1:C:311:GLU:CG	2.51	0.41
1:C:374:TYR:O	1:C:375:PRO:C	2.60	0.41
1:D:13:ASN:HB3	1:D:404:GLY:O	2.21	0.41
1:D:37:VAL:C	1:D:38:TYR:CD2	2.98	0.41
1:D:188:ALA:HB1	1:D:236:LEU:CD1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:HIS:HB2	1:C:27:ILE:HD13	1.99	0.40
1:C:24:HIS:NE2	1:C:407:ARG:HD2	2.37	0.40
1:C:69:GLU:OE1	1:C:407:ARG:NH2	2.54	0.40
1:C:313:TRP:O	1:C:314:ILE:C	2.64	0.40
1:C:323:ARG:HG2	1:C:352:LEU:CD2	2.50	0.40
1:C:413:MET:O	1:C:449:THR:N	2.52	0.40
1:D:46:MET:HE3	1:D:46:MET:HB2	1.95	0.40
1:D:75:PRO:C	1:D:77:ARG:H	2.29	0.40
1:D:94:MET:HB2	1:D:99:PHE:CE1	2.56	0.40
1:D:168:GLY:O	1:D:170:ASP:OD2	2.39	0.40
1:D:264:LYS:C	1:D:266:TRP:N	2.79	0.40
1:D:352:LEU:N	1:D:352:LEU:CD2	2.84	0.40
1:D:359:SER:OG	1:D:371:VAL:HG21	2.21	0.40
1:D:373:ASN:OD1	1:D:373:ASN:C	2.61	0.40
1:D:560:THR:O	1:D:561:ALA:C	2.63	0.40
1:C:20:GLY:O	1:C:21:THR:HB	2.21	0.40
1:C:84:LEU:O	1:C:85:LEU:C	2.64	0.40
1:C:115:PHE:CD1	1:C:116:ILE:N	2.89	0.40
1:C:135:GLN:NE2	1:C:453:TYR:HD1	2.19	0.40
1:C:299:HIS:HB3	1:C:302:VAL:HB	2.04	0.40
1:D:179:ASP:O	1:D:180:HIS:C	2.64	0.40
1:D:252:VAL:C	1:D:254:VAL:N	2.78	0.40
1:D:268:HIS:HB2	1:D:284:ASP:HB2	2.03	0.40
1:D:377:THR:O	1:D:378:ASN:C	2.65	0.40
1:D:452:ILE:HD13	1:D:452:ILE:HA	1.80	0.40
1:C:235:VAL:H	1:C:320:ASP:CB	2.28	0.40
1:C:438:LEU:HD11	1:C:575:PHE:HA	2.04	0.40
1:D:37:VAL:HG23	1:D:37:VAL:O	2.20	0.40
1:D:38:TYR:HA	1:D:54:VAL:O	2.21	0.40
1:D:85:LEU:HD12	1:D:85:LEU:N	2.37	0.40
1:D:193:PRO:CG	1:D:202:LYS:O	2.70	0.40
1:D:262:LYS:C	1:D:264:LYS:H	2.28	0.40
1:D:346:ASN:OD1	1:D:348:ASP:N	2.54	0.40
1:C:410:SER:HA	1:C:413:MET:HG2	2.03	0.40
1:C:439:ALA:C	1:C:441:LEU:N	2.79	0.40
1:D:133:PHE:CD2	1:D:188:ALA:HB3	2.57	0.40
1:D:224:LEU:O	1:D:225:VAL:C	2.65	0.40
1:D:238:ASP:OD1	1:D:239:ALA:N	2.55	0.40
1:D:303:LYS:O	1:D:304:GLU:C	2.65	0.40
1:D:374:TYR:O	1:D:377:THR:N	2.55	0.40
1:D:376:PHE:CE2	1:D:415:ASN:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:GLN:HA	1:D:411:GLU:OE1	2.19	0.40
1:D:579:LYS:HE2	1:D:580:ALA:N	2.35	0.40
1:D:579:LYS:HB2	1:D:580:ALA:H	1.75	0.40
1:C:11:ARG:CG	1:C:11:ARG:HH11	2.35	0.40
1:C:119:VAL:CG1	1:C:120:ASP:N	2.85	0.40
1:C:424:ARG:HH12	1:C:460:LEU:CD1	2.27	0.40
1:D:118:PRO:HA	1:D:121:VAL:CG2	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LYS:NZ	1:C:12:LYS:NZ[4_566]	1.77	0.43

