



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 04:11 AM EST

PDB ID : 6U5U
EMDB ID : EMD-20656
Title : Electron cryomicroscopy Structure of *S. cerevisiae* FAS in the KS-stalled state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2019-08-28
Resolution : 2.80 Å (reported)
Based on initial model : 2UV8

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

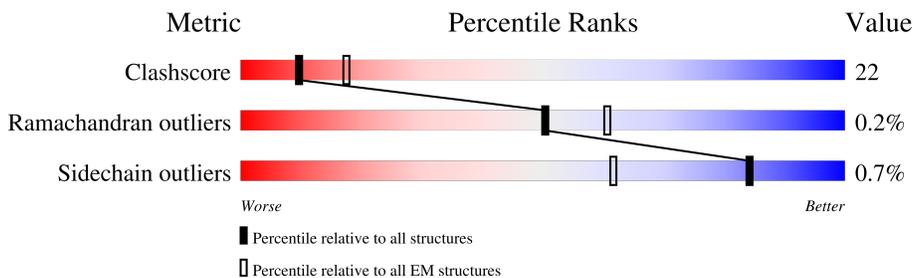
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1887	
2	G	2073	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAP	G	2102	-	-	X	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 28298 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1611	12171	7684	2081	2362	44	0	0

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	2033	15995	10253	2660	3026	56	0	0

There are 22 discrepancies between the modelled and reference sequences:

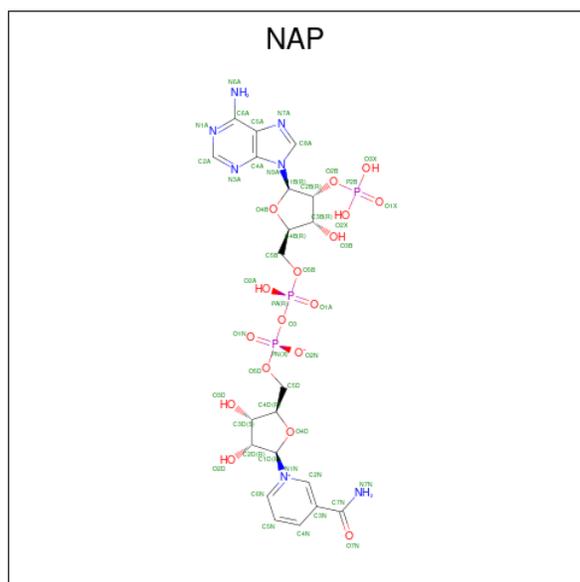
Chain	Residue	Modelled	Actual	Comment	Reference
G	2052	ASP	-	expression tag	UNP P07149
G	2053	TYR	-	expression tag	UNP P07149
G	2054	LYS	-	expression tag	UNP P07149
G	2055	ASP	-	expression tag	UNP P07149
G	2056	HIS	-	expression tag	UNP P07149
G	2057	ASP	-	expression tag	UNP P07149
G	2058	GLY	-	expression tag	UNP P07149
G	2059	ASP	-	expression tag	UNP P07149
G	2060	TYR	-	expression tag	UNP P07149
G	2061	LYS	-	expression tag	UNP P07149
G	2062	ASP	-	expression tag	UNP P07149
G	2063	HIS	-	expression tag	UNP P07149
G	2064	ASP	-	expression tag	UNP P07149
G	2065	ILE	-	expression tag	UNP P07149
G	2066	ASP	-	expression tag	UNP P07149
G	2067	TYR	-	expression tag	UNP P07149
G	2068	LYS	-	expression tag	UNP P07149
G	2069	ASP	-	expression tag	UNP P07149
G	2070	ASP	-	expression tag	UNP P07149
G	2071	ASP	-	expression tag	UNP P07149
G	2072	ASP	-	expression tag	UNP P07149

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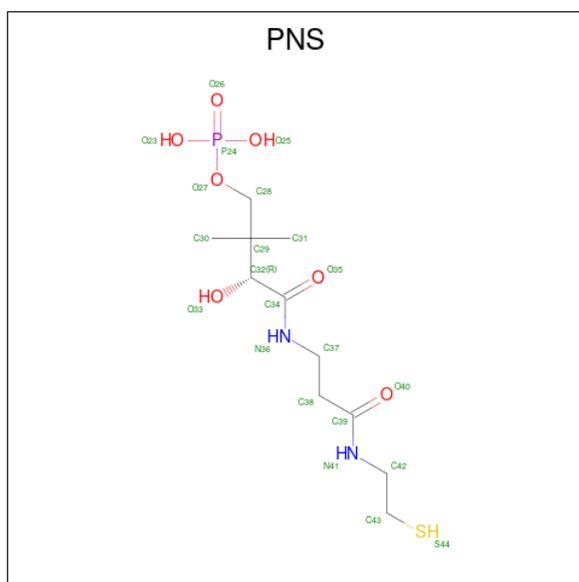
Chain	Residue	Modelled	Actual	Comment	Reference
G	2073	LYS	-	expression tag	UNP P07149

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



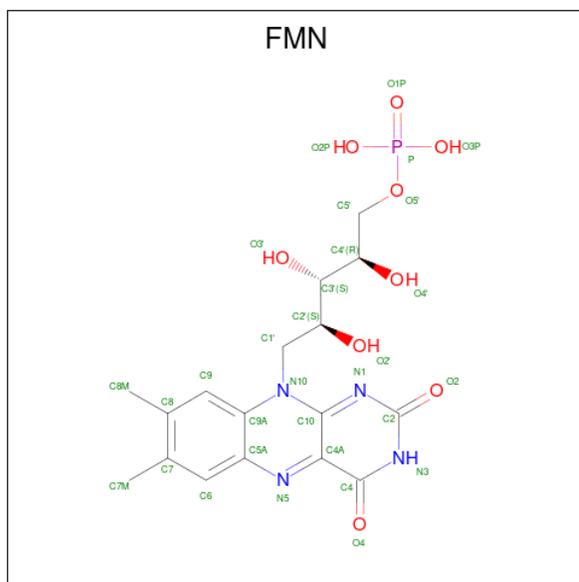
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
3	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	G	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			5	1	3	1	

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).

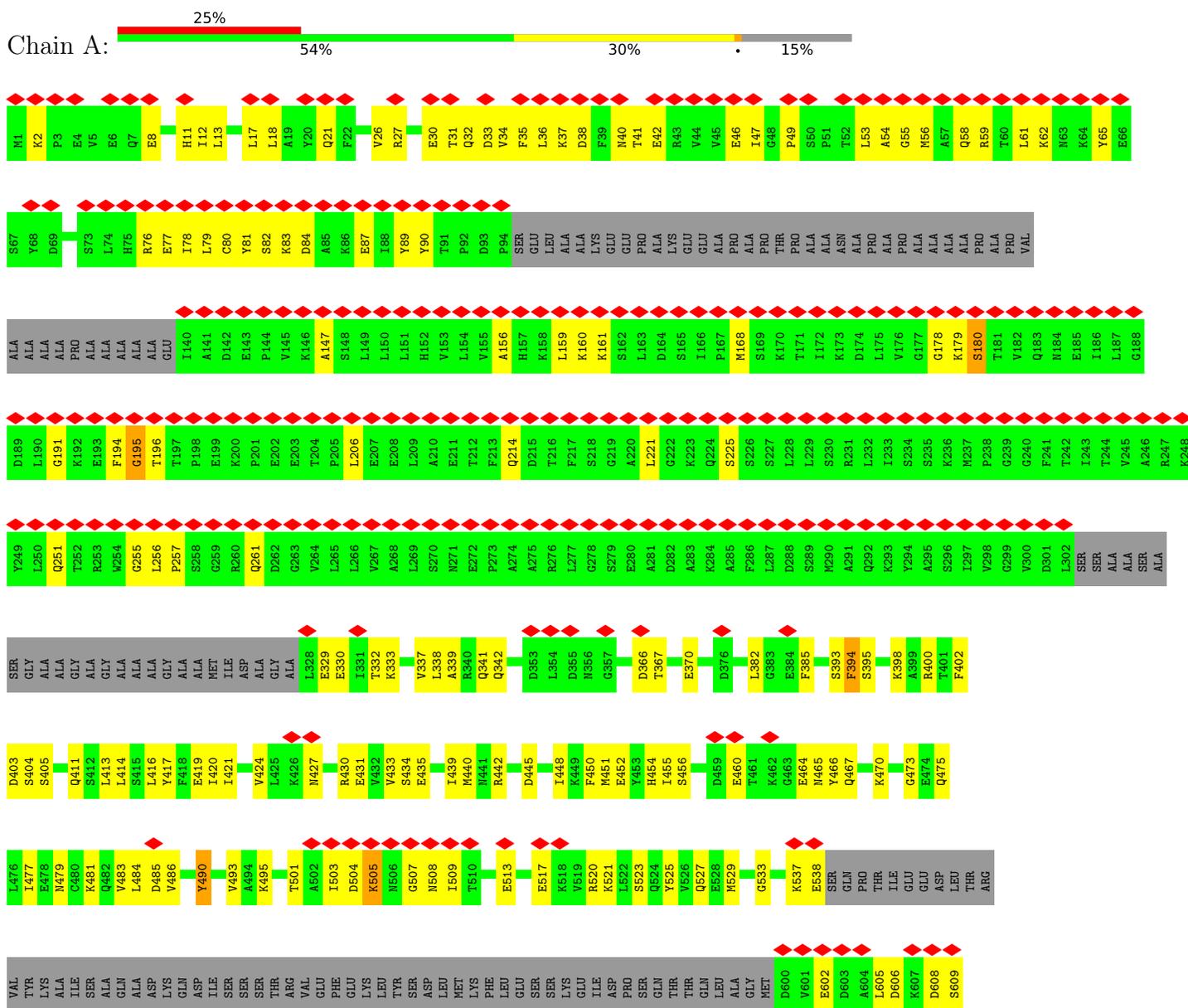


Mol	Chain	Residues	Atoms				AltConf	
5	G	1	Total	C	N	O	P	0
			31	17	4	9	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fatty acid synthase subunit alpha



T810	K611	E812	V613	L616	P617	N618	K619	S620	T621	I622	S623	K624	T625	V626	S627	S628	T629	I630	P631	R632	E633	T634	I635	L640	D652	R653	S656	S657	L658	D661	G662	F673	Y677	T681	G684	I688	L693	Q694	G695	Q698	V705	T706	S708	R709	F710									
S711	K712	Q713	V714	T715	D716	Y718	K724	Y725	G726	A727	K728	G729	T731	L732	I733	V734	P735	Q739	G740	R741	D744	V745	E746	A747	L640	E750	Y753	K757	N758	G759	G760	D764	L765	D766	I768	P770	F771	A772	I774	W775	E776	Q777	I779	I784	D785									
S786	K787	A791	I794	N798	M802	M803	G804	K807	K808	Q809	K810	R813	R818	P819	A820	Q821	V822	I823	L824	S827	P828	V829	N829	D836	G837	M838	Y839	S840	E841	S842	L844	S845	L846	E847	T848	F850	N851	R852	W853	E856	S857	W858	A859	N860	Q861	L862	C865							
I868	I869	R873	G874	T875	GLY	LEU	MET	SER	ALA	N881	N882	I883	I884	A885	E886	G892	V893	R894	E900	L906	T910	P911	E912	L916	P921	D925	N926	N927	L930	Q931	L938	D944	Q945	E949	E952	V953	R954	K955	A956	V957	S958	I959	E960											
T961	A962	L963	E964	H965	K966	N969	G970	N971	S972	A973	D974	A975	A976	Y977	A978	Q979	V980	E981	Q983	P984	R985	A986	I988	E994	L995	K996	V1001	I1004	E1010	D1014	L1015	E1016	R1017	I1019	V1020	F1024	A1025	E1026	P1029	W1030	R1034	T1035	R1036	W1037	M1038	E1040								
S1046	L1047	E1048	V1051	E1052	I1056	M1057	G1058	F1059	M1064	G1065	M1066	L1067	K1068	G1069	R1070	P1071	Y1072	D1077	S1078	K1079	E1082	D1086	K1087	D1088	V1089	Y1093	S1096	E1099	H1100	S1101	G1102	I1103	R1104	L1105	I1106	E1107	M1112	M1115	P1116	E1117	K1118	K1119	M1120	M1121	Q1123	E1124								
V1125	I1126	V1127	E1128	E1129	D1130	L1131	E1132	P1133	F1134	A1135	S1137	K1138	E1139	T1140	A1141	E1142	Q1143	F1144	K1145	H1148	G1149	D1150	V1152	D1153	I1154	F1155	E1156	I1157	P1158	E1159	T1160	G1161	E1162	Y1163	S1164	V1165	K1166	L1167	L1168	K1169	T1172	E1173	Y1174	I1175	P1176	K1177	A1178	L1179	R1180	D1182	R1183	L1184	V1185	A1186
G1187	Q1188	I1189	P1190	A1195	I1200	D1203	I1204	I1205	S1206	V1208	D1209	P1210	I1211	T1212	V1215	V1219	F1223	S1226	G1227	I1228	M1234	Y1235	V1238	H1239	V1240	E1241	E1242	M1245	G1246	S1247	G1248	A1249	G1250	G1253	V1254	S1255	A1256	L1257	R1258	G1259	M1260	F1261	K1262	D1263	E1267	E1268								
N1272	L1275	Q1276	S1277	F1278	F1279	T1282	M1283	S1284	A1285	W1286	M1289	I1292	R1293	M1294	S1295	T1298	P1301	V1302	G1303	A1304	C1305	T1307	S1311	S1312	D1313	I1314	G1315	V1316	E1317	L1320	S1321	G1322	A1323	A1324	R1325	G1331	D1333	D1334	F1335	Q1336	E1337	E1338	F1341	K1347	A1348	T1349								
S1350	M1351	E1354	E1355	F1356	E1357	R1360	T1361	R1367	P1368	A1369	T1370	T1371	L1372	R1373	M1374	G1375	F1376	M1377	Q1380	I1384	M1388	Q1389	A1390	D1391	L1392	A1393	G1397	V1398	P1399	I1400	Y1401	G1402	I1403	I1414	G1415	R1416	S1417	V1418	G1424	L1425	L1426	T1427	E1431	S1434	S1435	V1436	K1437	Y1438						
A1439	S1440	P1441	N1442	L1443	K1446	R1450	E1456	K1460	D1461	E1464	N1465	E1466	L1467	E1468	A1469	L1470	K1471	L1472	A1473	A1474	E1475	E1476	I1477	P1478	S1479	E1480	D1481	Q1482	N1483	E1484	F1485	L1486	L1487	E1488	R1489	T1490	R1491	A1492	I1493	H1494	N1495	E1496	A1497	E1498	S1499	Q1500	L1501	R1502	Q1505	G1509	M1510	D1511		
R1515	D1516	P1517	R1518	I1519	A1520	L1531	T1532	L1533	D1534	V1538	A1539	H1542	G1543	T1544	S1545	T1546	K1547	D1550	E1553	S1554	I1567	M1568	E1569	M1560	M1561	K1562	H1563	R1566	E1567	L1580	H1583	P1584	K1585	G1586	A1587	A1588	A1589	W1591	M1592	M1593	M1594	G1595	Q1598	I1604	L1605	P1606								
G1607	M1608	R1609	M1610	D1611	L1612	N1613	K1629	T1630	L1631	K1632	I1641	G1647	G1651	Y1660	L1661	A1664	D1668	V1674	A1675	K1676	V1677	M1678	S1679	A1680	T1707	D1708	E1709	L1710	E1711	E1712	L1716	D1717	P1718	L1719	K1724	D1725	K1726	K1727	S1728	G1729	S1730	L1731	M1734	S1735	K1736	M1737	I1738							

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L1464	T1465	F1466	E1467	T1468	T1469	T1470	K1475	N1476	A1477	N1478	S1481	K1484	G1485	F1486	G1487	P1488	V1491	K1496	E1500	I1501	G1502	I1503	V1504	Y1505	V1506	E1507	A1510	S1511	H1512	G1513	M1514	P1515	V1516	V1517	D1518	F1519	L1520	K1521	R1522	M1523	G1524	S1525	T1526	L1527	Q1529	M1530	V1531	M1532	N1533	E1534	M1535				
K1401	P1402	V1403	V1406	S1409	F1410	F1411	R1412	R1413	G1414	M1415	Y1416	T1417	D1418	F1419	E1420	M1421	T1422	F1423	Q1424	K1425	T1426	V1427	E1428	F1429	V1430	Y1431	Q1432	M1433	H1434	V1435	K1436	T1437	S1438	K1439	D1440	I1441	V1442	L1443	L1444	R1445	S1446	K1447	W1449	L1452	D1453	L1454	E1455	D1456	F1457	D1458	L1459	N1460	M1461	K1462	T1463
I1338	F1339	P1340	N1341	V1342	V1343	D1344	G1345	D1346	L1347	L1348	K1349	L1350	V1351	H1352	L1353	S1354	N1355	G1356	V1357	K1358	M1359	G1362	A1363	K1364	P1365	L1366	G1367	V1368	G1369	D1370	V1371	V1372	S1373	T1374	V1375	A1376	V1377	I1378	E1379	S1380	V1381	V1382	M1383	Q1384	P1385	T1386	K1387	L1388	V1390	D1391	G1394	S1397	N1398	M1399	G1400
F1275	N1276	L1277	D1278	F1279	D1280	P1281	R1282	D1283	V1284	I1285	K1286	G1287	K1288	D1289	F1290	E1291	T1292	T1293	A1294	V1297	Y1298	D1299	F1300	T1301	H1302	A1303	V1304	G1305	N1306	N1307	C1308	E1309	D1310	F1311	S1312	S1313	R1314	P1315	D1316	R1317	T1318	M1319	L1320	A1321	P1322	M1323	D1324	F1325	A1326	T1327	V1328	G1330	H1331	R1332	I1335
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P882	E885	A886	K887	R888	D889	Y890	I891	R894	L895	N896	A897	F899	Q900	K901	P902	T906	N907	N908	G909	Q910	A911	R912	D913	L914	M917	T918	Y919	R925	L926	I932	R933	S934	T935	W838	F939	D940	R944	R952	R953	V954	E955	F956	R957	F958	T959	D1045	Q1046	D1047	V1048	Q1049	R1050				
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T1051	C1052	L1053	L1054	H1055	G1056	V1058	Q1061	F1062	T1063	K1064	V1065	I1066	D1067	E1068	P1069	I1070	K1071	M1074	H1078	D1079	G1080	H1081	I1082	L1085	L1086	H1087	Y1090	G1091	D1092	D1093	E1094	S1095	I1096	I1097	F1098	A1099	V1100	E1101	S1107	P1108	V1109	ASP	GLN	SER	GLN	VAL	ASP	SER	SER	SER	VAL				
SER	GLU	D1123	S1124	A1125	V1126	K1127	A1129	T1130	S1131	K982	V983	F984	Y987	R991	E992	Q993	P994	D999	I1000	D1001	N1009	P1010	M1011	K1012	K1013	V1018	D1022	R1023	R1024	F1025	S1026	F1029	K1030	K1031	D1032	S1033	L1034	S1037	E1038	H1039	L1040	E1041	V1044	D1045	Q1046	D1047	V1048	Q1049	R1050						
E1199	P1200	V1201	Q1202	G1203	E1204	L1205	K1206	I1210	K1215	E1216	N1217	I1218	I1219	E1222	M1223	I1224	E1225	R1227	T1228	M1229	D1230	G1231	K1232	P1233	V1234	S1235	L1236	L1239	Y1240	N1241	F1242	N1243	P1250	L1251	M1255	E1256	D1257	Q1260	R1261	I1262	K1263	E1264	M1265	T1266	K1268	L1269	D1272	E1273	F1274						
F1275	N1276	L1277	D1278	F1279	D1280	P1281	R1282	D1283	V1284	I1285	K1286	G1287	K1288	D1289	F1290	E1291	T1292	T1293	A1294	V1297	Y1298	D1299	F1300	T1301	H1302	A1303	V1304	G1305	N1306	N1307	C1308	E1309	D1310	F1311	S1312	S1313	R1314	P1315	D1316	R1317	T1318	M1319	L1320	A1321	P1322	M1323	D1324	F1325	A1326	T1327	V1328	G1330	H1331	R1332	I1335
I1338	F1339	P1340	N1341	V1342	V1343	D1344	G1345	D1346	L1347	L1348	K1349	L1350	V1351	H1352	L1353	S1354	N1355	G1356	V1357	K1358	M1359	G1362	A1363	K1364	P1365	L1366	G1367	V1368	G1369	D1370	V1371	V1372	S1373	T1374	V1375	A1376	V1377	I1378	E1379	S1380	V1381	V1382	M1383	Q1384	P1385	T1386	K1387	L1388	V1390	D1391	G1394	S1397	N1398	M1399	G1400
K1401	P1402	V1403	V1406	S1409	F1410	F1411	R1412	R1413	G1414	M1415	Y1416	T1417	D1418	F1419	E1420	M1421	T1422	F1423	Q1424	K1425	T1426	V1427	E1428	F1429	V1430	Y1431	Q1432	M1433	H1434	V1435	K1436	T1437	S1438	K1439	D1440	I1441	V1442	L1443	L1444	R1445	S1446	K1447	W1449	L1452	D1453	L1454	E1455	D1456	F1457	D1458	L1459	N1460	M1461	K1462	T1463
L1464	T1465	F1466	E1467	T1468	T1469	T1470	K1475	N1476	A1477	N1478	S1481	K1484	G1485	F1486	G1487	P1488	V1491	K1496	E1500	I1501	G1502	I1503	V1504	Y1505	V1506	E1507	A1510	S1511	H1512	G1513	M1514	P1515	V1516	V1517	D1518	F1519	L1520	K1521	R1522	M1523	G1524	S1525	T1526	L1527	Q1529	M1530	V1531	M1532	N1533	E1534	M1535				