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	581/583 (100%)	384 (66%)	138 (24%)	59 (10%)	0 2
1	D	581/583 (100%)	360 (62%)	158 (27%)	63 (11%)	0 2
All	All	1162/1166 (100%)	744 (64%)	296 (26%)	122 (10%)	0 2

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	15	SER
1	C	31	LYS
1	C	49	HIS
1	C	70	CYS
1	C	114	PRO
1	C	152	GLY

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Mol	Chain	Res	Type
1	C	286	PHE
1	C	430	ASP
1	C	456	ASP
1	C	505	PHE
1	C	512	LYS
1	C	576	ALA
1	D	21	THR
1	D	31	LYS
1	D	46	MET
1	D	47	TRP
1	D	155	PRO
1	D	265	ASP
1	D	430	ASP
1	D	490	VAL
1	D	525	GLN
1	D	539	HIS
1	D	540	THR
1	D	563	HIS
1	D	565	GLN
1	D	566	LEU
1	D	568	VAL
1	C	2	PHE
1	C	21	THR
1	C	155	PRO
1	C	196	LYS
1	C	260	LYS
1	C	276	VAL
1	C	277	VAL
1	C	279	GLY
1	C	282	THR
1	C	455	GLY
1	C	476	GLU
1	C	511	GLU
1	C	513	ASN
1	C	549	GLN
1	C	555	GLN
1	D	86	GLN
1	D	139	GLU
1	D	169	GLY
1	D	179	ASP
1	D	258	GLY
1	D	259	GLU

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Mol	Chain	Res	Type
1	D	277	VAL
1	D	391	ALA
1	D	392	GLU
1	D	476	GLU
1	D	510	ALA
1	D	550	TRP
1	D	557	ASP
1	D	561	ALA
1	C	11	ARG
1	C	77	ARG
1	C	134	TYR
1	C	312	TYR
1	C	328	ASN
1	C	348	ASP
1	C	504	THR
1	C	535	ASP
1	D	10	PRO
1	D	44	LYS
1	D	48	ASP
1	D	114	PRO
1	D	175	ILE
1	D	198	THR
1	D	205	THR
1	D	278	ASP
1	D	297	THR
1	D	431	GLY
1	D	432	ASP
1	D	438	LEU
1	D	556	ASP
1	C	48	ASP
1	C	85	LEU
1	C	125	PRO
1	C	307	LEU
1	C	325	ASP
1	C	399	GLY
1	C	510	ALA
1	D	67	TYR
1	D	125	PRO
1	D	126	ALA
1	D	196	LYS
1	D	202	LYS
1	D	261	SER

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Mol	Chain	Res	Type
1	D	312	TYR
1	D	413	MET
1	D	551	THR
1	C	63	GLU
1	C	118	PRO
1	C	162	THR
1	C	480	ASP
1	D	8	HIS
1	D	407	ARG
1	D	481	LYS
1	D	492	ARG
1	C	133	PHE
1	C	154	LEU
1	C	248	PHE
1	C	291	LEU
1	C	303	LYS
1	C	525	GLN
1	D	578	LEU
1	D	213	PRO
1	D	380	VAL
1	C	55	PRO
1	C	249	PRO
1	C	319	ILE
1	C	577	VAL
1	D	361	ILE
1	D	375	PRO
1	C	491	ILE
1	D	103	PRO
1	D	107	PRO
1	D	173	GLY
1	C	240	VAL
1	C	538	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	508/508 (100%)	464 (91%)	44 (9%)	9	36
1	D	508/508 (100%)	456 (90%)	52 (10%)	7	29
All	All	1016/1016 (100%)	920 (91%)	96 (9%)	8	33