E2036	I1972	M1912	Y1852	K1793	E1730	V1601
F2037	S1973	V1913	G1853	S1794	E1731	S1602
I2038	V1974	L1914	M1854	K1795	M1732	S1603
K2039	L1914	L1914	I1855	K1796	Y1733	R1604
E2040	F1975	M1915	I1856	L1796	S1734	V1605
I2041	F1976	F1916	A1857	L1797	A1735	R1606
I2042	H1977	I1917	I1857	I1798	M1736	R1607
I2043	S1978	K1918	M1858	P1799	I1737	Y1608
D2044	T1979	L1919	P1859	A1800	F1738	T1609
W2045	M1982	Q1920	G1860	I1801	E1739	C1610
E2046	N1983	I1922	V1862	A1802	T1740	Q1611
K2047	G1984	D1923	A1863	T1803	I1741	F1612
Y2048	V1985	I1924	A1864	F1804	V1742	V1613
E2049	K1986	I1925	S1865	A1805	D1743	M1615
Q2050	P1987	E1926	F1866	H1807	G1744	V1616
SER	F1988	E1926	S1867	S1808	K1745	L1617
ASP	K1989	L1927	Q1868	L1809	L1746	M1618
TYR	S1990	Q1928	A1870	G1810	K1747	M1619
LYS	F1991	Q1929	E1869	E1811	T1748	T1620
ASP	L1992	S1930	A1871	Y1812	E1749	A1621
HIS	K1993	L1931	Q1872	A1813	K1750	L1622
GLY	M1994	S1932	I1873	A1814	I1751	K1623
ASP	M1995	L1933	I1874	A1815	F1752	T1624
ASP	I1996	E1934	V1874	A1816	K1753	S1625
ASP	I1997	E1935	V1875	S1817	E1754	I1626
HIS	K1998	V1936	E1876	L1818	I1755	Q1627
ASP	E1999	V1937	R1877	A1819	M1756	H1628
ILE	N2000	E1937	V1878	D1820	A1686	V1629
ASP	V2001	G1938	V1879	H1758	A1687	G1630
TYR	K2002	H1939	K1880	M1822	Q1688	M1631
LYS	R2005	F1940	R1881	S1823	V1690	I1632
ASP	G2008	F1941	T1882	I1824	W1691	M1633
ASP	K2009	E1942	G1883	E1825	D1695	G1634
LYS	Y2010	I1943	W1884	S1826	F1698	R1635
N2013	M2013	D1944	L1885	L1827	T1701	K1636
L2014	L2014	D1945	L1886	V1828	F1704	L1637
T2015	T2015	E1946	V1886	E1829	S1705	I1638
A2016	A2016	A1947	E1887	V1830	L1706	K1639
K2017	K2017	S1948	V1888	I1831	L1707	F1640
P2018	P2018	K1949	M1890	F1832	D1708	E1641
F2019	F2019	K1950	Y1891	Y1833	G1769	R1643
Q2020	Q2020	S1951	M1892	G1835	L1770	M1644
V2021	V2021	A1952	V1893	M1836	S1772	E1645
T2022	T2022	V1953	E1894	T1837	I1774	M1644
K2023	K2023	K1954	M1895	M1838	Q1775	E1645
E2024	E2024	P1955	Q1896	Q1839	F1776	D1646
Y2025	Y2025	P1956	Q1897	V1840	T1777	I1711
F2026	F2026	P1957	Y1898	A1841	Q1778	I1711
Q2027	Q2027	L1958	Y1899	V1842	P1779	V1648
D2028	D2028	K1959	A1900	P1844	A1780	V1649
V2029	V2029	L1960	A1901	R1844	L1781	V1650
Y2030	Y2030	L1961	G1902	D1845	T1782	L1651
D2031	D2031	R1962	D1903	E1846	T1783	T1652
L2032	L2032	G1963	L1904	L1847	L1784	G1653
T2033	T2033	F1964	L1905	L1848	M1784	E1654
G2034	G2034	A1965	A1906	R1849	F1721	A1655
S2035	S2035	C1966	L1907	S1850	G1722	E1656
		I1967	D1908	M1851	G1726	I1657
		P1968	T1909			E1658
		L1969	V1910			Q1659
		V1970	T1911			P1660
		I1971				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	594818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTFFIND4 within cryoSPARC2	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.727	Depositor
Minimum map value	-1.412	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.706	Depositor
Map size (\AA)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

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: PNS, FMN, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	3/12392 (0.0%)	0.60	3/16775 (0.0%)
2	G	0.44	0/16360	0.51	0/22198
All	All	0.52	3/28752 (0.0%)	0.55	3/38973 (0.0%)

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
1	A	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1174	TYR	CD1-CE1	-6.37	1.29	1.39
1	A	1174	TYR	CE1-CZ	-6.33	1.30	1.38
1	A	490	TYR	CD1-CE1	-5.27	1.31	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1173	LEU	CA-CB-CG	5.66	128.33	115.30
1	A	1719	LEU	CA-CB-CG	-5.06	103.67	115.30
1	A	1174	TYR	CB-CG-CD2	5.05	124.03	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1132	GLU	Peptide
1	A	1173	LEU	Peptide
1	A	1584	PRO	Peptide
1	A	1716	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12171	0	11679	490	0
2	G	15995	0	15978	772	0
3	A	48	0	22	19	0
3	G	48	0	25	27	0
4	A	5	0	0	0	0
5	G	31	0	19	3	0
All	All	28298	0	27723	1241	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1241) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:740:HIS:HB2	3:G:2102:NAP:C7N	1.22	1.59
1:A:147:ALA:CB	1:A:214:GLN:HA	1.50	1.41
2:G:740:HIS:HD2	3:G:2102:NAP:C2N	1.33	1.39
2:G:740:HIS:HD2	3:G:2102:NAP:C3N	1.40	1.34
2:G:740:HIS:CB	3:G:2102:NAP:C7N	2.06	1.32
1:A:147:ALA:HB2	1:A:214:GLN:CA	1.63	1.29
2:G:1034:LEU:HD13	3:G:2102:NAP:O1N	1.29	1.25
2:G:740:HIS:CD2	3:G:2102:NAP:C2N	2.19	1.24
1:A:147:ALA:CB	1:A:214:GLN:CA	2.14	1.23
2:G:740:HIS:HB2	3:G:2102:NAP:O7N	1.07	1.22
2:G:740:HIS:CD2	3:G:2102:NAP:C3N	2.22	1.20
2:G:1032:ASP:N	3:G:2102:NAP:O1A	1.74	1.20
1:A:688:ILE:CD1	3:A:1901:NAP:O4D	1.89	1.19
2:G:740:HIS:CB	3:G:2102:NAP:O7N	1.91	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:HB3	1:A:214:GLN:CB	1.78	1.12
1:A:688:ILE:HB	3:A:1901:NAP:H51N	1.30	1.10
2:G:740:HIS:HB2	3:G:2102:NAP:N7N	1.75	0.99
2:G:1034:LEU:CD1	3:G:2102:NAP:O1N	2.10	0.99
2:G:740:HIS:CG	3:G:2102:NAP:C7N	2.48	0.96
1:A:688:ILE:CB	3:A:1901:NAP:H51N	1.91	0.93
2:G:740:HIS:CD2	3:G:2102:NAP:C7N	2.52	0.92
1:A:1019:ILE:HG13	1:A:1316:VAL:HG23	1.52	0.92
1:A:688:ILE:HD13	3:A:1901:NAP:O4D	1.06	0.90
1:A:147:ALA:CB	1:A:214:GLN:CB	2.46	0.89
1:A:739:GLN:O	1:A:798:ASN:ND2	2.05	0.88
2:G:740:HIS:CB	3:G:2102:NAP:N7N	2.36	0.87
1:A:1125:VAL:HG12	1:A:1126:ILE:H	1.37	0.87
1:A:753:TYR:O	1:A:813:ARG:NH2	2.10	0.85
2:G:740:HIS:N	3:G:2102:NAP:O7N	2.10	0.84
1:A:771:PHE:HB3	3:A:1901:NAP:H52N	1.57	0.84
1:A:178:GLY:O	1:A:180:SER:N	2.12	0.83
1:A:971:ASN:HA	1:A:974:ASP:HB2	1.60	0.83
2:G:706:LYS:NZ	5:G:2101:FMN:O2'	2.11	0.83
2:G:1888:ILE:HD13	2:G:1900:ALA:HB2	1.60	0.82
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.44	0.82
1:A:709:ARG:NH2	3:A:1901:NAP:O2X	2.06	0.81
1:A:843:LYS:HE3	3:A:1901:NAP:O2D	1.80	0.81
2:G:1313:SER:N	2:G:1319:MET:SD	2.54	0.80
1:A:1123:GLN:HG2	1:A:1124:GLU:H	1.46	0.80
2:G:821:ILE:HG13	2:G:857:ILE:HD11	1.63	0.80
2:G:394:ARG:HA	2:G:397:LYS:HG3	1.64	0.80
2:G:1839:GLN:O	2:G:1844:ARG:NH1	2.15	0.79
1:A:194:PHE:O	1:A:196:THR:N	2.15	0.79
2:G:610:THR:HB	2:G:617:ILE:HD11	1.65	0.79
2:G:1430:VAL:HG13	2:G:1527:LEU:HB3	1.64	0.78
2:G:736:ARG:HD2	2:G:1058:VAL:HG11	1.65	0.78
1:A:395:SER:HB3	1:A:398:LYS:HB2	1.66	0.77
1:A:1219:VAL:HG22	1:A:1384:ILE:HD13	1.67	0.77
1:A:490:TYR:OH	1:A:906:LEU:HB3	1.85	0.77
2:G:739:GLY:HA2	2:G:1054:LEU:HD13	1.67	0.77
2:G:881:VAL:HG13	2:G:882:PRO:HD3	1.67	0.77
2:G:1855:ILE:HD13	2:G:1960:LEU:HD21	1.64	0.77
1:A:1584:PRO:HB2	1:A:1587:ALA:HB3	1.65	0.76
1:A:41:THR:O	1:A:76:ARG:NH1	2.18	0.76
1:A:1183:ARG:NH1	1:A:1350:SER:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:456:GLN:O	2:G:469:ARG:NH2	2.18	0.76
2:G:688:LEU:HD22	2:G:715:GLN:HE22	1.50	0.76
2:G:1881:ARG:HH12	2:G:1949:LYS:HE3	1.50	0.76
1:A:1241:SER:HA	1:A:1295:SER:HB2	1.68	0.76
3:A:1901:NAP:O2X	3:A:1901:NAP:O3B	2.04	0.75
1:A:1067:LEU:HD23	1:A:1068:LYS:HG2	1.69	0.75
2:G:688:LEU:HD13	2:G:719:ILE:HD13	1.69	0.75
2:G:1842:VAL:O	2:G:1844:ARG:NH1	2.20	0.75
2:G:1890:ASN:HB2	2:G:1899:VAL:HG22	1.67	0.75
2:G:524:GLY:O	2:G:526:ARG:NH1	2.20	0.74
2:G:1319:MET:HB3	2:G:1368:VAL:HG21	1.68	0.74
2:G:1704:PHE:CE1	2:G:1709:ILE:HD11	2.22	0.74
2:G:914:LEU:HD23	2:G:1000:ILE:HG23	1.68	0.74
2:G:1623:LYS:HB2	2:G:1643:ARG:HB2	1.69	0.74
2:G:1636:LYS:HB2	2:G:1657:ILE:HG23	1.69	0.74
2:G:1037:SER:HB2	2:G:1053:ILE:HG22	1.69	0.74
1:A:1533:ILE:O	1:A:1566:ARG:NH1	2.19	0.74
2:G:952:ARG:NH2	2:G:967:ILE:O	2.21	0.74
2:G:1621:ALA:N	2:G:1645:GLU:OE1	2.19	0.73
2:G:1210:ILE:HB	2:G:1222:GLU:HB2	1.68	0.73
2:G:128:THR:O	2:G:132:MET:HB2	1.89	0.73
1:A:768:ILE:HG22	1:A:770:PRO:HD3	1.71	0.73
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.22	0.73
2:G:183:LEU:HD11	2:G:254:LYS:HG2	1.69	0.73
2:G:1022:ASP:OD2	2:G:1024:ARG:NH2	2.19	0.72
2:G:1704:PHE:HE1	2:G:1709:ILE:HD11	1.54	0.72
1:A:40:ASN:HA	1:A:76:ARG:HH22	1.53	0.72
1:A:1249:SER:OG	1:A:1250:GLY:N	2.21	0.72
2:G:896:ASN:O	2:G:1050:ARG:NH2	2.22	0.72
2:G:1034:LEU:HD13	3:G:2102:NAP:PN	2.29	0.72
2:G:2047:LYS:O	2:G:2050:GLN:NE2	2.22	0.72
2:G:716:VAL:HG21	2:G:730:LEU:HD21	1.71	0.72
2:G:1739:GLU:HB2	2:G:1987:PRO:HB3	1.70	0.72
2:G:1701:THR:O	2:G:1732:ASN:ND2	2.23	0.72
1:A:1182:ASP:OD2	1:A:1183:ARG:N	2.21	0.72
2:G:1904:LEU:HB3	2:G:1958:LEU:HD22	1.72	0.71
2:G:1031:LYS:HD2	3:G:2102:NAP:O5B	1.90	0.71
1:A:827:SER:OG	3:A:1901:NAP:C5N	2.38	0.71
2:G:1201:VAL:HG11	2:G:1226:ASN:HD21	1.54	0.71
2:G:175:ASP:O	2:G:179:THR:N	2.16	0.71
2:G:596:GLY:N	2:G:618:GLU:OE1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1279:PHE:HB3	2:G:1340:PRO:HB3	1.73	0.71
2:G:1350:LEU:HD11	2:G:1410:PHE:HB3	1.71	0.71
2:G:11:LEU:HB3	2:G:13:HIS:HE1	1.56	0.70
1:A:411:GLN:HE21	1:A:1629:LYS:HE2	1.56	0.70
2:G:56:THR:OG1	2:G:59:GLU:OE1	2.09	0.70
1:A:1077:ASP:OD2	1:A:1078:SER:N	2.24	0.70
2:G:1284:VAL:HG23	2:G:1377:VAL:HB	1.72	0.70
1:A:26:VAL:HG13	2:G:2013:ASN:HB3	1.74	0.70
2:G:326:ASP:O	2:G:330:ASN:ND2	2.22	0.70
2:G:907:VAL:HG23	2:G:917:MET:HE2	1.73	0.70
2:G:1013:LYS:NZ	2:G:1032:ASP:OD2	2.24	0.70
1:A:507:GLY:O	1:A:955:LYS:NZ	2.19	0.70
2:G:1549:THR:HG23	2:G:1552:PRO:HD3	1.74	0.70
2:G:1180:MET:HG2	2:G:1199:GLU:HG2	1.74	0.69
1:A:430:ARG:NH2	1:A:520:ARG:O	2.21	0.69
1:A:17:LEU:HD23	2:G:2014:LEU:HD23	1.74	0.69
1:A:727:ALA:O	1:A:730:SER:OG	2.07	0.69
1:A:843:LYS:CE	3:A:1901:NAP:O2D	2.40	0.69
2:G:174:ARG:NH2	2:G:218:TRP:O	2.25	0.69
2:G:686:PRO:HB2	2:G:691:ALA:HB2	1.72	0.69
1:A:1545:SER:OG	1:A:1545:SER:O	2.10	0.69
2:G:596:GLY:HA3	2:G:650:ASN:HD22	1.57	0.69
2:G:2023:LYS:HD2	2:G:2045:TRP:CE2	2.28	0.69
1:A:1470:LEU:O	1:A:1474:ALA:N	2.26	0.69
2:G:1738:PHE:HB2	2:G:1751:ILE:HD13	1.73	0.69
2:G:1199:GLU:OE2	2:G:1567:ARG:NH2	2.24	0.69
1:A:1123:GLN:HB3	1:A:1177:LYS:HD3	1.75	0.69
2:G:218:TRP:HB3	2:G:225:THR:HG22	1.75	0.68
2:G:626:SER:OG	2:G:627:ALA:N	2.26	0.68
2:G:740:HIS:CA	3:G:2102:NAP:O7N	2.40	0.68
1:A:1414:ILE:O	1:A:1416:ARG:HG2	1.93	0.68
1:A:1186:ALA:O	1:A:1188:GLN:NE2	2.27	0.68
1:A:1373:ARG:HH11	1:A:1547:LYS:HA	1.57	0.68
2:G:1893:VAL:HG23	2:G:1896:GLN:HB3	1.74	0.68
2:G:1800:ALA:O	2:G:2009:LYS:NZ	2.26	0.67
1:A:479:ASN:ND2	1:A:613:VAL:O	2.26	0.67
2:G:517:HIS:HB2	2:G:527:VAL:HG11	1.74	0.67
1:A:332:THR:OG1	1:A:333:LYS:NZ	2.27	0.67
2:G:56:THR:N	2:G:59:GLU:OE2	2.20	0.67
1:A:1259:GLY:HA2	1:A:1263:ASP:HB2	1.75	0.67
2:G:1319:MET:H	2:G:1368:VAL:HB	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:409:PHE:HA	2:G:412:ARG:HD2	1.77	0.67
1:A:985:ARG:N	2:G:956:GLU:O	2.27	0.67
2:G:245:GLN:HG2	2:G:505:GLY:HA2	1.75	0.67
1:A:147:ALA:HB2	1:A:214:GLN:HA	0.71	0.66
2:G:1878:VAL:HG22	2:G:1944:ILE:HD11	1.77	0.66
1:A:1138:LYS:NZ	1:A:1163:TYR:O	2.25	0.66
2:G:1135:GLU:HA	2:G:1176:PRO:HG2	1.77	0.66
1:A:21:GLN:NE2	2:G:1811:GLU:OE2	2.29	0.66
2:G:297:ARG:NH2	2:G:447:ASN:OD1	2.29	0.66
2:G:1126:VAL:HG12	2:G:1183:GLU:HG2	1.77	0.66
2:G:1629:VAL:HB	2:G:1639:LYS:HZ3	1.60	0.66
1:A:46:GLU:OE1	1:A:54:ALA:N	2.25	0.66
2:G:174:ARG:HA	2:G:177:TYR:CE1	2.31	0.66
2:G:362:ALA:HA	2:G:365:GLN:HG3	1.77	0.66
2:G:1863:ALA:HB3	2:G:1866:PHE:HB2	1.76	0.66
3:G:2102:NAP:O2N	3:G:2102:NAP:H3D	1.94	0.66
1:A:1034:ARG:NH2	1:A:1052:GLU:OE2	2.29	0.66
2:G:1424:GLN:HE22	2:G:1426:THR:HB	1.60	0.66
2:G:1767:GLU:HG2	2:G:1768:LYS:HG3	1.78	0.66
2:G:1550:ASN:ND2	2:G:1564:HIS:O	2.26	0.66
2:G:1742:VAL:HG23	2:G:1745:LYS:HB3	1.76	0.66
1:A:688:ILE:HB	3:A:1901:NAP:C5D	2.18	0.66
2:G:1877:ARG:HD3	2:G:1940:LEU:HD13	1.78	0.66
2:G:130:ARG:NH2	2:G:136:PRO:O	2.27	0.65
2:G:1032:ASP:CA	3:G:2102:NAP:O1A	2.44	0.65
1:A:776:GLU:HB2	1:A:779:ILE:HD13	1.78	0.65
1:A:1203:ASP:OD2	1:A:1204:ILE:N	2.28	0.65
1:A:490:TYR:HB3	1:A:698:GLN:HB2	1.79	0.65
1:A:517:GLU:N	1:A:517:GLU:OE1	2.29	0.65
1:A:1403:ILE:HD11	1:A:1661:LEU:HB2	1.77	0.65
2:G:56:THR:HG21	2:G:108:LEU:HD11	1.79	0.65
2:G:818:LYS:HB3	2:G:1066:ILE:HD11	1.78	0.65
2:G:590:PRO:HB3	2:G:1078:HIS:CD2	2.31	0.65
1:A:852:ARG:NH1	1:A:856:GLU:OE2	2.29	0.65
2:G:1775:GLN:HE22	2:G:1836:MET:HB2	1.62	0.65
2:G:23:PRO:HD2	2:G:86:LEU:HD11	1.77	0.65
2:G:740:HIS:CD2	3:G:2102:NAP:H2N	2.27	0.64
2:G:1695:ASP:OD1	2:G:1707:LEU:N	2.21	0.64
1:A:36:LEU:O	1:A:76:ARG:NH2	2.31	0.64
1:A:1144:PHE:HZ	1:A:1174:TYR:CZ	2.15	0.64
1:A:513:GLU:OE2	1:A:873:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:343:ASN:HB2	2:G:416:PHE:HB3	1.80	0.64
2:G:1716:ASN:HD22	2:G:1765:ARG:HA	1.63	0.64
1:A:1584:PRO:O	1:A:1587:ALA:N	2.29	0.64
2:G:720:ALA:HB2	2:G:728:ILE:HD11	1.80	0.64
1:A:394:PHE:HB3	1:A:744:ASP:OD1	1.98	0.64
2:G:213:LEU:HD12	2:G:236:ILE:HG13	1.80	0.64
2:G:1041:GLU:HA	2:G:1046:GLN:HE22	1.62	0.64
2:G:1674:GLN:HE22	2:G:1713:ASN:HB2	1.63	0.64
2:G:707:PRO:HG3	2:G:730:LEU:HD22	1.79	0.63
1:A:464:GLU:OE2	1:A:465:ASN:ND2	2.32	0.63
2:G:993:GLN:NE2	2:G:994:PHE:O	2.32	0.63
1:A:445:ASP:OD1	1:A:445:ASP:N	2.31	0.63
2:G:161:GLY:O	2:G:245:GLN:NE2	2.31	0.63
2:G:2036:GLU:HA	2:G:2039:LYS:HG2	1.80	0.63
1:A:32:GLN:HA	1:A:35:PHE:HE2	1.64	0.63
1:A:413:LEU:HB2	1:A:439:ILE:HD12	1.80	0.63
1:A:1102:GLY:O	1:A:1104:ARG:HG3	1.99	0.63
2:G:740:HIS:CG	3:G:2102:NAP:N7N	2.65	0.63
2:G:1885:LEU:O	2:G:1903:ASP:N	2.30	0.63
1:A:1121:MET:N	1:A:1177:LYS:O	2.23	0.63
2:G:1040:LEU:HD21	2:G:1048:VAL:HB	1.81	0.63
2:G:1491:VAL:HB	2:G:1501:ILE:HD11	1.79	0.63
2:G:37:PHE:CE1	2:G:64:PHE:HA	2.34	0.62
1:A:843:LYS:NZ	3:A:1901:NAP:O2D	2.31	0.62
1:A:1414:ILE:HD13	1:A:1416:ARG:HH21	1.64	0.62
1:A:1070:ARG:HE	1:A:1071:PRO:HD2	1.62	0.62
2:G:54:PRO:HB3	2:G:59:GLU:HG2	1.80	0.62
2:G:148:ALA:HB1	2:G:153:ASN:HB3	1.81	0.62
2:G:259:THR:HG22	2:G:262:GLU:HB2	1.80	0.62
1:A:433:VAL:HG23	1:A:493:VAL:HG11	1.82	0.62
1:A:442:ARG:HD3	1:A:726:GLY:O	2.00	0.62
2:G:199:ILE:HD11	2:G:213:LEU:HD22	1.80	0.62
1:A:400:ARG:NH1	1:A:1367:ARG:HH22	1.97	0.62
1:A:1139:GLU:N	1:A:1139:GLU:OE1	2.33	0.62
2:G:1737:ILE:HG21	2:G:1748:THR:HG23	1.81	0.62
2:G:1866:PHE:HE2	2:G:1871:LEU:HG	1.64	0.62
1:A:1089:VAL:HG23	1:A:1093:TYR:HD2	1.64	0.62
2:G:1366:LEU:HD23	2:G:1366:LEU:H	1.65	0.62
1:A:251:GLN:HA	1:A:256:LEU:H	1.65	0.62
1:A:1120:GLU:OE1	1:A:1120:GLU:N	2.32	0.62
2:G:1172:LYS:NZ	2:G:1574:ASN:OD1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:GLN:O	1:A:1177:LYS:NZ	2.21	0.62
2:G:180:TYR:HB3	2:G:183:LEU:HB3	1.81	0.62
1:A:503:ILE:HG12	1:A:509:ILE:HG13	1.81	0.62
1:A:1134:PHE:HE1	1:A:1168:LEU:O	1.83	0.62
1:A:1334:ASP:OD1	1:A:1335:PHE:N	2.33	0.62
2:G:11:LEU:HD11	2:G:20:LEU:HB2	1.81	0.62
2:G:1550:ASN:ND2	2:G:1579:ILE:O	2.32	0.62
2:G:1685:LYS:NZ	2:G:1689:ASP:OD2	2.33	0.62
2:G:1546:THR:OG1	2:G:1620:THR:N	2.30	0.61
1:A:931:GLN:OE1	1:A:931:GLN:N	2.27	0.61
1:A:1268:GLU:N	1:A:1268:GLU:OE1	2.33	0.61
1:A:1367:ARG:NH1	1:A:1612:ASP:OD1	2.34	0.61
2:G:55:THR:HG23	2:G:56:THR:HG23	1.83	0.61
2:G:696:GLU:N	2:G:696:GLU:OE1	2.33	0.61
2:G:860:ARG:NH1	2:G:898:ASP:OD1	2.32	0.61
2:G:1189:THR:O	2:G:1193:THR:OG1	2.18	0.61
2:G:1468:THR:HA	2:G:1487:GLY:HA3	1.82	0.61
1:A:32:GLN:HA	1:A:35:PHE:CE2	2.34	0.61
2:G:1376:ALA:HA	2:G:1394:GLY:HA2	1.83	0.61
1:A:1474:ALA:O	1:A:1482:GLN:NE2	2.34	0.61
2:G:1963:GLY:N	2:G:1966:CYS:SG	2.72	0.61
1:A:764:ASP:OD2	1:A:818:ARG:NH1	2.33	0.61
1:A:1604:ILE:HG12	1:A:1632:LYS:HG3	1.83	0.61
2:G:96:LEU:HD23	2:G:98:GLY:H	1.66	0.61
2:G:875:LEU:HG	2:G:876:PRO:HD2	1.82	0.61
2:G:723:HIS:HB3	2:G:726:PHE:CD2	2.36	0.61
2:G:1475:LYS:HB3	2:G:1481:SER:HB2	1.82	0.61
1:A:631:PRO:O	1:A:653:ARG:NH2	2.31	0.61
1:A:1176:PRO:C	1:A:1177:LYS:HD2	2.21	0.61
2:G:1667:THR:OG1	2:G:1785:GLU:OE2	2.16	0.61
1:A:191:GLY:O	1:A:195:GLY:N	2.33	0.61
1:A:856:GLU:OE1	1:A:858:TRP:NE1	2.34	0.61
1:A:1544:THR:HG23	1:A:1546:THR:H	1.65	0.61
2:G:953:ARG:HA	2:G:956:GLU:HB2	1.83	0.61
2:G:1828:VAL:HA	2:G:1831:VAL:HG12	1.83	0.60
1:A:1584:PRO:O	1:A:1586:GLY:N	2.35	0.60
2:G:569:LEU:HD21	2:G:1085:LEU:HB3	1.82	0.60
2:G:703:LEU:HB3	2:G:728:ILE:HG22	1.84	0.60
2:G:1877:ARG:HD2	2:G:1944:ILE:HB	1.82	0.60
1:A:1505:GLN:O	1:A:1509:GLY:N	2.34	0.60
2:G:11:LEU:HB3	2:G:13:HIS:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1277:LEU:HB3	2:G:1341:ASN:HB2	1.83	0.60
1:A:1183:ARG:NE	1:A:1349:THR:OG1	2.35	0.60
1:A:1337:GLU:OE1	1:A:1337:GLU:N	2.26	0.60
2:G:305:PHE:CD2	2:G:442:ASP:HB3	2.35	0.60
2:G:919:TYR:OH	2:G:999:ASP:OD2	2.13	0.60
1:A:56:MET:HG2	1:A:59:ARG:HH21	1.66	0.60
1:A:983:GLN:HB3	1:A:1087:LYS:HG3	1.82	0.60
1:A:1719:LEU:HD12	1:A:1744:TYR:HA	1.84	0.60
1:A:807:LYS:HD2	1:A:858:TRP:HB3	1.83	0.60
2:G:868:PHE:HB3	2:G:873:PHE:CE2	2.37	0.60
2:G:1227:ARG:HD3	2:G:1555:ARG:HH12	1.65	0.60
2:G:1844:ARG:HB3	2:G:1848:GLY:HA2	1.84	0.60
1:A:1718:PRO:HD2	1:A:1744:TYR:CE1	2.37	0.60
2:G:1142:LEU:O	2:G:1150:ARG:NE	2.29	0.60
1:A:739:GLN:HB2	1:A:794:ILE:HG23	1.83	0.59
1:A:807:LYS:NZ	1:A:861:GLN:OE1	2.32	0.59
1:A:1550:ASP:O	1:A:1554:SER:OG	2.16	0.59
2:G:156:LEU:HD22	2:G:502:LEU:HD22	1.84	0.59
2:G:1925:ILE:H	2:G:1925:ILE:HD12	1.66	0.59
1:A:1035:THR:O	1:A:1035:THR:OG1	2.16	0.59
2:G:59:GLU:CB	2:G:122:LEU:HD21	2.32	0.59
2:G:121:GLU:OE2	2:G:125:ASN:ND2	2.35	0.59
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.85	0.59
1:A:1020:VAL:HG21	1:A:1400:ILE:HG12	1.84	0.59
1:A:1590:ALA:O	1:A:1594:ASN:HB2	2.02	0.59
2:G:37:PHE:CZ	2:G:67:TYR:HB3	2.37	0.59
2:G:459:VAL:HG23	2:G:468:LEU:HB2	1.85	0.59
2:G:515:LEU:O	2:G:519:ASN:ND2	2.35	0.59
1:A:1067:LEU:HB3	1:A:1072:TYR:CD2	2.38	0.59
2:G:408:PRO:HB2	2:G:411:GLU:HG2	1.85	0.59
2:G:1380:SER:HB2	2:G:1424:GLN:HA	1.85	0.59
2:G:1427:VAL:HG22	2:G:1469:GLU:HG2	1.85	0.59
2:G:241:ILE:HB	2:G:275:GLN:HE22	1.68	0.59
1:A:1185:VAL:HG23	1:A:1377:MET:HE1	1.84	0.59
2:G:666:ILE:HG22	2:G:698:LEU:HD22	1.84	0.59
2:G:1243:ASN:N	2:G:1250:PRO:O	2.36	0.59
1:A:1301:PRO:HG3	1:A:1314:ILE:HD13	1.84	0.59
1:A:1542:HIS:N	1:A:1553:GLU:OE2	2.32	0.59
2:G:1034:LEU:CD1	3:G:2102:NAP:PN	2.88	0.59
2:G:1905:ARG:NH1	2:G:1955:PRO:O	2.36	0.59
1:A:81:TYR:HH	1:A:89:TYR:HH	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:580:GLU:OE2	2:G:585:LYS:HE2	2.03	0.58
2:G:1037:SER:HA	2:G:1051:THR:HG21	1.84	0.58
1:A:1247:SER:HG	1:A:1332:TYR:HE1	1.51	0.58
1:A:1168:LEU:HG	1:A:1169:LYS:H	1.68	0.58
2:G:745:ASP:OD1	2:G:746:ALA:N	2.35	0.58
2:G:1936:VAL:O	2:G:1940:LEU:HG	2.03	0.58
1:A:938:GLU:HA	1:A:941:ALA:HB3	1.85	0.58
1:A:1256:ALA:O	1:A:1259:GLY:N	2.36	0.58
2:G:1432:GLN:HG2	2:G:1465:THR:HG22	1.86	0.58
1:A:404:SER:O	1:A:404:SER:OG	2.16	0.58
1:A:1037:TRP:HB2	1:A:1598:GLN:NE2	2.19	0.58
1:A:1377:MET:O	1:A:1583:HIS:N	2.34	0.57
2:G:329:GLU:OE1	2:G:329:GLU:N	2.37	0.57
1:A:1014:ASP:HB2	1:A:1505:GLN:HB2	1.86	0.57
1:A:1675:ALA:O	1:A:1678:SER:OG	2.22	0.57
2:G:1871:LEU:HA	2:G:1874:VAL:HG12	1.85	0.57
2:G:37:PHE:HD1	2:G:63:LYS:HZ2	1.51	0.57
1:A:147:ALA:CB	1:A:214:GLN:N	2.67	0.57
1:A:1589:GLY:HA2	1:A:1592:MET:HG2	1.87	0.57
2:G:1386:THR:HG23	2:G:1411:PHE:HZ	1.69	0.57
1:A:1360:ARG:HG2	1:A:1367:ARG:NH2	2.19	0.57
1:A:1499:SER:HA	1:A:1502:ARG:HG2	1.87	0.57
2:G:582:LYS:HE2	2:G:1108:PRO:HB3	1.86	0.57
2:G:860:ARG:NH2	2:G:1047:ASP:OD2	2.37	0.57
1:A:984:PRO:HG2	1:A:1087:LYS:HD3	1.87	0.57
1:A:1010:GLU:HA	1:A:1664:ALA:HA	1.86	0.57
1:A:1235:TYR:OH	1:A:1292:ILE:O	2.11	0.57
2:G:156:LEU:HD23	2:G:500:HIS:HB2	1.86	0.57
2:G:1101:GLU:HB3	2:G:1147:ILE:HG22	1.86	0.57
1:A:442:ARG:HG3	1:A:727:ALA:HA	1.87	0.57
1:A:708:SER:OG	3:A:1901:NAP:O3X	2.22	0.57
2:G:440:ASN:ND2	2:G:477:GLU:HG2	2.20	0.57
2:G:571:LYS:HB2	2:G:1097:ILE:HG12	1.86	0.57
1:A:1388:MET:HE1	1:A:1398:VAL:HG21	1.87	0.56
2:G:1859:PRO:HB3	2:G:1866:PHE:HD2	1.69	0.56
2:G:740:HIS:HA	2:G:854:ILE:HD13	1.87	0.56
1:A:1189:ILE:HG12	1:A:1380:GLN:HE21	1.71	0.56
2:G:130:ARG:NE	2:G:135:ARG:O	2.35	0.56
2:G:869:ASP:HA	2:G:873:PHE:HD2	1.70	0.56
1:A:986:ALA:HB1	1:A:1051:VAL:HG11	1.87	0.56
1:A:1139:GLU:HG2	1:A:1140:THR:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:161:GLY:H	2:G:505:GLY:HA3	1.70	0.56
1:A:984:PRO:HB3	2:G:959:THR:HG23	1.87	0.56
2:G:1138:TRP:O	2:G:1142:LEU:HG	2.06	0.56
1:A:681:THR:HG21	1:A:802:MET:HE3	1.87	0.56
2:G:260:PRO:HD3	2:G:289:TRP:CE2	2.41	0.56
2:G:1264:GLU:HA	2:G:1267:TRP:HD1	1.69	0.56
1:A:677:TYR:H	1:A:766:ASP:HB2	1.71	0.56
1:A:810:LYS:HB3	1:A:861:GLN:HG2	1.88	0.56
2:G:389:LEU:HA	2:G:392:THR:HG22	1.87	0.56
1:A:840:SER:OG	1:A:841:GLU:N	2.38	0.56
1:A:1239:HIS:CD2	1:A:1241:SER:H	2.23	0.56
2:G:662:GLY:O	2:G:666:ILE:N	2.23	0.56
2:G:688:LEU:HD22	2:G:715:GLN:NE2	2.21	0.56
1:A:442:ARG:HA	1:A:728:LYS:HG3	1.87	0.56
1:A:1360:ARG:NH2	1:A:1372:THR:O	2.38	0.56
2:G:1300:PHE:HA	2:G:1556:VAL:HG11	1.87	0.56
1:A:893:VAL:HG11	1:A:930:LEU:HD21	1.87	0.55
1:A:1239:HIS:CE1	1:A:1718:PRO:HA	2.41	0.55
1:A:1333:ASP:OD2	1:A:1334:ASP:N	2.37	0.55
2:G:220:GLU:HG2	2:G:221:ASN:N	2.21	0.55
2:G:404:GLN:NE2	2:G:413:LYS:H	2.05	0.55
2:G:581:THR:H	2:G:584:SER:HG	1.54	0.55
2:G:586:LEU:HD21	2:G:1107:SER:HA	1.88	0.55
2:G:1227:ARG:NE	2:G:1551:GLU:OE2	2.30	0.55
2:G:1924:ILE:HA	2:G:1927:LEU:HD12	1.87	0.55
1:A:520:ARG:HH12	1:A:521:LYS:NZ	2.04	0.55
2:G:475:ILE:O	2:G:479:ILE:HG13	2.05	0.55
1:A:1137:SER:O	1:A:1138:LYS:HE2	2.06	0.55
1:A:1515:ARG:HH12	1:A:1517:PRO:HD3	1.72	0.55
2:G:1706:ILE:O	2:G:1709:ILE:N	2.39	0.55
1:A:339:ALA:HA	1:A:342:GLN:HG3	1.89	0.55
1:A:804:GLY:O	1:A:808:LYS:NZ	2.24	0.55
2:G:1789:PHE:CD2	2:G:1817:SER:HB2	2.42	0.55
1:A:484:LEU:HD23	1:A:485:ASP:HB2	1.89	0.55
1:A:625:THR:HG22	1:A:627:SER:H	1.72	0.55
1:A:1096:SER:HA	1:A:1099:GLU:HB3	1.87	0.55
2:G:1543:ASP:HA	2:G:1622:LEU:O	2.07	0.55
2:G:1547:PRO:HD3	2:G:1584:PHE:CE2	2.42	0.55
2:G:1637:LEU:O	2:G:1639:LYS:NZ	2.39	0.55
2:G:1914:LEU:HA	2:G:1917:ILE:HG22	1.89	0.55
1:A:960:GLU:O	1:A:964:GLU:N	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:404:GLN:HB3	2:G:412:ARG:HG2	1.88	0.55
2:G:940:ASP:OD2	2:G:1013:LYS:HD2	2.07	0.55
2:G:2015:THR:HG22	2:G:2017:LYS:H	1.71	0.55
2:G:528:ILE:HD12	2:G:547:ILE:HG12	1.88	0.55
2:G:529:VAL:HB	2:G:543:PHE:HD1	1.72	0.55
2:G:881:VAL:CG1	2:G:882:PRO:HD3	2.35	0.55
2:G:1830:VAL:HG12	2:G:1991:PHE:HE2	1.72	0.55
2:G:2041:ILE:HG12	2:G:2047:LYS:NZ	2.22	0.55
1:A:1104:ARG:NH2	1:A:1107:GLU:OE1	2.34	0.55
1:A:1148:HIS:ND1	1:A:1151:LYS:HD3	2.22	0.55
1:A:1189:ILE:H	1:A:1380:GLN:HE21	1.53	0.55
1:A:1286:TRP:HA	1:A:1289:MET:HB2	1.88	0.55
2:G:9:LEU:N	2:G:20:LEU:O	2.32	0.55
2:G:37:PHE:CZ	2:G:64:PHE:HA	2.42	0.55
2:G:879:LYS:C	2:G:882:PRO:HD2	2.26	0.55
2:G:1321:ALA:HB3	2:G:1366:LEU:HG	1.88	0.55
1:A:684:GLY:HA3	1:A:709:ARG:HH22	1.72	0.54
2:G:668:GLU:N	2:G:668:GLU:OE1	2.40	0.54
2:G:695:ILE:HD11	2:G:723:HIS:CD2	2.42	0.54
2:G:582:LYS:HA	2:G:585:LYS:HE3	1.88	0.54
2:G:1339:PHE:N	2:G:1340:PRO:HD2	2.22	0.54