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	LEU
1	C	9	ARG
1	C	11	ARG
1	C	19	ASN
1	C	27	ILE
1	C	40	LEU
1	C	43	ASP
1	C	48	ASP
1	C	49	HIS
1	C	64	LEU
1	C	93	TRP
1	C	100	LEU
1	C	106	ASN
1	C	109	ARG
1	C	114	PRO
1	C	139	GLU
1	C	140	ARG
1	C	155	PRO
1	C	166	PHE
1	C	180	HIS
1	C	194	LEU
1	C	214	GLN
1	C	229	HIS
1	C	233	ILE
1	C	236	LEU
1	C	246	ARG
1	C	253	ASP
1	C	266	TRP
1	C	328	ASN
1	C	382	ASP
1	C	430	ASP
1	C	457	GLU
1	C	465	ASP
1	C	479	HIS
1	C	509	THR

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Mol	Chain	Res	Type
1	C	525	GLN
1	C	528	ILE
1	C	529	LEU
1	C	534	ASN
1	C	543	LEU
1	C	553	LEU
1	C	555	GLN
1	C	573	TYR
1	C	579	LYS
1	D	3	LEU
1	D	19	ASN
1	D	25	LEU
1	D	44	LYS
1	D	64	LEU
1	D	68	TRP
1	D	69	GLU
1	D	98	ASP
1	D	106	ASN
1	D	109	ARG
1	D	114	PRO
1	D	123	GLN
1	D	148	ASN
1	D	156	TRP
1	D	178	LEU
1	D	184	LEU
1	D	194	LEU
1	D	196	LYS
1	D	199	THR
1	D	234	ARG
1	D	236	LEU
1	D	237	LEU
1	D	265	ASP
1	D	272	LEU
1	D	275	GLU
1	D	317	THR
1	D	322	TRP
1	D	328	ASN
1	D	329	GLU
1	D	352	LEU
1	D	368	PHE
1	D	373	ASN
1	D	377	THR

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Mol	Chain	Res	Type
1	D	382	ASP
1	D	393	LYS
1	D	434	ARG
1	D	452	ILE
1	D	457	GLU
1	D	458	VAL
1	D	482	ASP
1	D	502	THR
1	D	517	ILE
1	D	522	GLU
1	D	525	GLN
1	D	528	ILE
1	D	539	HIS
1	D	543	LEU
1	D	549	GLN
1	D	550	TRP
1	D	553	LEU
1	D	578	LEU
1	D	579	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	HIS
1	C	19	ASN
1	C	106	ASN
1	C	117	ASN
1	C	123	GLN
1	C	135	GLN
1	C	143	ASN
1	C	148	ASN
1	C	177	HIS
1	C	201	HIS
1	C	296	ASN
1	C	299	HIS
1	C	328	ASN
1	C	333	GLN
1	C	344	GLN
1	C	415	ASN
1	C	420	HIS
1	C	479	HIS
1	C	488	GLN

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Mol	Chain	Res	Type
1	C	495	GLN
1	C	497	HIS
1	C	534	ASN
1	C	539	HIS
1	D	19	ASN
1	D	106	ASN
1	D	123	GLN
1	D	148	ASN
1	D	177	HIS
1	D	187	ASN
1	D	296	ASN
1	D	299	HIS
1	D	328	ASN
1	D	332	HIS
1	D	344	GLN
1	D	367	GLN
1	D	378	ASN
1	D	386	HIS
1	D	387	GLN
1	D	401	GLN
1	D	415	ASN
1	D	428	GLN
1	D	495	GLN
1	D	534	ASN
1	D	552	HIS
1	D	563	HIS
1	D	565	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 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.