2:G:1433:MET:N	2:G:1464:LEU:O	2.39	0.54
2:G:1511:SER:OG	2:G:1512:HIS:N	2.40	0.54
2:G:573:LYS:HG2	2:G:1101:GLU:HA	1.89	0.54
2:G:669:LEU:HD22	2:G:674:TYR:CE2	2.42	0.54
2:G:1590:ARG:NH2	2:G:1594:GLU:OE2	2.40	0.54
1:A:1141:ALA:HB1	1:A:1145:LYS:HE2	1.90	0.54
1:A:1148:HIS:HB3	1:A:1151:LYS:HD3	1.90	0.54
2:G:1431:TYR:HE1	2:G:1526:THR:HG22	1.71	0.54
1:A:777:GLN:N	1:A:777:GLN:OE1	2.41	0.54
2:G:881:VAL:O	2:G:885:GLU:HG2	2.08	0.54
2:G:1130:THR:N	2:G:1133:THR:OG1	2.28	0.54
1:A:1173:LEU:HB2	1:A:1174:TYR:CD2	2.42	0.54
1:A:1584:PRO:HG3	1:A:1591:TRP:CE3	2.43	0.54
2:G:1738:PHE:O	2:G:1749:GLU:HG3	2.08	0.54
2:G:2024:GLU:O	2:G:2028:ASP:N	2.38	0.54
1:A:53:LEU:HD13	2:G:1665:VAL:HB	1.89	0.54
1:A:58:GLN:HB3	1:A:78:ILE:HD13	1.89	0.54
2:G:349:VAL:HG21	2:G:377:LEU:HD22	1.89	0.54
2:G:619:LEU:H	2:G:649:ILE:HA	1.73	0.54
2:G:1698:PHE:CZ	2:G:1828:VAL:HG22	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HD21	1:A:87:GLU:HB2	1.89	0.54
1:A:1245:ASN:ND2	1:A:1284:SER:OG	2.41	0.54
2:G:9:LEU:O	2:G:20:LEU:N	2.32	0.54
1:A:194:PHE:C	1:A:196:THR:H	2.07	0.53
2:G:404:GLN:HE22	2:G:413:LYS:H	1.56	0.53
1:A:403:ASP:OD1	1:A:1613:ASN:ND2	2.28	0.53
1:A:1544:THR:O	1:A:1545:SER:HB3	2.08	0.53
2:G:259:THR:HG23	2:G:262:GLU:H	1.73	0.53
2:G:264:ARG:NH2	2:G:456:GLN:OE1	2.42	0.53
2:G:1138:TRP:CD1	2:G:1176:PRO:HG3	2.43	0.53
2:G:2026:PHE:HB3	2:G:2038:ILE:HG23	1.89	0.53
1:A:652:ASP:OD1	1:A:653:ARG:N	2.41	0.53
1:A:753:TYR:CE1	1:A:764:ASP:HA	2.43	0.53
2:G:1123:ASP:OD2	2:G:1187:GLY:N	2.41	0.53
2:G:1539:ILE:HB	2:G:1626:ILE:HG22	1.89	0.53
2:G:1691:TRP:HB3	2:G:1707:LEU:HD21	1.91	0.53
1:A:1105:LEU:HA	1:A:1185:VAL:HG12	1.91	0.53
1:A:1137:SER:C	1:A:1138:LYS:HE2	2.29	0.53
1:A:1595:GLY:HA2	1:A:1598:GLN:HG3	1.90	0.53
2:G:1148:ASN:H	2:G:1151:HIS:HB2	1.72	0.53
2:G:1607:GLY:O	2:G:1656:GLU:N	2.29	0.53
1:A:1239:HIS:HD2	1:A:1241:SER:H	1.57	0.53
2:G:55:THR:N	2:G:59:GLU:OE2	2.42	0.53
2:G:220:GLU:HG2	2:G:221:ASN:H	1.74	0.53
2:G:382:PRO:HD3	2:G:431:LEU:HD11	1.89	0.53
2:G:526:ARG:CG	2:G:558:ASN:H	2.22	0.53
2:G:1533:LEU:HD23	2:G:1534:GLU:N	2.23	0.53
2:G:1895:ASN:H	2:G:1898:TYR:HE2	1.57	0.53
2:G:2023:LYS:HD2	2:G:2045:TRP:CZ2	2.44	0.53
2:G:160:PHE:CE2	2:G:504:PHE:HB2	2.43	0.53
2:G:728:ILE:HG13	2:G:763:ILE:HD13	1.91	0.53
2:G:1517:VAL:O	2:G:1521:LYS:N	2.42	0.53
2:G:1754:GLU:OE1	2:G:1754:GLU:N	2.42	0.53
2:G:803:SER:N	5:G:2101:FMN:O1P	2.38	0.53
2:G:1226:ASN:HA	2:G:1233:PRO:HA	1.90	0.53
2:G:1866:PHE:HA	2:G:1925:ILE:HD11	1.91	0.53
2:G:1997:ILE:HG22	2:G:1999:GLU:H	1.74	0.53
1:A:1077:ASP:HB3	1:A:1082:GLU:H	1.73	0.53
1:A:1136:ALA:O	1:A:1164:SER:OG	2.18	0.53
1:A:1174:TYR:O	1:A:1175:ILE:HG13	2.09	0.53
1:A:1397:GLY:O	1:A:1680:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:461:ASP:HB3	2:G:465:GLY:H	1.74	0.53
2:G:1281:PRO:HG2	2:G:1342:THR:OG1	2.09	0.53
2:G:1356:GLY:HA2	2:G:1609:THR:HA	1.89	0.53
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.23	0.53
1:A:483:VAL:O	1:A:486:VAL:HG12	2.08	0.53
1:A:490:TYR:CZ	1:A:906:LEU:HD13	2.43	0.53
1:A:533:GLY:O	1:A:537:LYS:HG2	2.09	0.53
1:A:707:THR:HG21	1:A:718:TYR:HE2	1.74	0.53
2:G:720:ALA:HB2	2:G:763:ILE:HD11	1.90	0.53
2:G:847:ARG:HB3	2:G:851:GLY:HA2	1.89	0.53
2:G:1146:GLU:HG2	2:G:1148:ASN:ND2	2.24	0.53
2:G:1698:PHE:CD2	2:G:1706:ILE:HD11	2.43	0.53
2:G:860:ARG:HB3	2:G:898:ASP:HB3	1.90	0.52
2:G:873:PHE:CD1	2:G:1026:GLU:HB3	2.44	0.52
2:G:1830:VAL:HG12	2:G:1991:PHE:CE2	2.44	0.52
1:A:661:ASP:OD2	1:A:662:GLY:N	2.42	0.52
2:G:145:LEU:HG	2:G:146:PHE:HD1	1.74	0.52
2:G:306:ILE:HD11	2:G:480:VAL:HG12	1.89	0.52
2:G:610:THR:HB	2:G:617:ILE:CD1	2.38	0.52
2:G:1323:MET:H	2:G:1590:ARG:NH2	2.06	0.52
1:A:42:GLU:N	1:A:42:GLU:OE2	2.42	0.52
1:A:87:GLU:OE2	1:A:87:GLU:N	2.33	0.52
1:A:774:ILE:CG2	3:A:1901:NAP:N7A	2.73	0.52
2:G:59:GLU:HB2	2:G:122:LEU:HD21	1.91	0.52
2:G:148:ALA:O	2:G:151:GLU:HG2	2.09	0.52
2:G:843:ILE:HG21	2:G:1057:PRO:HA	1.91	0.52
1:A:858:TRP:HE3	1:A:862:LEU:HB2	1.74	0.52
1:A:1247:SER:OG	1:A:1332:TYR:HE1	1.92	0.52
1:A:520:ARG:HH12	1:A:521:LYS:HZ3	1.55	0.52
1:A:966:LYS:HD3	1:A:971:ASN:HB3	1.91	0.52
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	1.91	0.52
2:G:1234:VAL:HG11	2:G:1269:LEU:HD21	1.92	0.52
2:G:1026:GLU:HA	2:G:1029:PHE:HB3	1.91	0.52
2:G:1709:ILE:HG22	2:G:1771:LEU:HD11	1.91	0.52
1:A:1360:ARG:NH1	1:A:1367:ARG:HG3	2.25	0.52
2:G:716:VAL:HG11	2:G:730:LEU:HD21	1.92	0.52
2:G:1614:ASP:OD1	2:G:1650:VAL:HG12	2.09	0.52
2:G:509:ALA:O	2:G:514:VAL:HG21	2.10	0.52
2:G:741:HIS:HB3	2:G:853:PRO:HG2	1.92	0.52
2:G:1338:ILE:HG22	2:G:1390:VAL:HG21	1.92	0.52
2:G:1359:MET:HE3	2:G:1365:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:ILE:HG21	1:A:1253:GLY:H	1.75	0.52
2:G:569:LEU:HB3	2:G:1097:ILE:CD1	2.40	0.52
2:G:1859:PRO:HG3	2:G:1871:LEU:HD21	1.91	0.52
1:A:490:TYR:HB3	1:A:698:GLN:CB	2.40	0.52
1:A:995:LEU:HD13	1:A:1674:VAL:HG22	1.90	0.52
1:A:1037:TRP:HB2	1:A:1598:GLN:HE21	1.75	0.52
1:A:1139:GLU:HG2	1:A:1140:THR:N	2.25	0.52
2:G:37:PHE:CE2	2:G:67:TYR:HD2	2.28	0.52
2:G:116:LEU:O	2:G:119:THR:HG22	2.10	0.52
1:A:501:THR:HG21	1:A:883:ILE:O	2.10	0.51
2:G:747:HIS:O	2:G:751:LEU:N	2.43	0.51
1:A:711:SER:OG	1:A:713:GLN:OE1	2.14	0.51
1:A:741:SER:OG	1:A:744:ASP:HB2	2.10	0.51
1:A:1104:ARG:HH22	1:A:1188:GLN:HB2	1.75	0.51
1:A:1132:GLU:O	1:A:1132:GLU:HG2	2.10	0.51
2:G:1311:PHE:HA	2:G:1320:LEU:HD21	1.92	0.51
2:G:1678:MET:HG3	2:G:1711:ILE:HG22	1.92	0.51
2:G:873:PHE:CE1	2:G:1026:GLU:HB3	2.45	0.51
1:A:77:GLU:HG3	1:A:79:LEU:CD1	2.40	0.51
1:A:953:VAL:HG12	2:G:1439:LYS:HB2	1.92	0.51
2:G:162:GLY:N	2:G:273:HIS:HB3	2.25	0.51
2:G:205:ALA:O	2:G:208:VAL:HG12	2.10	0.51
1:A:1115:ASN:HD22	1:A:1118:LYS:HB2	1.75	0.51
2:G:1911:THR:HG23	2:G:1966:CYS:SG	2.51	0.51
1:A:1718:PRO:HD2	1:A:1744:TYR:HE1	1.74	0.51
2:G:955:GLU:HG2	2:G:987:TYR:HE2	1.75	0.51
1:A:221:LEU:O	1:A:225:SER:CB	2.59	0.51
1:A:430:ARG:NH2	1:A:606:ASP:OD2	2.42	0.51
1:A:1215:VAL:O	1:A:1219:VAL:HG23	2.10	0.51
1:A:1279:PHE:HB2	1:A:1282:THR:HG23	1.92	0.51
1:A:1370:THR:HG22	1:A:1372:THR:H	1.76	0.51
2:G:785:TRP:NE1	2:G:794:MET:O	2.35	0.51
2:G:1519:PHE:O	2:G:1523:ASN:ND2	2.44	0.51
1:A:684:GLY:CA	1:A:709:ARG:HH22	2.23	0.51
1:A:1262:LYS:NZ	1:A:1338:GLU:OE2	2.38	0.51
1:A:1668:ASP:OD2	1:A:1668:ASP:N	2.43	0.51
1:A:608:ASP:OD2	1:A:611:LYS:HG2	2.11	0.51
1:A:329:GLU:O	1:A:333:LYS:NZ	2.34	0.51
1:A:1017:ARG:HH11	1:A:1320:LEU:HD12	1.74	0.51
1:A:1148:HIS:CD2	1:A:1167:LEU:HD22	2.46	0.51
2:G:116:LEU:HA	2:G:119:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1804:PHE:CD1	2:G:1818:LEU:HG	2.46	0.51
2:G:695:ILE:HD11	2:G:723:HIS:CG	2.46	0.50
2:G:1458:ASP:OD1	2:G:1458:ASP:N	2.44	0.50
1:A:1425:ILE:CG1	1:A:1651:GLY:H	2.24	0.50
2:G:145:LEU:H	2:G:145:LEU:HD23	1.75	0.50
2:G:234:ILE:HG13	2:G:235:PRO:HD3	1.93	0.50
2:G:569:LEU:HD23	2:G:1090:TYR:HE1	1.75	0.50
2:G:1383:ASN:ND2	2:G:1416:TYR:HB2	2.25	0.50
2:G:1906:ALA:O	2:G:1910:VAL:HG23	2.12	0.50
1:A:416:LEU:HD22	1:A:420:ILE:HD11	1.93	0.50
2:G:619:LEU:N	2:G:648:GLY:O	2.44	0.50
2:G:694:TYR:O	2:G:698:LEU:HB2	2.12	0.50
2:G:737:GLY:O	2:G:855:HIS:ND1	2.32	0.50
2:G:740:HIS:CD2	3:G:2102:NAP:N7N	2.79	0.50
2:G:1452:LEU:HB3	2:G:1501:ILE:HG22	1.92	0.50
1:A:828:PRO:HG3	1:A:927:ASN:ND2	2.26	0.50
1:A:846:LEU:O	1:A:849:LEU:HB2	2.10	0.50
1:A:1226:SER:O	1:A:1226:SER:OG	2.23	0.50
2:G:480:VAL:O	2:G:484:ILE:HG12	2.11	0.50
2:G:625:PHE:HD2	3:G:2102:NAP:C6A	1.85	0.50
2:G:900:GLN:HE21	2:G:1052:CYS:H	1.60	0.50
2:G:1300:PHE:CZ	2:G:1304:VAL:HG21	2.46	0.50
2:G:1397:SER:HA	2:G:1403:VAL:HG23	1.93	0.50
2:G:1562:PRO:HB2	2:G:1569:PHE:CD2	2.46	0.50
1:A:609:SER:O	1:A:613:VAL:HG23	2.12	0.50
1:A:1360:ARG:HH21	1:A:1372:THR:HG23	1.77	0.50
2:G:9:LEU:HB3	2:G:20:LEU:HB3	1.94	0.50
2:G:1855:ILE:HB	2:G:1907:LEU:HD21	1.94	0.50
1:A:868:ILE:HG13	1:A:925:ASP:HA	1.94	0.50
1:A:1077:ASP:OD2	1:A:1079:LYS:N	2.39	0.50
1:A:1303:GLY:H	1:A:1307:THR:HB	1.77	0.50
2:G:72:VAL:HG21	2:G:84:LEU:HD22	1.93	0.50
2:G:1318:THR:OG1	2:G:1369:GLY:N	2.44	0.50
2:G:1668:GLY:HA2	2:G:1809:LEU:HB3	1.94	0.50
2:G:118:LYS:O	2:G:122:LEU:HD23	2.10	0.50
2:G:1206:LYS:HD3	2:G:1226:ASN:HD22	1.76	0.50
2:G:1595:ASN:OD1	2:G:1596:TRP:N	2.44	0.50
1:A:42:GLU:OE2	2:G:1661:VAL:HB	2.11	0.50
1:A:403:ASP:O	1:A:405:SER:N	2.44	0.50
1:A:753:TYR:CB	1:A:809:GLN:HG2	2.42	0.50
2:G:1440:ASP:OD1	2:G:1441:ILE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1878:VAL:HG21	2:G:1910:VAL:HG22	1.92	0.50
1:A:1136:ALA:H	1:A:1164:SER:HB3	1.75	0.49
2:G:1320:LEU:H	2:G:1320:LEU:HD23	1.77	0.49
1:A:1373:ARG:HD2	1:A:1547:LYS:HA	1.92	0.49
2:G:139:LYS:NZ	2:G:140:LYS:O	2.38	0.49
2:G:426:PRO:HG3	2:G:431:LEU:HD12	1.95	0.49
2:G:670:ARG:HH11	2:G:670:ARG:HA	1.77	0.49
2:G:1884:TRP:HB2	2:G:1906:ALA:HB2	1.93	0.49
2:G:2015:THR:OG1	2:G:2029:VAL:HG12	2.13	0.49
1:A:431:GLU:OE1	1:A:434:SER:OG	2.31	0.49
1:A:1476:GLU:OE2	1:A:1477:ILE:HG13	2.12	0.49
2:G:1294:ALA:HA	2:G:1368:VAL:HG11	1.94	0.49
1:A:47:ILE:HD13	1:A:81:TYR:HB2	1.93	0.49
1:A:168:MET:O	1:A:206:LEU:CB	2.60	0.49
1:A:460:GLU:OE1	1:A:470:LYS:NZ	2.41	0.49
1:A:475:GLN:O	1:A:479:ASN:N	2.40	0.49
1:A:1335:PHE:O	1:A:1336:GLN:HG2	2.12	0.49
2:G:368:ILE:HG22	2:G:379:VAL:HG12	1.93	0.49
2:G:1706:ILE:HA	2:G:1709:ILE:HD12	1.95	0.49
1:A:520:ARG:HH21	1:A:602:GLU:CD	2.15	0.49
1:A:1207:GLN:NE2	1:A:1277:GLU:OE2	2.45	0.49
2:G:615:TYR:CZ	2:G:1074:MET:HB3	2.47	0.49
2:G:844:VAL:HG12	2:G:845:THR:N	2.27	0.49
2:G:1635:ARG:HD2	2:G:1656:GLU:OE1	2.12	0.49
2:G:1874:VAL:HA	2:G:1877:ARG:CZ	2.42	0.49
2:G:1941:PHE:HA	2:G:1944:ILE:HG22	1.94	0.49
1:A:994:GLU:OE1	1:A:994:GLU:N	2.46	0.49
1:A:1135:GLU:OE1	1:A:1135:GLU:N	2.44	0.49
2:G:818:LYS:O	2:G:821:ILE:HG22	2.13	0.49
1:A:1026:GLU:HB2	1:A:1594:ASN:ND2	2.28	0.49
2:G:435:ALA:O	2:G:439:ILE:HG13	2.12	0.49
2:G:1485:CYS:SG	2:G:1514:ASN:ND2	2.77	0.49
1:A:784:ILE:HD13	1:A:838:MET:HG3	1.93	0.49
2:G:31:SER:HA	2:G:34:GLN:HE21	1.78	0.49
2:G:59:GLU:HB3	2:G:122:LEU:HD21	1.95	0.49
2:G:691:ALA:HA	2:G:694:TYR:CD2	2.47	0.49
2:G:736:ARG:NE	2:G:769:SER:O	2.33	0.49
1:A:521:LYS:HZ3	1:A:605:LEU:HD12	1.78	0.49
2:G:549:ASP:HB3	2:G:554:GLY:HA3	1.93	0.49
2:G:698:LEU:O	2:G:700:LEU:N	2.44	0.49
2:G:902:PRO:HG3	2:G:1044:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1447:LYS:HG2	2:G:1449:TRP:CE2	2.46	0.49
2:G:1452:LEU:HA	2:G:1502:GLY:HA3	1.94	0.49
1:A:1138:LYS:N	1:A:1139:GLU:OE1	2.46	0.49
2:G:202:THR:HG21	2:G:205:ALA:HB3	1.94	0.49
2:G:275:GLN:HE21	2:G:303:LEU:HD13	1.77	0.49
2:G:1215:LYS:O	2:G:1218:ILE:HG12	2.13	0.49
2:G:1695:ASP:OD1	2:G:1705:SER:OG	2.24	0.49
1:A:411:GLN:NE2	1:A:1629:LYS:HG2	2.27	0.48
1:A:727:ALA:N	1:A:730:SER:OG	2.46	0.48
1:A:1354:GLU:OE2	1:A:1374:ASN:ND2	2.28	0.48
2:G:59:GLU:HA	2:G:122:LEU:HD11	1.95	0.48
2:G:610:THR:OG1	2:G:1070:ILE:HG12	2.12	0.48
2:G:1604:ARG:O	2:G:1657:ILE:HD12	2.13	0.48
2:G:1917:ILE:O	2:G:1921:LYS:N	2.43	0.48
1:A:1141:ALA:O	1:A:1145:LYS:HD3	2.13	0.48
2:G:35:GLU:HA	2:G:38:ASN:HD21	1.78	0.48
1:A:1189:ILE:HG12	1:A:1380:GLN:NE2	2.27	0.48
1:A:750:GLU:OE1	1:A:750:GLU:N	2.37	0.48
1:A:827:SER:HG	3:A:1901:NAP:C5N	2.25	0.48
2:G:1738:PHE:HB2	2:G:1751:ILE:CD1	2.43	0.48
1:A:159:LEU:O	1:A:161:LYS:N	2.45	0.48
2:G:887:LYS:O	2:G:891:ILE:HG23	2.13	0.48
2:G:1359:MET:HG3	2:G:1606:ARG:HH21	1.79	0.48
2:G:1484:LYS:NZ	2:G:1507:GLU:HB2	2.28	0.48
2:G:1778:GLN:HB2	2:G:1779:PRO:HD3	1.95	0.48
1:A:30:GLU:HB2	2:G:2016:ALA:CB	2.43	0.48
1:A:974:ASP:HA	1:A:977:TYR:CD2	2.49	0.48
2:G:733:THR:OG1	2:G:769:SER:HB3	2.12	0.48
2:G:1224:ILE:O	2:G:1568:HIS:NE2	2.46	0.48
2:G:1373:SER:N	2:G:1397:SER:O	2.42	0.48
2:G:1454:ASP:OD1	2:G:1454:ASP:N	2.45	0.48
2:G:1822:MET:HG3	2:G:1827:LEU:HB2	1.94	0.48
1:A:27:ARG:HH21	2:G:2016:ALA:H	1.60	0.48
1:A:440:MET:CE	1:A:479:ASN:HB3	2.43	0.48
1:A:1317:GLU:O	1:A:1321:SER:HB3	2.13	0.48
2:G:214:ASN:HB3	2:G:217:GLU:OE2	2.13	0.48
2:G:1924:ILE:HD12	2:G:1924:ILE:H	1.77	0.48
2:G:215:ILE:HD12	2:G:240:LEU:HD21	1.94	0.48
2:G:646:THR:HG21	2:G:677:GLN:HB2	1.95	0.48
2:G:1079:ASP:OD2	2:G:1080:GLY:N	2.46	0.48
2:G:1129:ALA:HB2	2:G:1138:TRP:CH2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1957:PRO:HB2	2:G:1959:LYS:HE2	1.95	0.48
1:A:1116:PRO:HB2	1:A:1184:LEU:HD13	1.96	0.48
1:A:1144:PHE:HZ	1:A:1174:TYR:HH	1.62	0.48
2:G:45:THR:O	2:G:48:PHE:N	2.47	0.48
2:G:246:LEU:O	2:G:250:VAL:HG13	2.13	0.48
2:G:809:LYS:HB3	2:G:1067:ASP:O	2.13	0.48
2:G:2046:GLU:N	2:G:2046:GLU:OE1	2.46	0.48
1:A:421:ILE:HA	1:A:465:ASN:HB3	1.96	0.48
1:A:1052:GLU:O	1:A:1056:ILE:HG23	2.14	0.48
2:G:543:PHE:HB2	2:G:545:GLN:HE22	1.79	0.48
2:G:725:ASN:HA	2:G:1109:VAL:HG11	1.96	0.48
2:G:1839:GLN:HE21	2:G:1844:ARG:HD2	1.79	0.48
1:A:985:ARG:HG3	2:G:956:GLU:HB3	1.95	0.47
1:A:1334:ASP:CG	1:A:1335:PHE:H	2.17	0.47
2:G:270:ALA:O	2:G:459:VAL:HA	2.13	0.47
1:A:1608:ASN:O	1:A:1610:ASN:N	2.47	0.47
2:G:16:LEU:HD23	2:G:48:PHE:CD2	2.50	0.47
2:G:155:GLN:HG2	2:G:499:THR:HG23	1.95	0.47
2:G:336:SER:OG	2:G:423:VAL:O	2.32	0.47
2:G:710:ILE:HD13	2:G:749:PRO:HB3	1.96	0.47
2:G:1889:VAL:HG23	2:G:1899:VAL:HG23	1.97	0.47
1:A:33:ASP:O	1:A:37:LYS:N	2.45	0.47
2:G:20:LEU:HD12	2:G:90:GLU:CD	2.35	0.47
2:G:900:GLN:NE2	2:G:1052:CYS:H	2.11	0.47
2:G:1491:VAL:CB	2:G:1501:ILE:HD11	2.44	0.47
2:G:1908:ASP:OD2	2:G:1954:LYS:HD3	2.14	0.47
2:G:1976:PHE:HD1	2:G:1977:HIS:HD1	1.59	0.47
1:A:1125:VAL:CG1	1:A:1126:ILE:H	2.16	0.47
2:G:109:LEU:HG	2:G:114:THR:HG23	1.95	0.47
2:G:864:LEU:HD11	2:G:868:PHE:CZ	2.49	0.47
2:G:1038:GLU:H	2:G:1038:GLU:HG2	1.53	0.47
2:G:1485:CYS:HB2	2:G:1506:TYR:HB3	1.95	0.47
2:G:1850:SER:HB3	2:G:1973:SER:OG	2.14	0.47
1:A:385:PHE:CD2	1:A:787:LYS:HA	2.50	0.47
1:A:810:LYS:CB	1:A:861:GLN:HG2	2.45	0.47
1:A:1040:GLU:HA	1:A:1580:LEU:HD11	1.97	0.47
1:A:1390:ALA:O	1:A:1393:ALA:N	2.48	0.47
2:G:1310:ASP:OD1	2:G:1602:SER:N	2.45	0.47
2:G:1730:ARG:NH2	2:G:1757:GLU:O	2.47	0.47
2:G:259:THR:HA	2:G:289:TRP:NE1	2.30	0.47
2:G:865:TRP:HE1	2:G:1030:LYS:HZ3	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1058:VAL:O	2:G:1061:GLN:HG2	2.15	0.47
2:G:1517:VAL:O	2:G:1521:LYS:HG2	2.13	0.47
1:A:413:LEU:HD23	1:A:450:PHE:CD2	2.49	0.47
1:A:433:VAL:HG13	1:A:609:SER:HB2	1.95	0.47
1:A:1584:PRO:HG2	1:A:1588:ALA:N	2.30	0.47
2:G:598:THR:OG1	2:G:599:PRO:HD3	2.14	0.47
2:G:633:ALA:O	2:G:637:VAL:HG13	2.14	0.47
2:G:895:LEU:HD13	2:G:1018:VAL:HG21	1.95	0.47
2:G:1201:VAL:HG11	2:G:1226:ASN:ND2	2.27	0.47
2:G:1287:GLY:HA3	2:G:1374:THR:HG23	1.97	0.47
2:G:1718:THR:HA	2:G:1763:THR:HA	1.96	0.47
2:G:1858:ASN:ND2	2:G:1861:ARG:HG3	2.30	0.47
2:G:1960:LEU:HD23	2:G:1968:PRO:HB3	1.96	0.47
1:A:13:LEU:HD22	2:G:2026:PHE:CE1	2.50	0.47
1:A:695:GLY:HA3	1:A:906:LEU:HD11	1.97	0.47
1:A:1120:GLU:H	1:A:1120:GLU:CD	2.18	0.47
2:G:66:GLY:O	2:G:69:SER:OG	2.22	0.47
2:G:530:ALA:HA	2:G:547:ILE:HD11	1.95	0.47
2:G:1263:LYS:HD3	2:G:1347:LEU:HD11	1.96	0.47
2:G:1323:MET:H	2:G:1590:ARG:HH22	1.60	0.47
2:G:1775:GLN:HE22	2:G:1836:MET:CB	2.26	0.47
2:G:1956:ARG:O	2:G:1956:ARG:NE	2.48	0.47
1:A:712:LYS:HB3	1:A:1361:THR:HG21	1.96	0.47
2:G:6:THR:HA	2:G:23:PRO:HA	1.96	0.47
2:G:421:LEU:O	2:G:423:VAL:N	2.48	0.47
2:G:589:ARG:HG2	2:G:590:PRO:HD2	1.96	0.47
2:G:1381:VAL:HG12	2:G:1390:VAL:HG12	1.97	0.47
2:G:1799:PRO:HD2	2:G:1802:ALA:HB2	1.96	0.47
1:A:640:LEU:N	1:A:656:SER:OG	2.48	0.47
1:A:1059:PHE:HA	1:A:1079:LYS:NZ	2.30	0.47
1:A:1298:ILE:HD13	1:A:1298:ILE:HA	1.65	0.47
2:G:67:TYR:CZ	2:G:71:LEU:HD11	2.50	0.47
2:G:831:LYS:HE2	2:G:834:GLN:HG3	1.97	0.47
2:G:857:ILE:O	2:G:862:VAL:HG11	2.15	0.47
1:A:257:PRO:O	1:A:261:GLN:N	2.41	0.46
1:A:338:LEU:O	1:A:342:GLN:N	2.28	0.46
1:A:1064:ASN:HA	1:A:1072:TYR:O	2.15	0.46
2:G:1324:ASP:O	2:G:1327:ILE:HG22	2.15	0.46
2:G:1342:THR:O	2:G:1421:ASN:ND2	2.48	0.46
2:G:1351:VAL:HG21	2:G:1413:ARG:NH2	2.30	0.46
1:A:49:PRO:HD3	2:G:1784:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:VAL:HG11	1:A:1154:ILE:HG23	1.96	0.46
2:G:138:ASP:OD1	2:G:138:ASP:N	2.48	0.46
2:G:264:ARG:HH21	2:G:456:GLN:HB2	1.80	0.46
1:A:1119:LYS:HE3	1:A:1341:PHE:CD1	2.49	0.46
1:A:1397:GLY:O	1:A:1680:ARG:HG3	2.15	0.46
1:A:1446:LYS:O	1:A:1450:ARG:HG3	2.14	0.46
2:G:748:THR:HA	2:G:751:LEU:HB3	1.98	0.46
2:G:932:ILE:HD11	2:G:939:PHE:HB2	1.97	0.46
2:G:1323:MET:HE1	2:G:1608:TYR:HB3	1.97	0.46
2:G:1550:ASN:HB3	2:G:1581:HIS:CE1	2.51	0.46
2:G:2030:TYR:HB2	2:G:2038:ILE:HG21	1.97	0.46
1:A:1360:ARG:NH2	1:A:1367:ARG:HD2	2.30	0.46
2:G:36:GLN:O	2:G:40:ILE:HG13	2.16	0.46
2:G:1737:ILE:O	2:G:1833:TYR:OH	2.34	0.46
1:A:46:GLU:HB3	1:A:80:CYS:HA	1.97	0.46
1:A:693:LEU:HD13	1:A:705:VAL:HG11	1.97	0.46
1:A:858:TRP:CE3	1:A:862:LEU:HB2	2.50	0.46
2:G:273:HIS:CG	2:G:274:SER:H	2.34	0.46
2:G:573:LYS:CG	2:G:1101:GLU:HA	2.45	0.46
2:G:804:ARG:NH2	2:G:1068:GLU:OE1	2.37	0.46
2:G:1643:ARG:HB3	2:G:1647:ASP:HA	1.96	0.46
2:G:1812:TYR:OH	2:G:1834:ARG:NE	2.48	0.46
2:G:1924:ILE:O	2:G:1928:GLN:NE2	2.48	0.46
2:G:239:PRO:O	2:G:243:VAL:HG13	2.16	0.46
2:G:1093:ASP:OD1	2:G:1096:LYS:HB2	2.16	0.46
2:G:1138:TRP:NE1	2:G:1142:LEU:HD11	2.30	0.46
2:G:1722:GLY:N	2:G:1726:GLY:HA3	2.31	0.46
1:A:467:GLN:O	1:A:467:GLN:NE2	2.49	0.46
2:G:490:TRP:CH2	2:G:512:LEU:HD21	2.51	0.46
2:G:649:ILE:HD13	2:G:666:ILE:HD11	1.98	0.46
1:A:803:MET:HE1	1:A:849:LEU:HD21	1.98	0.46
1:A:1029:PRO:HG3	1:A:1187:GLY:O	2.16	0.46
2:G:2036:GLU:CD	2:G:2037:PRO:HD3	2.36	0.46
1:A:55:GLY:O	1:A:59:ARG:HG2	2.16	0.46
1:A:1534:ASP:OD2	1:A:1567:SER:OG	2.32	0.46
2:G:978:GLU:OE1	2:G:978:GLU:N	2.49	0.46
2:G:1149:TRP:HB2	2:G:1219:ILE:HD11	1.98	0.46
1:A:395:SER:HB3	1:A:398:LYS:HD2	1.97	0.46
1:A:452:GLU:O	1:A:456:SER:OG	2.29	0.46
1:A:521:LYS:HD2	1:A:523:SER:OG	2.15	0.46
1:A:527:GLN:HG2	1:A:626:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:GLU:CD	1:A:1135:GLU:H	2.19	0.46
1:A:1461:ASP:O	1:A:1464:GLU:HG2	2.15	0.46
2:G:310:CYS:O	2:G:313:ALA:N	2.49	0.46
2:G:410:SER:OG	2:G:411:GLU:OE2	2.33	0.46
2:G:1741:ILE:HD11	2:G:1986:LYS:HG2	1.97	0.46
2:G:142:ASN:HD21	2:G:147:ARG:NE	2.13	0.45
2:G:502:LEU:HD23	2:G:502:LEU:H	1.81	0.45
2:G:634:ILE:O	2:G:637:VAL:HG22	2.17	0.45
1:A:430:ARG:HG3	1:A:495:LYS:HG3	1.98	0.45
1:A:821:GLN:OE1	1:A:823:ILE:HD11	2.16	0.45
1:A:957:VAL:HG23	2:G:1443:VAL:HG12	1.99	0.45
1:A:1606:PRO:HA	1:A:1630:THR:HG23	1.99	0.45
2:G:540:ASP:OD1	2:G:540:ASP:N	2.49	0.45
2:G:646:THR:CG2	2:G:677:GLN:HB2	2.46	0.45
2:G:906:THR:OG1	2:G:925:ARG:NH2	2.49	0.45
2:G:1488:PRO:HA	2:G:1503:ILE:HD13	1.98	0.45
2:G:1669:GLN:HB3	2:G:1809:LEU:HD13	1.99	0.45
2:G:1716:ASN:ND2	2:G:1765:ARG:HA	2.29	0.45
2:G:1819:ALA:HA	2:G:2005:ARG:HD2	1.98	0.45
2:G:273:HIS:HB2	2:G:512:LEU:HD22	1.98	0.45
2:G:479:ILE:O	2:G:483:ILE:HG13	2.16	0.45
2:G:938:TRP:CD2	2:G:944:ARG:HG3	2.51	0.45
2:G:1611:GLN:N	2:G:1652:THR:O	2.35	0.45
2:G:1644:ASN:HB3	2:G:1646:ASP:OD2	2.16	0.45
1:A:1001:VAL:HA	1:A:1004:ILE:HG22	1.98	0.45
1:A:1036:ARG:HH21	1:A:1598:GLN:HE21	1.65	0.45
1:A:1209:ASP:OD2	1:A:1253:GLY:HA2	2.17	0.45
2:G:430:HIS:HA	2:G:433:VAL:HG23	1.99	0.45
2:G:1641:GLU:OE2	2:G:1643:ARG:NE	2.48	0.45
2:G:1712:ASN:OD1	2:G:1712:ASN:N	2.50	0.45
1:A:329:GLU:O	1:A:332:THR:OG1	2.25	0.45
1:A:1020:VAL:HG23	1:A:1402:GLY:O	2.16	0.45
1:A:1046:SER:OG	1:A:1047:LEU:N	2.48	0.45
1:A:1123:GLN:HB3	1:A:1177:LYS:CD	2.45	0.45
1:A:1182:ASP:O	1:A:1184:LEU:HB2	2.16	0.45
1:A:1207:GLN:HE22	1:A:1286:TRP:HZ2	1.65	0.45
1:A:1238:VAL:HG22	1:A:1242:GLU:HB2	1.98	0.45
1:A:1355:GLU:CD	1:A:1360:ARG:HD2	2.37	0.45
2:G:126:TYR:HD2	2:G:127:ILE:HD13	1.80	0.45
2:G:1168:ASN:O	2:G:1172:LYS:HG2	2.17	0.45
2:G:1291:GLU:HA	2:G:1371:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1531:VAL:HG13	2:G:1631:MET:HB2	1.99	0.45
1:A:90:TYR:O	2:G:1533:LEU:HD21	2.17	0.45
1:A:1559:GLU:O	1:A:1563:HIS:N	2.39	0.45
2:G:1357:TYR:CD1	2:G:1406:VAL:HG12	2.52	0.45
2:G:1681:TYR:CE2	2:G:1691:TRP:HB2	2.52	0.45
1:A:413:LEU:HD23	1:A:450:PHE:CE2	2.52	0.45
1:A:739:GLN:HG3	1:A:772:ALA:HB3	1.98	0.45
1:A:819:PRO:HB3	1:A:860:ASN:O	2.16	0.45
1:A:1431:GLU:HB3	1:A:1520:ALA:HB2	1.99	0.45
2:G:2041:ILE:HG12	2:G:2047:LYS:HZ1	1.82	0.45
1:A:27:ARG:NH2	2:G:2015:THR:HA	2.32	0.45
2:G:109:LEU:HD12	2:G:119:THR:HG21	1.98	0.45
2:G:268:LYS:O	2:G:458:PRO:HD2	2.16	0.45
2:G:877:LYS:HG3	2:G:878:ASN:N	2.31	0.45
2:G:938:TRP:CE2	2:G:944:ARG:HG3	2.52	0.45
2:G:1745:LYS:NZ	2:G:1747:LYS:HA	2.32	0.45
1:A:333:LYS:O	1:A:337:VAL:HG13	2.16	0.45
1:A:853:TRP:CE3	1:A:921:PRO:HD3	2.51	0.45
1:A:1026:GLU:OE1	1:A:1594:ASN:ND2	2.47	0.45
1:A:1245:ASN:O	1:A:1298:ILE:HG23	2.17	0.45
1:A:1707:THR:O	1:A:1710:LEU:N	2.46	0.45
2:G:68:VAL:O	2:G:72:VAL:HG23	2.17	0.45
2:G:297:ARG:NE	2:G:447:ASN:HD21	2.15	0.45
2:G:391:LEU:O	2:G:394:ARG:N	2.42	0.45
2:G:612:ASN:HD21	2:G:641:ILE:HA	1.82	0.45
2:G:872:ILE:O	2:G:875:LEU:HB3	2.17	0.45
2:G:1514:ASN:ND2	2:G:1516:VAL:HG22	2.32	0.45
1:A:1418:VAL:HG12	1:A:1647:GLY:HA2	1.99	0.45
2:G:812:LYS:HD3	2:G:812:LYS:HA	1.56	0.45
2:G:1151:HIS:CD2	2:G:1155:LEU:HD12	2.51	0.45
2:G:1669:GLN:HA	2:G:1781:LEU:HD13	1.99	0.45
2:G:1892:ASN:HB2	2:G:1897:GLN:HB3	1.99	0.45
1:A:945:LYS:O	1:A:949:GLU:HG2	2.17	0.44
1:A:981:GLU:OE2	2:G:962:LYS:HB2	2.17	0.44
1:A:1211:ILE:O	1:A:1215:VAL:HG23	2.17	0.44
1:A:1368:PRO:HG2	1:A:1608:ASN:ND2	2.31	0.44
1:A:1717:ASP:OD2	1:A:1739:GLN:HB2	2.17	0.44
2:G:408:PRO:HB3	2:G:833:GLU:OE2	2.17	0.44
2:G:1257:ASP:OD1	2:G:1260:GLN:HB2	2.18	0.44
2:G:1598:ALA:HB2	2:G:1657:ILE:HD11	1.98	0.44
2:G:1767:GLU:HG2	2:G:1768:LYS:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1804:PHE:CG	2:G:1818:LEU:HG	2.52	0.44
2:G:1854:MET:HA	2:G:1901:ALA:HA	1.98	0.44
1:A:330:GLU:HA	1:A:333:LYS:HG2	1.99	0.44
1:A:711:SER:H	1:A:714:VAL:HG12	1.82	0.44
2:G:230:TYR:O	2:G:236:ILE:HG21	2.17	0.44
2:G:437:ASP:OD1	2:G:437:ASP:N	2.50	0.44
2:G:587:ILE:HG13	2:G:589:ARG:H	1.82	0.44
2:G:665:LEU:HD21	2:G:669:LEU:HD12	1.99	0.44
2:G:734:GLY:H	2:G:769:SER:HB3	1.81	0.44
2:G:1539:ILE:HD11	2:G:1628:HIS:HB2	1.97	0.44
2:G:1786:LYS:NZ	2:G:1816:ALA:O	2.50	0.44
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.53	0.44
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.77	0.44
1:A:930:LEU:HD23	1:A:930:LEU:HA	1.71	0.44
2:G:124:LYS:HB2	2:G:179:THR:HA	1.99	0.44
2:G:423:VAL:HG12	2:G:424:ALA:H	1.81	0.44
2:G:1357:TYR:HD1	2:G:1406:VAL:HG12	1.82	0.44
2:G:1713:ASN:ND2	2:G:1771:LEU:HB2	2.33	0.44
2:G:297:ARG:NH1	2:G:301:THR:HG21	2.32	0.44
2:G:330:ASN:HB3	2:G:394:ARG:HH12	1.83	0.44
2:G:543:PHE:HB2	2:G:545:GLN:NE2	2.32	0.44
1:A:1123:GLN:HG2	1:A:1124:GLU:N	2.24	0.44
1:A:1254:VAL:HA	1:A:1257:LEU:HD12	1.99	0.44
1:A:1351:ASN:HB3	1:A:1354:GLU:HG2	2.00	0.44
1:A:1460:LYS:HE3	1:A:1460:LYS:HB3	1.87	0.44
2:G:597:MET:HB2	2:G:601:THR:HG23	2.00	0.44
2:G:604:PRO:HA	2:G:607:VAL:HG12	2.00	0.44
2:G:1624:THR:HA	2:G:1642:THR:HA	2.00	0.44
1:A:11:HIS:HB2	2:G:2001:VAL:HG11	2.00	0.44
1:A:843:LYS:CE	3:A:1901:NAP:HO2N	2.30	0.44
1:A:1086:ASP:O	1:A:1089:VAL:HG12	2.18	0.44
2:G:81:ASP:OD1	2:G:81:ASP:N	2.48	0.44
2:G:615:TYR:CE2	2:G:1074:MET:HB3	2.53	0.44
2:G:821:ILE:HD11	2:G:1055:HIS:ND1	2.32	0.44
2:G:861:GLY:HA2	2:G:898:ASP:O	2.17	0.44
1:A:774:ILE:HD11	1:A:791:ALA:HB2	2.00	0.44
1:A:1087:LYS:HA	1:A:1087:LYS:HD2	1.81	0.44
1:A:1234:MET:O	1:A:1238:VAL:HG12	2.18	0.44
2:G:148:ALA:O	2:G:153:ASN:N	2.50	0.44
2:G:368:ILE:HA	2:G:379:VAL:HG12	2.00	0.44
2:G:608:ALA:HA	2:G:611:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:810:GLU:CD	2:G:1070:ILE:H	2.21	0.44
2:G:2037:PRO:HA	2:G:2040:GLU:OE2	2.17	0.44
1:A:477:ILE:O	1:A:481:LYS:HG3	2.18	0.44
1:A:985:ARG:HB2	2:G:957:ARG:HA	2.00	0.44
1:A:1125:VAL:HG12	1:A:1126:ILE:N	2.18	0.44
1:A:1248:GLY:O	1:A:1331:GLY:HA2	2.17	0.44
2:G:848:SER:OG	2:G:849:GLU:N	2.51	0.44
2:G:1001:ASP:OD2	2:G:1001:ASP:N	2.48	0.44
2:G:1297:VAL:HG23	2:G:1319:MET:HG2	2.00	0.44
2:G:1561:ASN:HD21	2:G:1563:ILE:HG12	1.82	0.44
1:A:658:LEU:HD11	1:A:916:LEU:HD22	1.99	0.44
2:G:457:ILE:C	2:G:469:ARG:HH21	2.21	0.44
2:G:686:PRO:HB3	2:G:690:VAL:HG13	2.00	0.44
2:G:741:HIS:CE1	2:G:855:HIS:NE2	2.86	0.44
2:G:1624:THR:OG1	2:G:1642:THR:HG22	2.18	0.44
1:A:8:GLU:O	1:A:12:ILE:HG12	2.18	0.43
1:A:448:ILE:HD13	1:A:481:LYS:HG2	2.00	0.43
1:A:1298:ILE:HD11	1:A:1323:LYS:HZ1	1.83	0.43
2:G:394:ARG:HA	2:G:397:LYS:CG	2.43	0.43
2:G:461:ASP:OD2	2:G:478:ARG:HD3	2.18	0.43
2:G:736:ARG:NH1	2:G:829:ASP:OD2	2.51	0.43
2:G:1224:ILE:HA	2:G:1235:SER:HA	1.99	0.43
2:G:1299:ASP:OD2	2:G:1556:VAL:HG22	2.18	0.43
2:G:1594:GLU:HG2	2:G:1605:VAL:HG21	2.00	0.43
1:A:402:PHE:HB2	1:A:732:LEU:CD2	2.48	0.43
1:A:1015:LEU:O	1:A:1390:ALA:HB3	2.18	0.43
2:G:123:ILE:HD12	2:G:123:ILE:H	1.82	0.43
2:G:240:LEU:HA	2:G:243:VAL:HG22	2.00	0.43
2:G:517:HIS:HB2	2:G:527:VAL:CG1	2.46	0.43
2:G:1078:HIS:O	2:G:1082:ILE:HG12	2.18	0.43
2:G:1533:LEU:HD23	2:G:1534:GLU:H	1.82	0.43
1:A:1208:VAL:CG1	1:A:1212:THR:HB	2.48	0.43
2:G:355:LYS:O	2:G:358:SER:OG	2.31	0.43
2:G:856:LYS:HB2	2:G:862:VAL:HG21	2.00	0.43
2:G:1353:LEU:HD23	2:G:1353:LEU:HA	1.84	0.43
1:A:46:GLU:HA	2:G:1665:VAL:HG23	1.99	0.43
1:A:83:LYS:HD2	1:A:84:ASP:OD1	2.18	0.43
1:A:724:LYS:HE3	1:A:725:TYR:CZ	2.53	0.43
1:A:960:GLU:OE2	1:A:961:THR:HG23	2.19	0.43
2:G:391:LEU:HD23	2:G:394:ARG:HE	1.83	0.43
2:G:1087:HIS:HA	2:G:1092:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:VAL:O	1:A:341:GLN:N	2.42	0.43
1:A:1740:SER:OG	1:A:1742:ASP:OD1	2.27	0.43
2:G:807:ILE:HD11	2:G:822:ALA:HB2	2.01	0.43
2:G:1225:GLU:OE1	2:G:1227:ARG:N	2.52	0.43
2:G:1434:HIS:CD2	2:G:1436:LYS:HE3	2.53	0.43
2:G:1537:ILE:O	2:G:1537:ILE:HG13	2.19	0.43
2:G:1623:LYS:HA	2:G:1623:LYS:HE2	2.00	0.43
2:G:1845:ASP:CG	2:G:1849:ARG:HG2	2.39	0.43
1:A:31:THR:HA	1:A:34:VAL:HG12	2.01	0.43
1:A:440:MET:HE3	1:A:479:ASN:HB3	1.99	0.43
1:A:823:ILE:HD13	1:A:865:CYS:HB3	1.99	0.43
1:A:1101:SER:N	1:A:1104:ARG:HD3	2.32	0.43
2:G:45:THR:OG1	2:G:50:ALA:HB2	2.19	0.43
2:G:525:VAL:C	2:G:526:ARG:HD3	2.39	0.43
2:G:527:VAL:HG13	2:G:541:TYR:HB3	2.00	0.43
2:G:1045:ASP:OD1	2:G:1045:ASP:N	2.46	0.43
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.85	0.43
1:A:841:GLU:OE2	1:A:845:SER:OG	2.37	0.43
2:G:113:ASP:OD1	2:G:113:ASP:N	2.50	0.43
2:G:268:LYS:HE2	2:G:268:LYS:HB3	1.68	0.43
2:G:1869:GLU:HA	2:G:1872:GLN:HG2	2.00	0.43
2:G:2023:LYS:H	2:G:2023:LYS:HD3	1.83	0.43
2:G:256:LEU:HD23	2:G:256:LEU:HA	1.82	0.43
2:G:740:HIS:CE1	2:G:854:ILE:HD11	2.53	0.43
2:G:910:GLN:HE22	2:G:912:ARG:NH2	2.17	0.43
2:G:1428:GLU:OE2	2:G:1470:THR:OG1	2.23	0.43
2:G:1886:VAL:HA	2:G:1901:ALA:O	2.18	0.43
1:A:505:LYS:HA	1:A:954:ARG:HD2	2.01	0.43
1:A:883:ILE:HG13	1:A:884:ILE:HG23	2.01	0.43
2:G:767:PHE:HD2	2:G:771:PHE:CE2	2.37	0.43
2:G:1974:VAL:HG13	2:G:1976:PHE:HD2	1.83	0.43
1:A:430:ARG:CZ	1:A:605:LEU:HD13	2.49	0.43
1:A:694:GLN:O	1:A:698:GLN:HG3	2.19	0.43
1:A:1030:TRP:CZ2	1:A:1102:GLY:HA3	2.54	0.43
1:A:1165:VAL:H	1:A:1165:VAL:HG22	1.63	0.43
2:G:571:LYS:HD3	2:G:571:LYS:HA	1.67	0.43
2:G:1614:ASP:OD1	2:G:1614:ASP:N	2.51	0.43
2:G:1775:GLN:NE2	2:G:1836:MET:SD	2.91	0.43
2:G:1784:MET:HE3	2:G:1784:MET:HB3	1.89	0.43
2:G:1821:VAL:HG23	2:G:1822:MET:HG2	2.00	0.43
2:G:1847:LEU:HD23	2:G:1847:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:LYS:NZ	1:A:716:ASP:OD1	2.51	0.42
1:A:774:ILE:HG22	3:A:1901:NAP:N7A	2.34	0.42
2:G:350:GLN:HA	2:G:353:VAL:HG22	2.00	0.42
2:G:1176:PRO:HA	2:G:1180:MET:HE1	2.01	0.42
2:G:1475:LYS:HG3	2:G:1476:ASN:HD22	1.85	0.42
2:G:1547:PRO:HD3	2:G:1584:PHE:CZ	2.53	0.42
1:A:413:LEU:CD2	1:A:451:MET:HB3	2.49	0.42
1:A:733:ILE:HG22	1:A:735:VAL:HG13	2.01	0.42
1:A:745:VAL:C	1:A:747:ALA:H	2.23	0.42
1:A:1312:VAL:O	1:A:1316:VAL:HG12	2.19	0.42
2:G:16:LEU:HB3	2:G:60:LEU:HD12	2.00	0.42
2:G:48:PHE:HD1	2:G:53:GLU:HB3	1.84	0.42
2:G:569:LEU:HD23	2:G:1090:TYR:CE1	2.52	0.42
2:G:1085:LEU:HA	2:G:1085:LEU:HD23	1.70	0.42
2:G:1383:ASN:HD22	2:G:1388:LYS:HB3	1.83	0.42
2:G:1762:TYR:HE2	2:G:1764:PHE:CE1	2.37	0.42
2:G:1923:ASP:HB2	2:G:1926:GLU:HG3	2.01	0.42
2:G:2039:LYS:HG3	2:G:2040:GLU:N	2.34	0.42
1:A:366:ASP:OD2	1:A:367:THR:N	2.52	0.42
1:A:1165:VAL:HB	1:A:1167:LEU:HD11	2.01	0.42
1:A:1323:LYS:HD3	1:A:1324:ALA:HB2	1.99	0.42
1:A:1443:LEU:HA	1:A:1443:LEU:HD23	1.73	0.42
1:A:1538:VAL:HG12	1:A:1539:ALA:N	2.34	0.42
2:G:198:LEU:HA	2:G:201:THR:HG22	2.00	0.42
2:G:216:LEU:HD12	2:G:216:LEU:H	1.83	0.42
2:G:1181:VAL:O	2:G:1181:VAL:HG23	2.19	0.42
2:G:1447:LYS:HA	2:G:1447:LYS:HD3	1.81	0.42
2:G:1515:PRO:HB2	2:G:1519:PHE:CE2	2.54	0.42
2:G:1923:ASP:O	2:G:1927:LEU:HG	2.20	0.42
1:A:1260:MET:HG3	1:A:1261:PHE:N	2.34	0.42
1:A:1316:VAL:O	1:A:1320:LEU:HD23	2.19	0.42
2:G:7:ARG:N	2:G:22:VAL:O	2.43	0.42
2:G:309:ARG:NE	2:G:442:ASP:OD2	2.28	0.42
2:G:346:GLN:HE21	2:G:368:ILE:HD13	1.84	0.42
2:G:370:LEU:HA	2:G:488:VAL:HG22	2.00	0.42
2:G:1679:ASP:OD1	2:G:1680:LEU:N	2.47	0.42
1:A:338:LEU:HA	1:A:341:GLN:HB2	2.02	0.42
1:A:824:LEU:HB3	1:A:846:LEU:HD23	2.02	0.42
1:A:1070:ARG:HB3	1:A:1072:TYR:CE1	2.55	0.42
1:A:1557:ILE:O	1:A:1561:MET:HG2	2.19	0.42
1:A:1559:GLU:HA	1:A:1562:LYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:ARG:HG3	2:G:24:THR:HG22	2.01	0.42
2:G:159:ILE:HA	2:G:271:THR:O	2.20	0.42
2:G:865:TRP:CD1	2:G:865:TRP:C	2.93	0.42
2:G:1143:ALA:HB1	2:G:1151:HIS:HA	2.02	0.42
2:G:1175:LYS:O	2:G:1180:MET:HE1	2.20	0.42
2:G:1514:ASN:HB3	2:G:1517:VAL:HG22	2.01	0.42
2:G:1902:GLY:H	2:G:1975:PRO:HB3	1.84	0.42
1:A:538:GLU:OE1	1:A:538:GLU:N	2.45	0.42
1:A:1115:ASN:O	1:A:1118:LYS:N	2.35	0.42
1:A:1223:PHE:HB3	1:A:1228:ILE:O	2.19	0.42
2:G:58:ALA:HA	2:G:95:TYR:CD1	2.54	0.42
2:G:526:ARG:HG2	2:G:558:ASN:H	1.85	0.42
2:G:607:VAL:HG11	2:G:619:LEU:HD13	2.01	0.42
2:G:1236:LEU:HD22	2:G:1265:MET:HE3	2.00	0.42
2:G:1301:THR:HG23	2:G:1306:ASN:ND2	2.35	0.42
2:G:1311:PHE:CE1	2:G:1322:PRO:HA	2.54	0.42
2:G:1673:GLU:N	2:G:1673:GLU:OE1	2.52	0.42
1:A:393:SER:O	1:A:736:PRO:HB2	2.19	0.42
1:A:402:PHE:HB2	1:A:732:LEU:HD23	2.02	0.42
1:A:630:ILE:HG22	1:A:653:ARG:NH2	2.35	0.42
1:A:803:MET:CE	1:A:849:LEU:HD21	2.49	0.42
2:G:598:THR:HA	2:G:620:ALA:HB1	2.00	0.42
2:G:1197:LEU:HD12	2:G:1198:SER:N	2.35	0.42
2:G:1325:PHE:O	2:G:1329:VAL:HG12	2.20	0.42
2:G:1431:TYR:CE1	2:G:1526:THR:HG22	2.52	0.42
2:G:1537:ILE:HG13	2:G:1628:HIS:HB3	2.02	0.42
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.82	0.42
1:A:1152:VAL:CG1	1:A:1154:ILE:HG23	2.49	0.42
1:A:1307:THR:O	1:A:1311:SER:OG	2.33	0.42
1:A:1498:GLU:OE2	1:A:1502:ARG:HD3	2.19	0.42
2:G:14:GLY:HA3	2:G:48:PHE:HZ	1.84	0.42
2:G:670:ARG:NH1	2:G:674:TYR:O	2.53	0.42
2:G:1226:ASN:OD1	2:G:1226:ASN:N	2.48	0.42
2:G:1449:TRP:HZ2	2:G:1519:PHE:HD2	1.67	0.42
2:G:1632:ILE:O	2:G:1635:ARG:HG2	2.19	0.42
1:A:367:THR:HA	1:A:370:GLU:HG3	2.02	0.42
1:A:504:ASP:HB2	1:A:508:ASN:H	1.84	0.42
1:A:1592:MET:HG3	1:A:1641:ILE:HG23	2.02	0.42
2:G:677:GLN:O	2:G:678:PHE:HB3	2.20	0.42
2:G:680:THR:HA	2:G:704:GLY:O	2.20	0.42
2:G:1815:LEU:HB3	2:G:1821:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1962:ARG:HB2	2:G:1968:PRO:HD3	2.02	0.42
1:A:82:SER:OG	1:A:83:LYS:N	2.53	0.42
1:A:1017:ARG:NH1	1:A:1320:LEU:HD12	2.35	0.42
1:A:1375:GLY:O	1:A:1545:SER:OG	2.29	0.42
1:A:1515:ARG:HA	1:A:1515:ARG:HD2	1.79	0.42
1:A:1516:ASP:OD1	1:A:1518:ARG:HG2	2.20	0.42
2:G:238:CYS:O	2:G:275:GLN:NE2	2.53	0.42
2:G:602:VAL:O	2:G:624:TYR:OH	2.32	0.42
2:G:1475:LYS:HE3	2:G:1476:ASN:ND2	2.35	0.42
2:G:1679:ASP:OD1	2:G:1679:ASP:N	2.52	0.42
2:G:1765:ARG:HB3	2:G:1847:LEU:O	2.19	0.42
2:G:1778:GLN:HA	2:G:1809:LEU:HD11	2.01	0.42
1:A:431:GLU:O	1:A:435:GLU:N	2.53	0.41
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.55	0.41
1:A:1680:ARG:H	1:A:1680:ARG:HG2	1.71	0.41
1:A:1734:ASN:HB3	1:A:1736:LYS:HE2	2.00	0.41
2:G:440:ASN:HD21	2:G:477:GLU:HG2	1.83	0.41
2:G:730:LEU:HD23	2:G:730:LEU:HA	1.60	0.41
2:G:1163:LYS:O	2:G:1164:MET:HG3	2.20	0.41
2:G:1263:LYS:NZ	2:G:1338:ILE:O	2.53	0.41
2:G:1306:ASN:OD1	2:G:1308:CYS:HB2	2.20	0.41
2:G:1322:PRO:HB2	2:G:1590:ARG:HH12	1.84	0.41
2:G:56:THR:HG1	2:G:59:GLU:CD	2.19	0.41
2:G:174:ARG:NH1	2:G:222:PRO:HG3	2.35	0.41
2:G:555:LEU:HD21	2:G:557:LYS:HE3	2.02	0.41
2:G:1319:MET:HB3	2:G:1368:VAL:CG2	2.46	0.41
1:A:2:LYS:HB2	1:A:2:LYS:HE2	1.78	0.41
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.87	0.41
1:A:807:LYS:HG3	1:A:861:GLN:OE1	2.21	0.41
1:A:1123:GLN:CB	1:A:1177:LYS:HD3	2.48	0.41
2:G:180:TYR:O	2:G:184:VAL:HG22	2.19	0.41
2:G:309:ARG:HB2	2:G:439:ILE:HG12	2.02	0.41
2:G:1127:PHE:HE2	2:G:1184:ILE:HD13	1.85	0.41
2:G:1381:VAL:O	2:G:1422:THR:HG23	2.20	0.41
2:G:1570:ALA:HA	2:G:1575:LEU:HD12	2.03	0.41
2:G:2015:THR:HG23	2:G:2017:LYS:HE2	2.01	0.41
1:A:251:GLN:O	1:A:255:GLY:HA2	2.20	0.41
1:A:417:TYR:OH	1:A:454:HIS:HB3	2.20	0.41
1:A:504:ASP:OD2	1:A:508:ASN:HB3	2.21	0.41
1:A:525:TYR:O	1:A:529:MET:HG2	2.21	0.41
1:A:1238:VAL:HG21	1:A:1325:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:268:LYS:NZ	2:G:497:LYS:O	2.45	0.41
2:G:765:LEU:HD12	2:G:765:LEU:HA	1.83	0.41
2:G:804:ARG:HD2	2:G:1063:THR:HG22	2.02	0.41
2:G:1066:ILE:HD12	2:G:1066:ILE:HA	1.94	0.41
2:G:1475:LYS:HG3	2:G:1476:ASN:ND2	2.35	0.41
1:A:191:GLY:O	1:A:195:GLY:HA2	2.21	0.41
1:A:1140:THR:HA	1:A:1142:GLU:OE1	2.21	0.41
1:A:1148:HIS:CD2	1:A:1167:LEU:CD2	3.03	0.41
1:A:1425:ILE:HD13	1:A:1425:ILE:HA	1.80	0.41
2:G:673:GLY:O	2:G:1164:MET:HG2	2.20	0.41
2:G:875:LEU:HD21	2:G:879:LYS:C	2.41	0.41
2:G:1331:TRP:CD1	2:G:1335:ILE:HD13	2.55	0.41
2:G:1496:LYS:HB2	2:G:1496:LYS:HE3	1.79	0.41
2:G:1576:PRO:HB2	2:G:1617:LEU:HD21	2.00	0.41
2:G:1924:ILE:HG22	2:G:1928:GLN:HE22	1.85	0.41
2:G:748:THR:OG1	2:G:749:PRO:HD3	2.21	0.41
2:G:830:ASP:N	2:G:830:ASP:OD1	2.54	0.41
2:G:1445:ARG:H	2:G:1445:ARG:HG2	1.69	0.41
2:G:1739:GLU:HA	2:G:1747:LYS:O	2.21	0.41
2:G:1989:LYS:HE2	2:G:2037:PRO:HG2	2.03	0.41
1:A:156:ALA:HB1	1:A:161:LYS:O	2.20	0.41
1:A:1496:GLU:O	1:A:1500:GLN:HB2	2.21	0.41
3:A:1901:NAP:O2N	3:A:1901:NAP:C3D	2.69	0.41
2:G:31:SER:O	2:G:35:GLU:HG3	2.21	0.41
2:G:964:LEU:HD13	2:G:964:LEU:HA	1.93	0.41
2:G:1177:SER:H	2:G:1180:MET:HE2	1.86	0.41
2:G:1955:PRO:HB2	2:G:1957:PRO:HD2	2.02	0.41
1:A:79:LEU:HA	1:A:84:ASP:OD2	2.21	0.41
1:A:427:ASN:ND2	1:A:608:ASP:OD1	2.54	0.41
1:A:1676:LYS:O	1:A:1680:ARG:HG2	2.21	0.41
2:G:119:THR:O	2:G:123:ILE:HD12	2.21	0.41
2:G:1301:THR:HG22	2:G:1306:ASN:O	2.21	0.41
2:G:1638:ILE:O	2:G:1654:GLU:HA	2.21	0.41
1:A:34:VAL:HG23	1:A:38:ASP:OD2	2.20	0.41
1:A:61:LEU:HD11	1:A:76:ARG:HD2	2.03	0.41
1:A:439:ILE:HD11	1:A:451:MET:CE	2.50	0.41
1:A:460:GLU:HA	1:A:466:TYR:HB3	2.01	0.41
1:A:490:TYR:HE1	1:A:673:PHE:CE2	2.39	0.41
1:A:771:PHE:HB3	3:A:1901:NAP:C5D	2.40	0.41
1:A:1238:VAL:HG23	1:A:1325:ARG:HG3	2.01	0.41
1:A:1584:PRO:O	1:A:1585:LYS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:74:PRO:HG3	2:G:132:MET:HG3	2.02	0.41
2:G:126:TYR:CD2	2:G:127:ILE:HD13	2.56	0.41
2:G:292:PHE:O	2:G:296:VAL:HG23	2.21	0.41
2:G:309:ARG:CB	2:G:439:ILE:HG12	2.51	0.41
2:G:597:MET:O	2:G:601:THR:N	2.54	0.41
2:G:774:ALA:HB1	2:G:1081:HIS:HD2	1.85	0.41
2:G:803:SER:HB3	2:G:1055:HIS:CE1	2.56	0.41
2:G:926:LEU:HD23	2:G:926:LEU:HA	1.80	0.41
2:G:1011:MET:C	3:G:2102:NAP:H2A	2.40	0.41
2:G:1313:SER:OG	2:G:1314:ARG:N	2.53	0.41
2:G:1484:LYS:HA	2:G:1484:LYS:HD3	1.82	0.41
2:G:1592:LEU:O	2:G:1592:LEU:HD23	2.21	0.41
2:G:1719:ILE:HG21	2:G:1733:TYR:HE2	1.85	0.41
2:G:1721:PHE:HE2	2:G:1755:ILE:HD11	1.86	0.41
2:G:1992:LEU:O	2:G:1996:ILE:HG12	2.21	0.41
1:A:473:GLY:O	1:A:477:ILE:HG23	2.21	0.41
1:A:1024:PHE:HE1	1:A:1401:TYR:CD1	2.38	0.41
1:A:1057:MET:HG2	1:A:1190:PRO:HB2	2.02	0.41
2:G:359:HIS:HB2	2:G:360:LEU:HD12	2.01	0.41
2:G:404:GLN:O	2:G:407:ILE:HG22	2.21	0.41
2:G:1123:ASP:OD1	2:G:1188:ASN:ND2	2.54	0.41
2:G:1680:LEU:HD21	2:G:1687:ALA:HB1	2.03	0.41
2:G:1979:THR:HA	2:G:1982:MET:HG2	2.03	0.41
1:A:419:GLU:O	1:A:424:VAL:N	2.51	0.40
1:A:910:THR:HG22	1:A:912:GLU:H	1.86	0.40
1:A:1065:GLY:O	1:A:1071:PRO:HA	2.20	0.40
1:A:1154:ILE:HD12	1:A:1156:GLU:OE1	2.20	0.40
1:A:1737:ASN:HA	1:A:1740:SER:HB3	2.02	0.40
1:A:1742:ASP:OD1	1:A:1743:SER:N	2.54	0.40
2:G:322:SER:HA	2:G:325:GLU:OE2	2.21	0.40
2:G:666:ILE:HD13	2:G:666:ILE:HA	1.84	0.40
2:G:847:ARG:HH22	2:G:873:PHE:HB2	1.86	0.40
2:G:932:ILE:HG22	2:G:935:THR:H	1.86	0.40
2:G:980:ILE:HG23	2:G:984:PHE:CD1	2.56	0.40
2:G:1241:ASN:O	2:G:1251:ILE:HA	2.21	0.40
2:G:1290:PHE:HB3	2:G:1329:VAL:HG23	2.03	0.40
2:G:1544:SER:O	2:G:1621:ALA:HA	2.21	0.40
1:A:37:LYS:HB2	1:A:65:TYR:OH	2.22	0.40
2:G:89:THR:HG23	2:G:135:ARG:HH22	1.86	0.40
2:G:597:MET:HA	5:G:2101:FMN:N5	2.36	0.40
2:G:1610:CYS:HA	2:G:1653:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:HB2	2:G:2016:ALA:HB1	2.02	0.40
1:A:59:ARG:HH12	2:G:1897:GLN:HE21	1.69	0.40
1:A:630:ILE:HG22	1:A:653:ARG:HH21	1.86	0.40
1:A:849:LEU:HD12	1:A:849:LEU:HA	1.83	0.40
1:A:1227:GLY:O	1:A:1680:ARG:NH2	2.42	0.40
1:A:1391:ASP:OD1	1:A:1392:LEU:N	2.54	0.40
2:G:814:SER:OG	2:G:1040:LEU:HD13	2.21	0.40
2:G:1564:HIS:ND1	2:G:1579:ILE:HG13	2.36	0.40
2:G:1679:ASP:O	2:G:1683:THR:HG23	2.21	0.40
2:G:1773:ALA:O	2:G:1777:THR:HG23	2.21	0.40
2:G:2045:TRP:CE2	2:G:2048:TYR:HB2	2.56	0.40
1:A:56:MET:HA	1:A:59:ARG:HE	1.86	0.40
1:A:455:ILE:HD13	1:A:455:ILE:HA	1.92	0.40
1:A:688:ILE:H	1:A:688:ILE:HG13	1.59	0.40
1:A:960:GLU:OE1	2:G:1447:LYS:NZ	2.36	0.40
1:A:988:ILE:HD13	1:A:1048:GLU:HB3	2.04	0.40
1:A:1089:VAL:HG23	1:A:1093:TYR:CD2	2.52	0.40
1:A:1305:CYS:HA	1:A:1585:LYS:O	2.21	0.40
1:A:1424:GLY:O	1:A:1427:THR:HG22	2.21	0.40
2:G:10:THR:HA	2:G:19:VAL:HA	2.03	0.40
2:G:408:PRO:HG3	2:G:836:TYR:CZ	2.57	0.40
2:G:602:VAL:HG21	2:G:623:GLY:HA3	2.04	0.40
2:G:648:GLY:HA3	2:G:678:PHE:CE2	2.56	0.40
2:G:738:GLY:HA2	2:G:1055:HIS:O	2.22	0.40
2:G:1756:ASN:OD1	2:G:1759:SER:N	2.54	0.40
2:G:1982:MET:O	2:G:1985:VAL:HG22	2.21	0.40
1:A:996:LYS:H	1:A:996:LYS:HG2	1.73	0.40
1:A:1056:ILE:HG21	1:A:1056:ILE:HD13	1.84	0.40
1:A:1064:ASN:HD22	2:G:1001:ASP:HB2	1.86	0.40
2:G:85:ASN:HB2	2:G:135:ARG:NH2	2.36	0.40
2:G:571:LYS:HD2	2:G:575:GLY:C	2.42	0.40
2:G:757:ILE:O	2:G:759:ARG:N	2.54	0.40
2:G:788:LYS:HE2	2:G:789:PHE:HE1	1.86	0.40
2:G:832:TRP:CE3	2:G:833:GLU:HG2	2.56	0.40
2:G:1354:SER:N	2:G:1409:SER:OG	2.55	0.40
2:G:1618:PRO:HB2	2:G:1619:ASN:HD22	1.86	0.40
2:G:1685:LYS:HA	2:G:1688:GLN:NE2	2.37	0.40
2:G:1893:VAL:HG22	2:G:1897:GLN:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1601/1887 (85%)	1433 (90%)	161 (10%)	7 (0%)	34	66
2	G	2029/2073 (98%)	1883 (93%)	146 (7%)	0	100	100
All	All	3630/3960 (92%)	3316 (91%)	307 (8%)	7 (0%)	50	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	LYS
1	A	179	LYS
1	A	195	GLY
1	A	1609	ARG
1	A	180	SER
1	A	851	ASN
1	A	1158	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1230/1566 (78%)	1223 (99%)	7 (1%)	86	96
2	G	1772/1810 (98%)	1757 (99%)	15 (1%)	81	94
All	All	3002/3376 (89%)	2980 (99%)	22 (1%)	84	95

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	394	PHE
1	A	505	LYS
1	A	712	LYS
1	A	894	ARG
1	A	1035	THR
1	A	1307	THR
2	G	63	LYS
2	G	76	LYS
2	G	140	LYS
2	G	297	ARG
2	G	395	LYS
2	G	415	LYS
2	G	419	ARG
2	G	809	LYS
2	G	993	GLN
2	G	1023	ARG
2	G	1315	PRO
2	G	1439	LYS
2	G	1680	LEU
2	G	1704	PHE
2	G	1765	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	11	HIS
1	A	411	GLN
1	A	465	ASN
1	A	479	ASN
1	A	669	ASN
1	A	830	HIS
1	A	1115	ASN
1	A	1146	HIS
1	A	1188	GLN
1	A	1207	GLN
1	A	1239	HIS
1	A	1272	ASN
1	A	1380	GLN
1	A	1507	GLN
1	A	1558	ASN
1	A	1598	GLN

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Mol	Chain	Res	Type
1	A	1601	ASN
1	A	1689	HIS
1	A	1734	ASN
2	G	34	GLN
2	G	99	ASN
2	G	142	ASN
2	G	273	HIS
2	G	275	GLN
2	G	343	ASN
2	G	354	ASN
2	G	404	GLN
2	G	428	HIS
2	G	440	ASN
2	G	612	ASN
2	G	650	ASN
2	G	715	GLN
2	G	723	HIS
2	G	740	HIS
2	G	741	HIS
2	G	747	HIS
2	G	900	GLN
2	G	910	GLN
2	G	985	ASN
2	G	993	GLN
2	G	1012	GLN
2	G	1046	GLN
2	G	1148	ASN
2	G	1302	HIS
2	G	1352	HIS
2	G	1355	ASN
2	G	1383	ASN
2	G	1424	GLN
2	G	1476	ASN
2	G	1514	ASN
2	G	1535	ASN
2	G	1581	HIS
2	G	1619	ASN
2	G	1674	GLN
2	G	1716	ASN
2	G	1839	GLN
2	G	1868	GLN
2	G	1896	GLN

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Mol	Chain	Res	Type
2	G	1897	GLN
2	G	1920	GLN
2	G	1939	HIS
2	G	2027	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are 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$
4	PNS	A	1902	1	1,4,21	0.66	0	0,4,29	-	-
5	FMN	G	2101	-	33,33,33	1.24	4 (12%)	48,50,50	1.25	8 (16%)
3	NAP	A	1901	-	45,52,52	2.41	24 (53%)	56,80,80	1.99	14 (25%)
3	NAP	G	2102	-	45,52,52	0.82	1 (2%)	56,80,80	1.23	4 (7%)

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
4	PNS	A	1902	1	-	0/0/2/27	-
5	FMN	G	2101	-	-	3/18/18/18	0/3/3/3
3	NAP	A	1901	-	-	6/31/67/67	0/5/5/5
3	NAP	G	2102	-	-	7/31/67/67	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1901	NAP	C3N-C7N	-5.40	1.42	1.50
3	A	1901	NAP	O4D-C4D	-4.89	1.34	1.45
3	A	1901	NAP	C4A-N3A	-4.10	1.30	1.35
3	A	1901	NAP	O7N-C7N	-3.92	1.16	1.24
3	A	1901	NAP	C2N-C3N	-3.80	1.33	1.39
3	A	1901	NAP	C2N-N1N	-3.77	1.30	1.35
3	A	1901	NAP	C4N-C3N	-3.53	1.33	1.39
5	G	2101	FMN	C4A-N5	3.33	1.37	1.30
3	A	1901	NAP	C2D-C1D	-3.24	1.48	1.53
3	A	1901	NAP	C5A-N7A	-2.84	1.29	1.39
3	A	1901	NAP	P2B-O2B	-2.80	1.54	1.59
3	A	1901	NAP	PN-O2N	-2.76	1.42	1.55
3	A	1901	NAP	C2A-N1A	-2.64	1.29	1.33
3	A	1901	NAP	P2B-O3X	-2.63	1.44	1.54
3	A	1901	NAP	P2B-O2X	-2.62	1.44	1.54
3	G	2102	NAP	C5A-C4A	2.52	1.47	1.40
3	A	1901	NAP	C3D-C4D	-2.51	1.46	1.53
3	A	1901	NAP	O4B-C4B	-2.47	1.39	1.45
3	A	1901	NAP	C7N-N7N	-2.46	1.28	1.33
3	A	1901	NAP	C3B-C4B	-2.41	1.46	1.53
3	A	1901	NAP	O4B-C1B	-2.39	1.37	1.41
3	A	1901	NAP	PN-O1N	-2.26	1.42	1.50
3	A	1901	NAP	PN-O5D	-2.25	1.50	1.59
5	G	2101	FMN	C9A-N10	-2.24	1.37	1.41
5	G	2101	FMN	C10-N1	2.15	1.37	1.33
5	G	2101	FMN	C4A-C10	-2.11	1.37	1.44
3	A	1901	NAP	O5D-C5D	-2.07	1.36	1.44
3	A	1901	NAP	C6A-N1A	-2.03	1.28	1.37
3	A	1901	NAP	C6N-N1N	-2.01	1.30	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1901	NAP	O3D-C3D-C4D	-5.25	95.86	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1901	NAP	O4D-C1D-C2D	-5.12	99.45	106.93
3	A	1901	NAP	C6N-N1N-C2N	-4.97	117.44	121.97
3	A	1901	NAP	O4B-C4B-C3B	-4.39	96.42	105.11
3	A	1901	NAP	PN-O3-PA	-4.36	117.86	132.83
3	A	1901	NAP	O4B-C1B-C2B	-4.06	99.54	106.59
3	G	2102	NAP	PN-O3-PA	-3.60	120.49	132.83
3	G	2102	NAP	C3D-C2D-C1D	3.37	106.06	100.98
5	G	2101	FMN	C4-N3-C2	-3.37	119.42	125.64
3	A	1901	NAP	N3A-C2A-N1A	-3.28	123.55	128.68
3	G	2102	NAP	N3A-C2A-N1A	-3.18	123.71	128.68
3	A	1901	NAP	C3N-C2N-N1N	3.03	123.39	120.43
5	G	2101	FMN	C4A-C4-N3	2.82	120.34	113.19
3	A	1901	NAP	C5B-C4B-C3B	-2.69	105.08	115.18
3	G	2102	NAP	C4A-C5A-N7A	-2.67	106.62	109.40
5	G	2101	FMN	O4-C4-C4A	-2.61	119.69	126.60
3	A	1901	NAP	O3X-P2B-O2X	2.43	116.93	107.64
3	A	1901	NAP	O5B-PA-O1A	-2.43	99.57	109.07
3	A	1901	NAP	O3X-P2B-O2B	-2.39	95.30	105.99
5	G	2101	FMN	C9A-C5A-N5	-2.23	120.01	122.43
5	G	2101	FMN	C4A-C10-N10	2.20	119.70	116.48
3	A	1901	NAP	O5B-C5B-C4B	2.19	116.54	108.99
5	G	2101	FMN	C5A-C9A-N10	2.18	120.20	117.95
5	G	2101	FMN	C4A-C10-N1	-2.16	119.72	124.73
3	A	1901	NAP	C5N-C4N-C3N	-2.15	117.80	120.34
5	G	2101	FMN	C10-C4A-N5	-2.07	120.46	124.86

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1901	NAP	C5B-O5B-PA-O1A
3	A	1901	NAP	C3B-C4B-C5B-O5B
3	A	1901	NAP	C5D-O5D-PN-O3
3	A	1901	NAP	C4D-C5D-O5D-PN
3	G	2102	NAP	C5D-O5D-PN-O1N
3	A	1901	NAP	O4B-C4B-C5B-O5B
5	G	2101	FMN	C5'-O5'-P-O1P
3	G	2102	NAP	C3B-C4B-C5B-O5B
3	G	2102	NAP	C5B-O5B-PA-O3
3	A	1901	NAP	C5D-O5D-PN-O2N
3	G	2102	NAP	C4D-C5D-O5D-PN
5	G	2101	FMN	C4'-C5'-O5'-P

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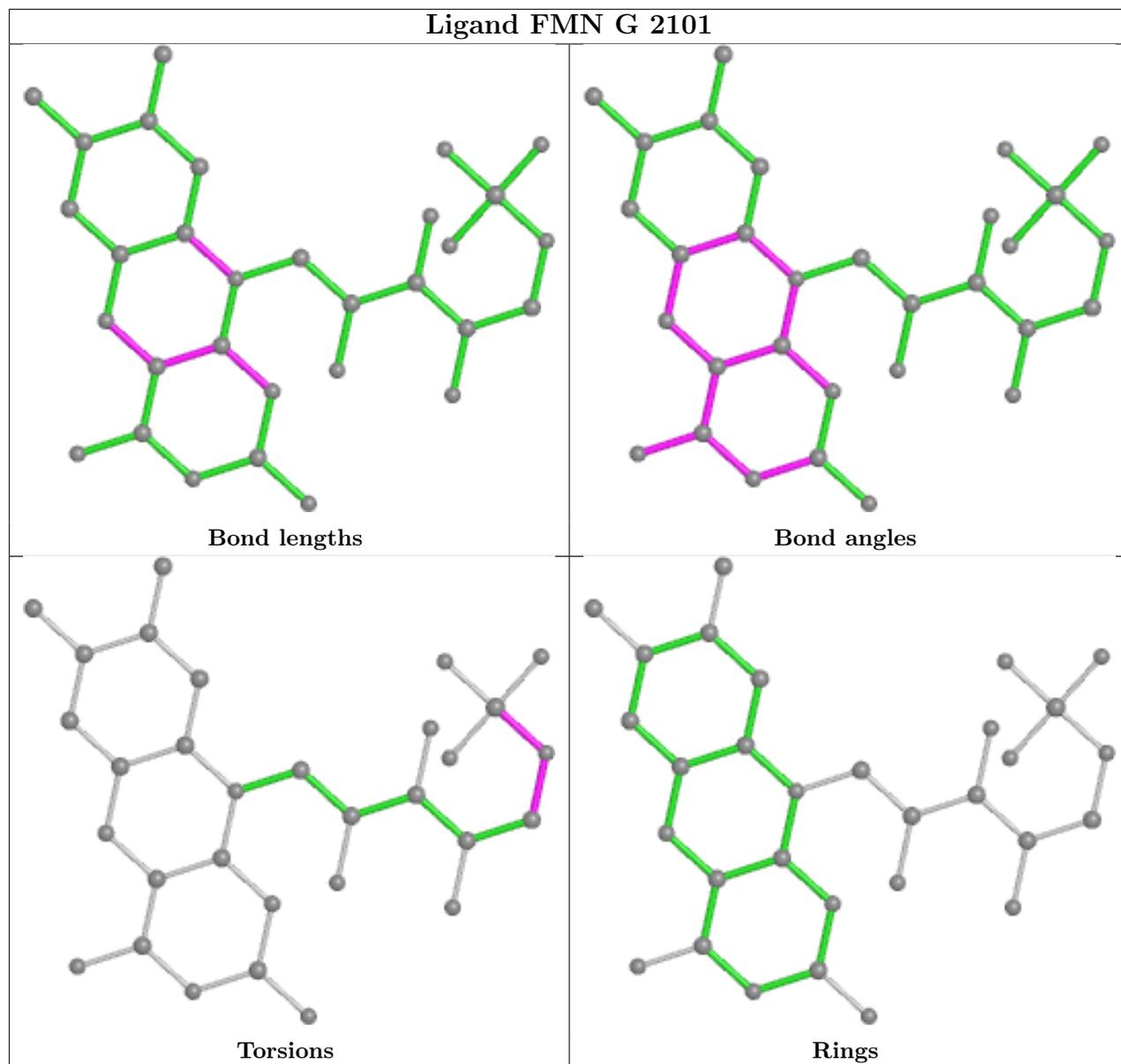
Mol	Chain	Res	Type	Atoms
5	G	2101	FMN	C5'-O5'-P-O2P
3	G	2102	NAP	O4D-C4D-C5D-O5D
3	G	2102	NAP	PA-O3-PN-O2N
3	G	2102	NAP	C5B-O5B-PA-O1A

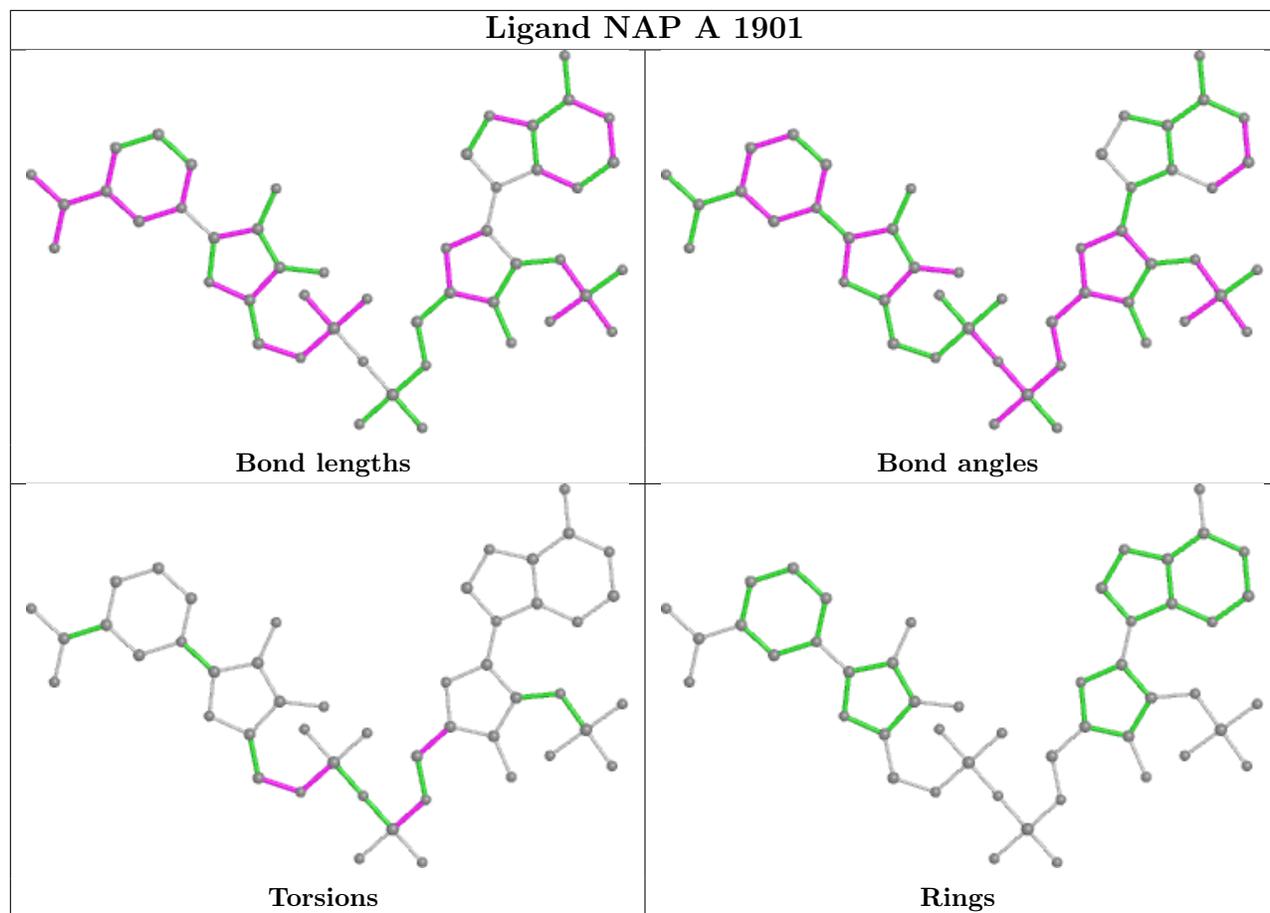
There are no ring outliers.

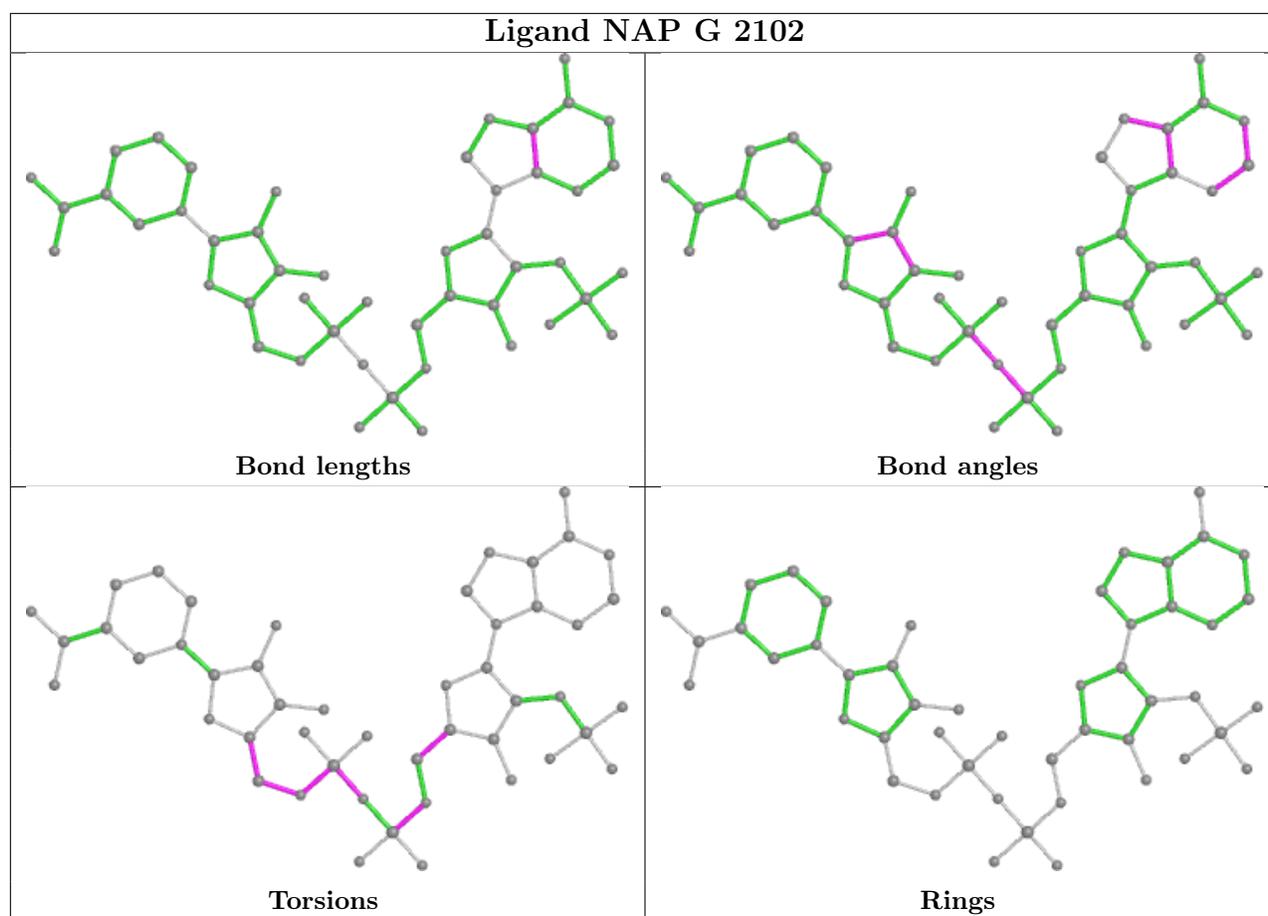
3 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2101	FMN	3	0
3	A	1901	NAP	19	0
3	G	2102	NAP	27	0

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







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

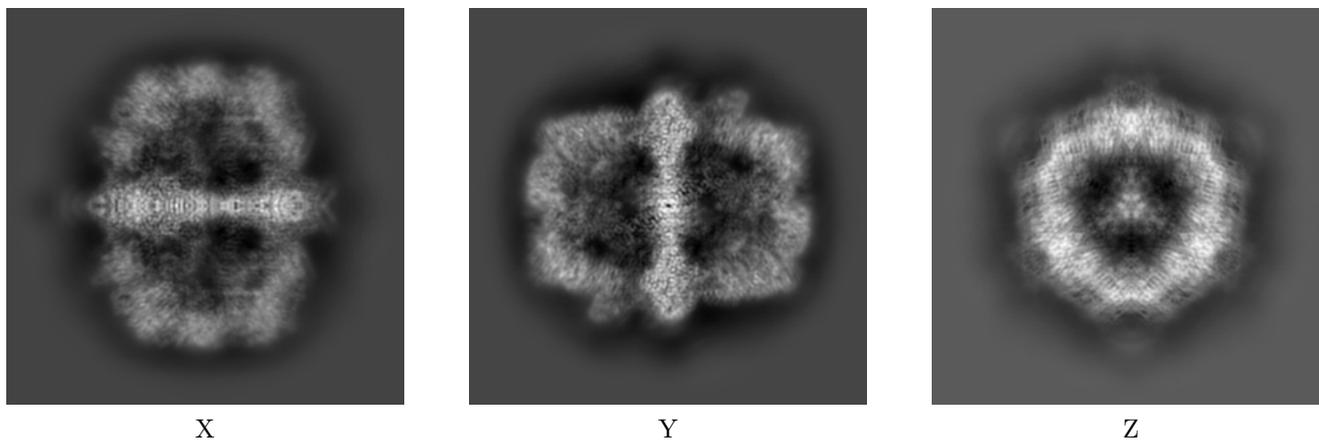
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20656. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

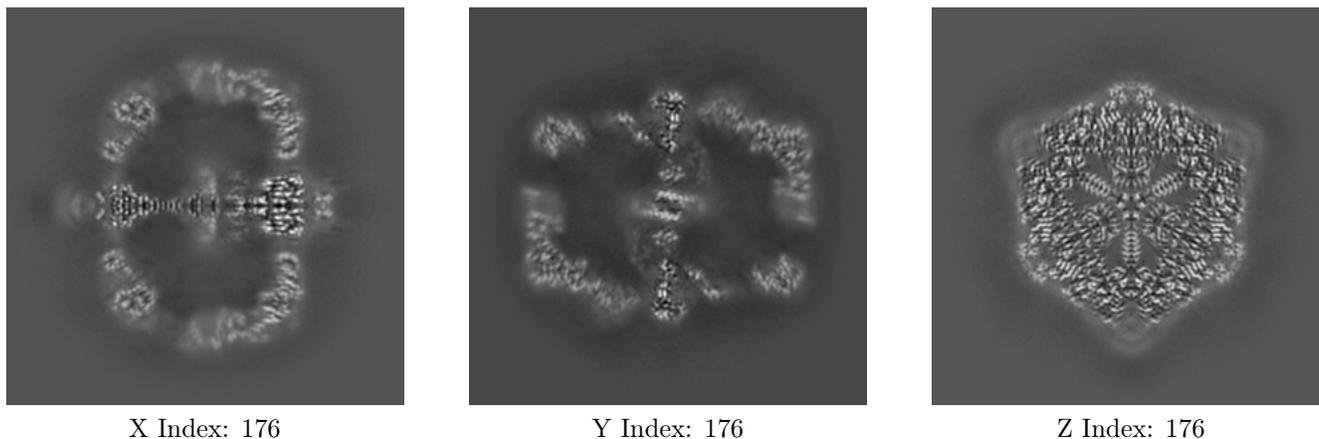
6.1.1 Primary map



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

6.2 Central slices [i](#)

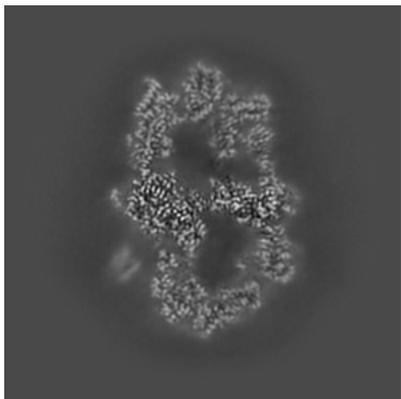
6.2.1 Primary map



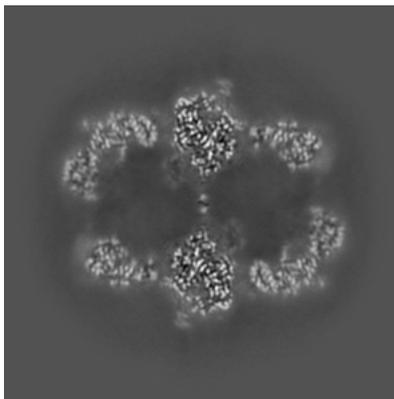
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

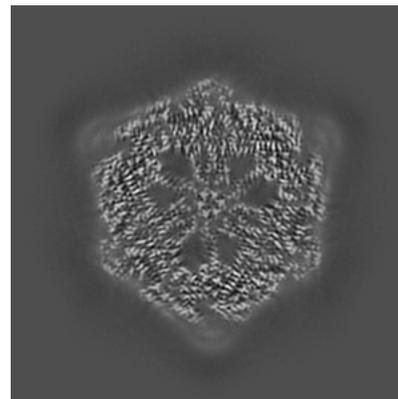
6.3.1 Primary map



X Index: 237



Y Index: 140



Z Index: 172

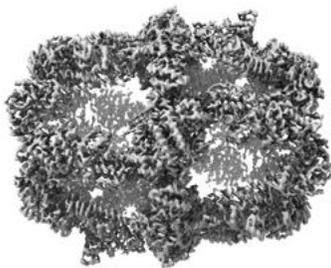
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

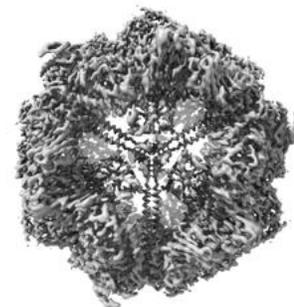
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.706. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

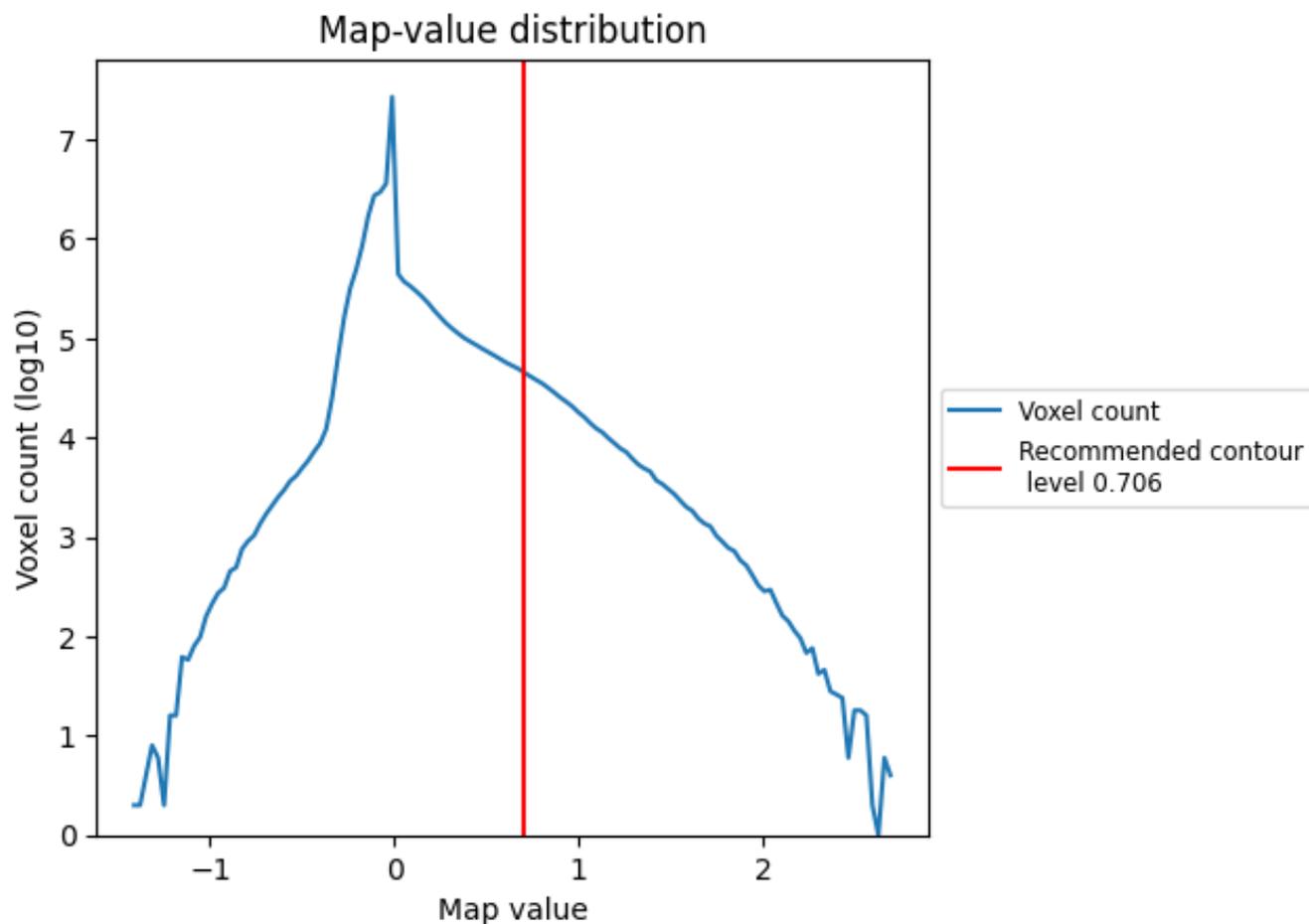
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

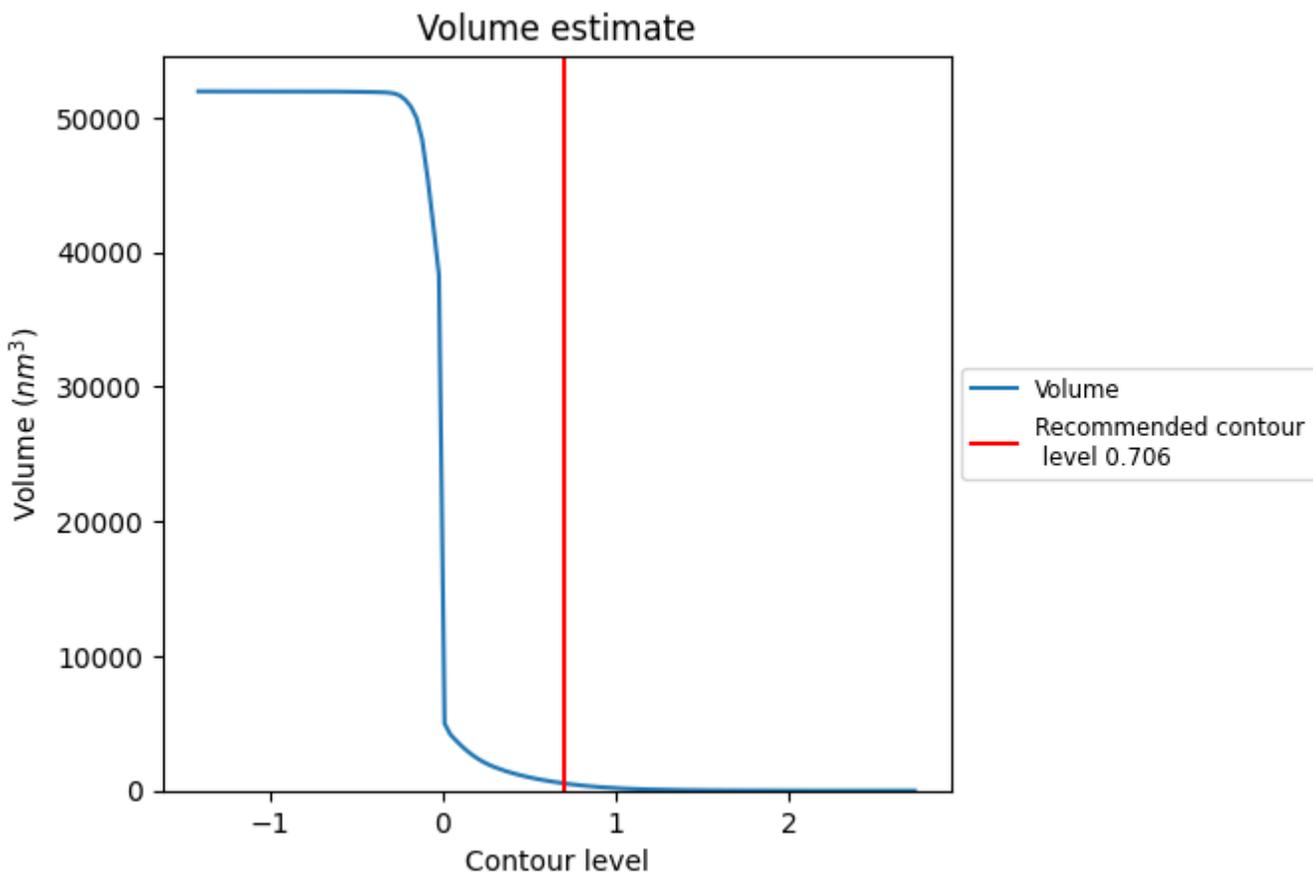
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

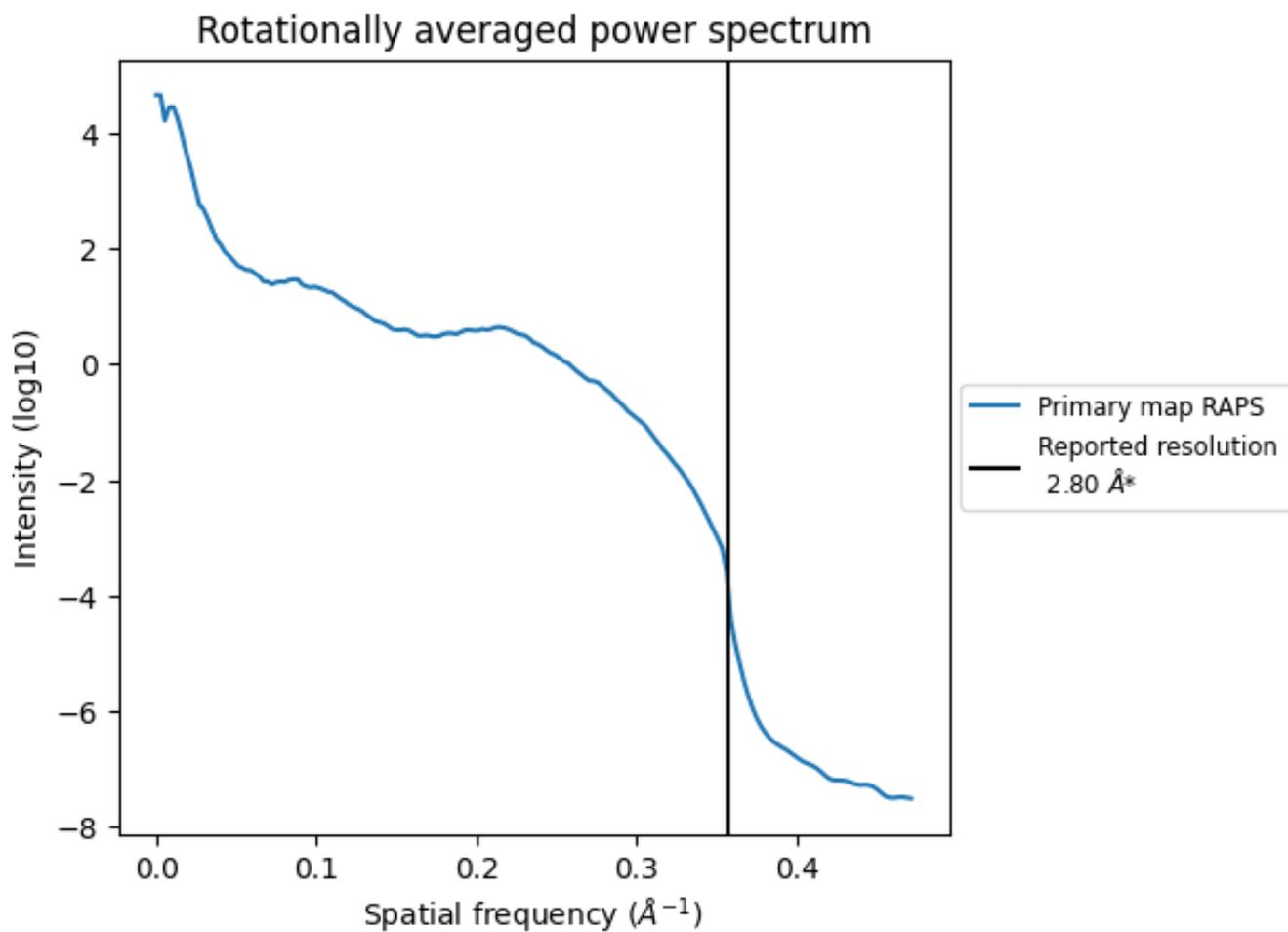
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 531 nm³; this corresponds to an approximate mass of 480 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.357\AA^{-1}

8 Fourier-Shell correlation

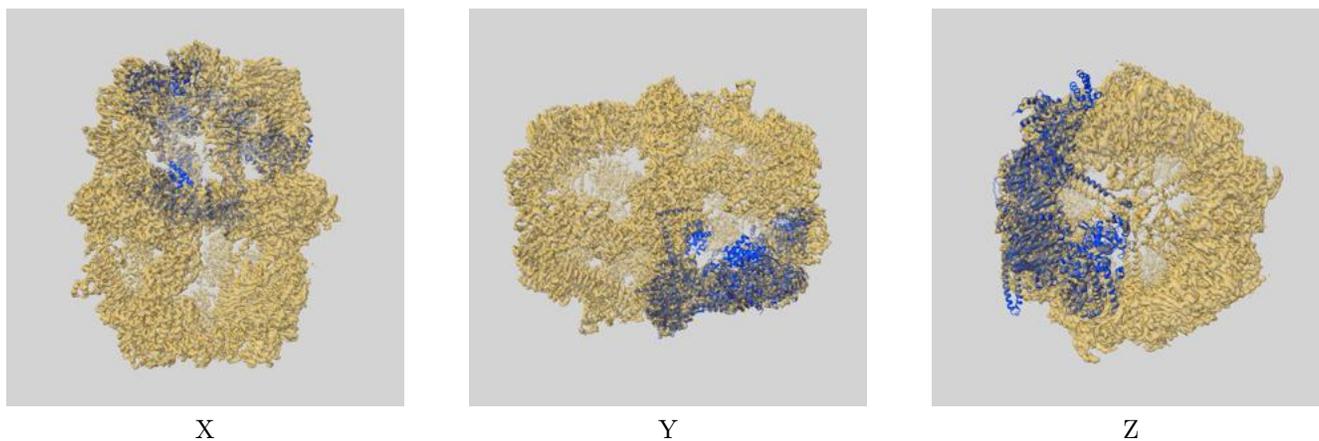
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

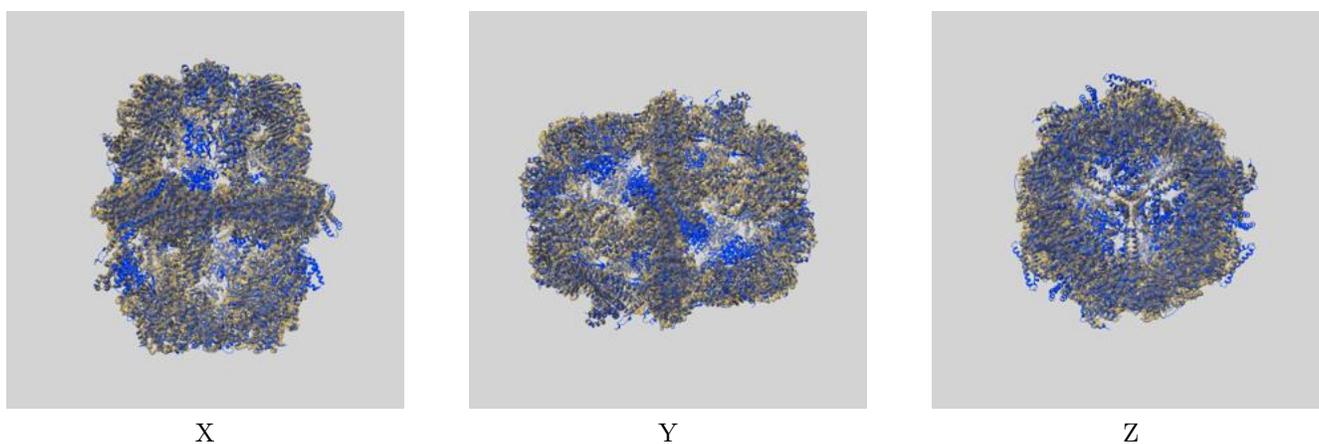
This section contains information regarding the fit between EMDB map EMD-20656 and PDB model 6U5U. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

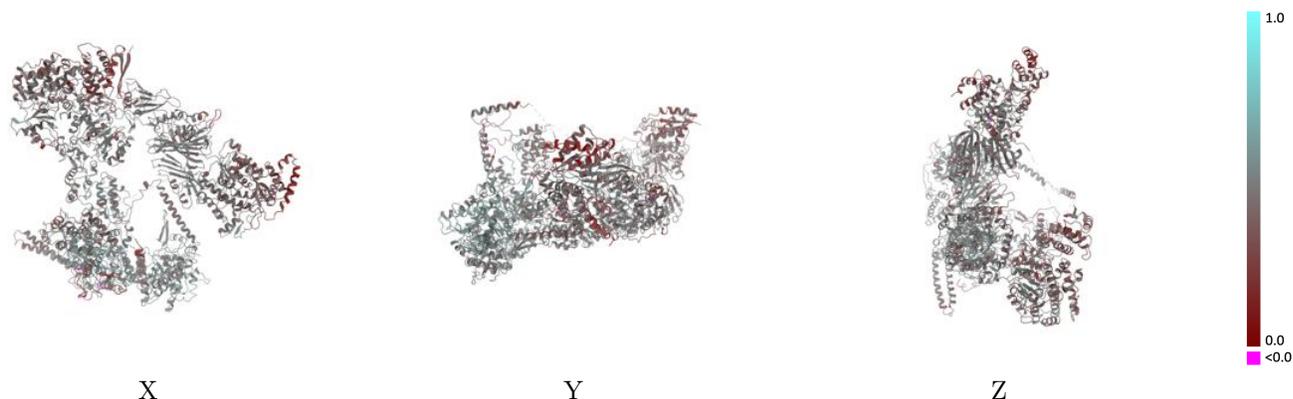


9.1.2 Map-model assembly overlay [i](#)



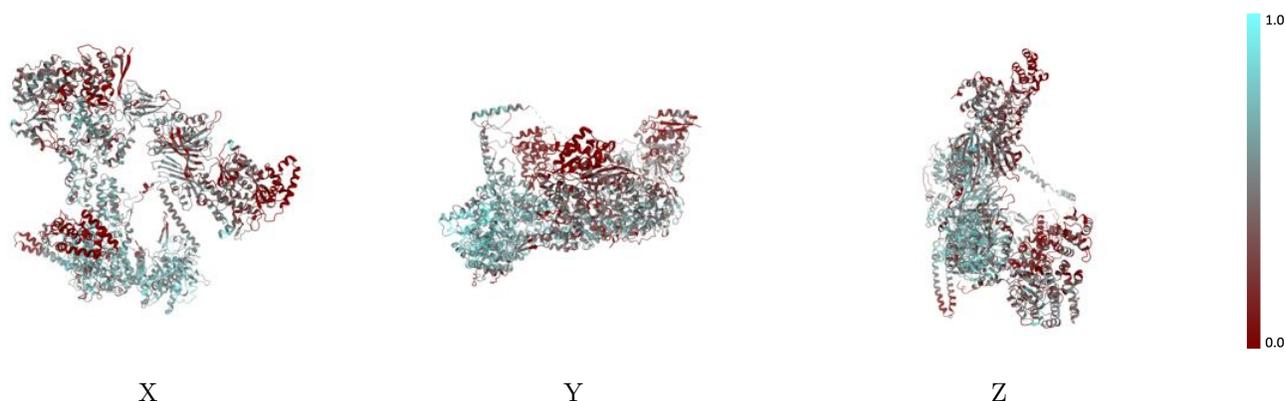
The images above show the 3D surface view of the map at the recommended contour level 0.706 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



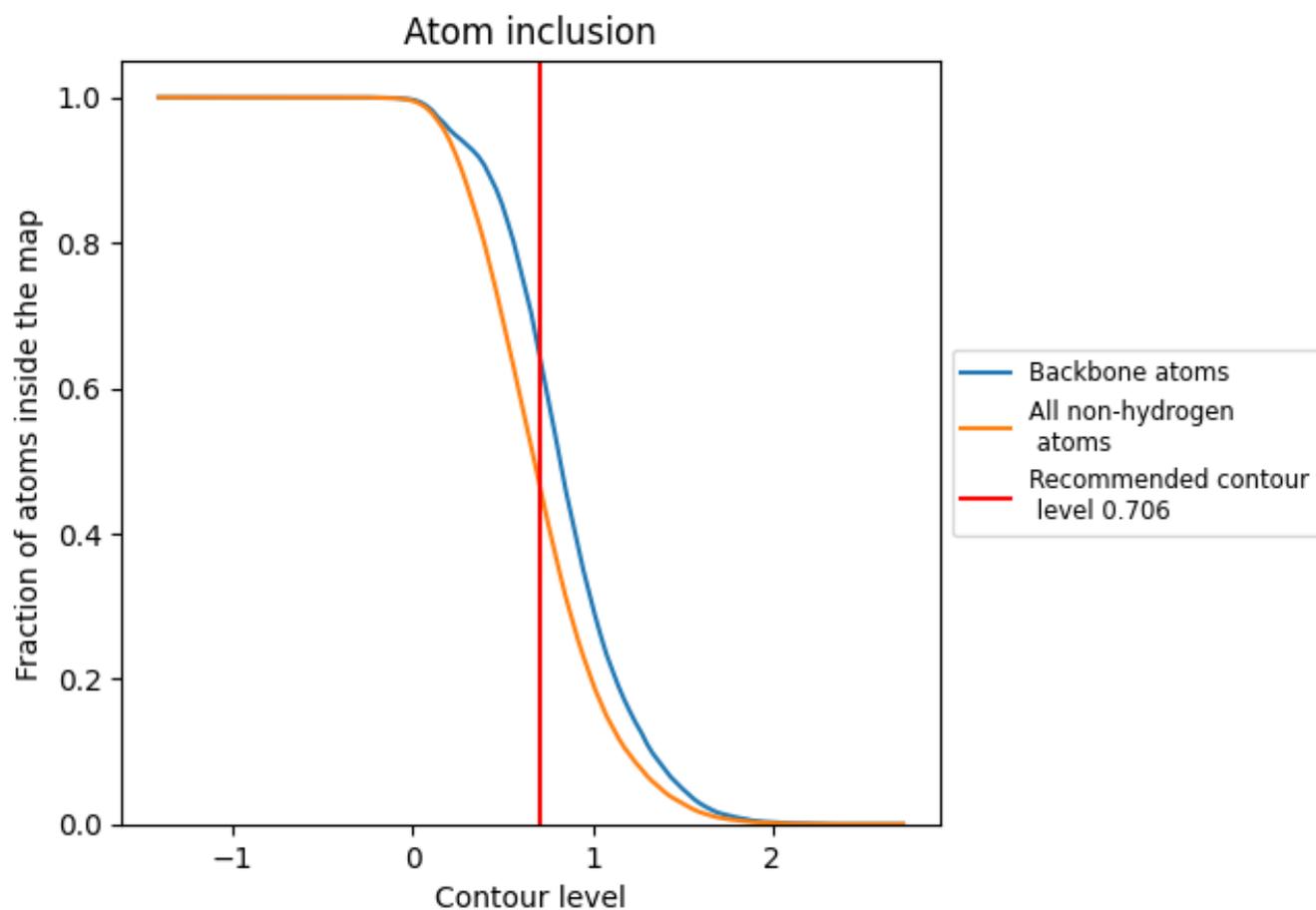
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.706).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.706) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4650	0.4490
A	0.5463	0.4800
G	0.4032	0.4260

