



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:59 PM UTC

PDB ID : 6U5T / pdb_00006u5t
EMDB ID : EMD-20655
Title : Electron cryomicroscopy Structure of *S. cerevisiae* FAS in the Apo state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2019-08-28
Resolution : 2.90 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

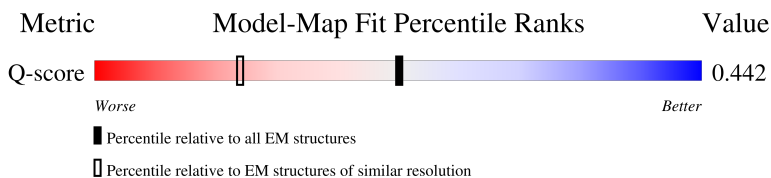
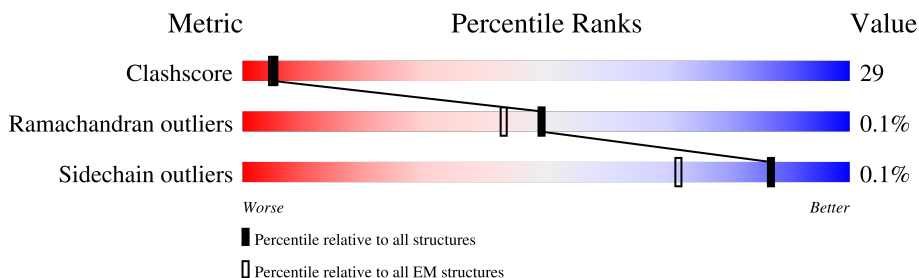
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	26% 45% 40% 14%
2	G	2073	46% 48% 50% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28233 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
1	A	1616	Total	C	N	O	S	0	0
			12202	7703	2086	2368	45		

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

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

There are 22 discrepancies between the modelled and reference sequences:

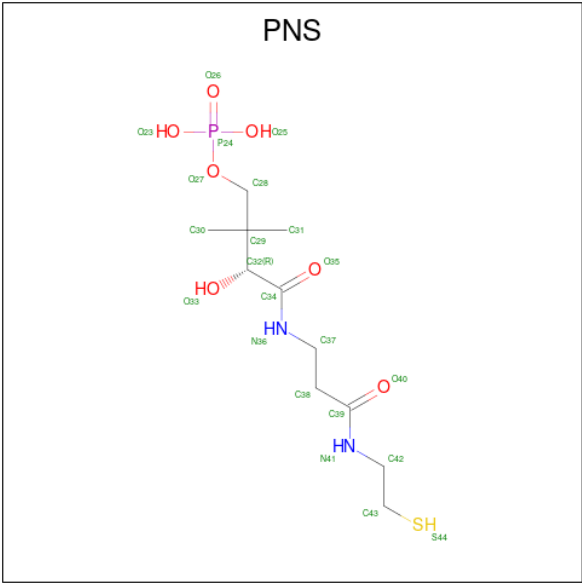
Chain	Residue	Modelled	Actual	Comment	Reference
G	2052	ASP	-	expression tag	UNP P07149
G	2053	TYR	-	expression tag	UNP P07149
G	2054	LYS	-	expression tag	UNP P07149
G	2055	ASP	-	expression tag	UNP P07149
G	2056	HIS	-	expression tag	UNP P07149
G	2057	ASP	-	expression tag	UNP P07149
G	2058	GLY	-	expression 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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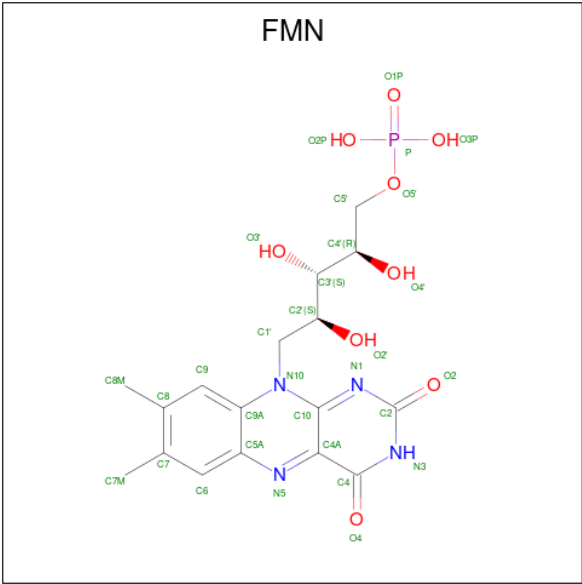
Chain	Residue	Modelled	Actual	Comment	Reference
G	2073	LYS	-	expression tag	UNP P07149

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).



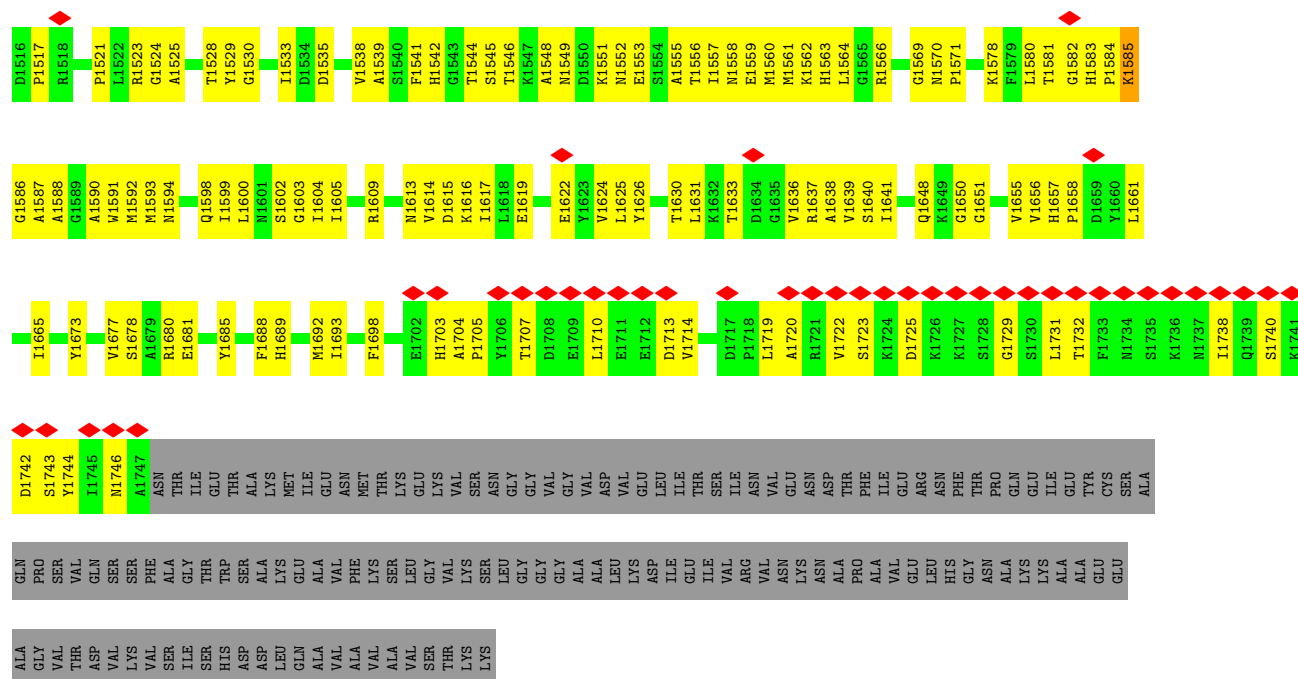
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			5	1	3	1	

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).

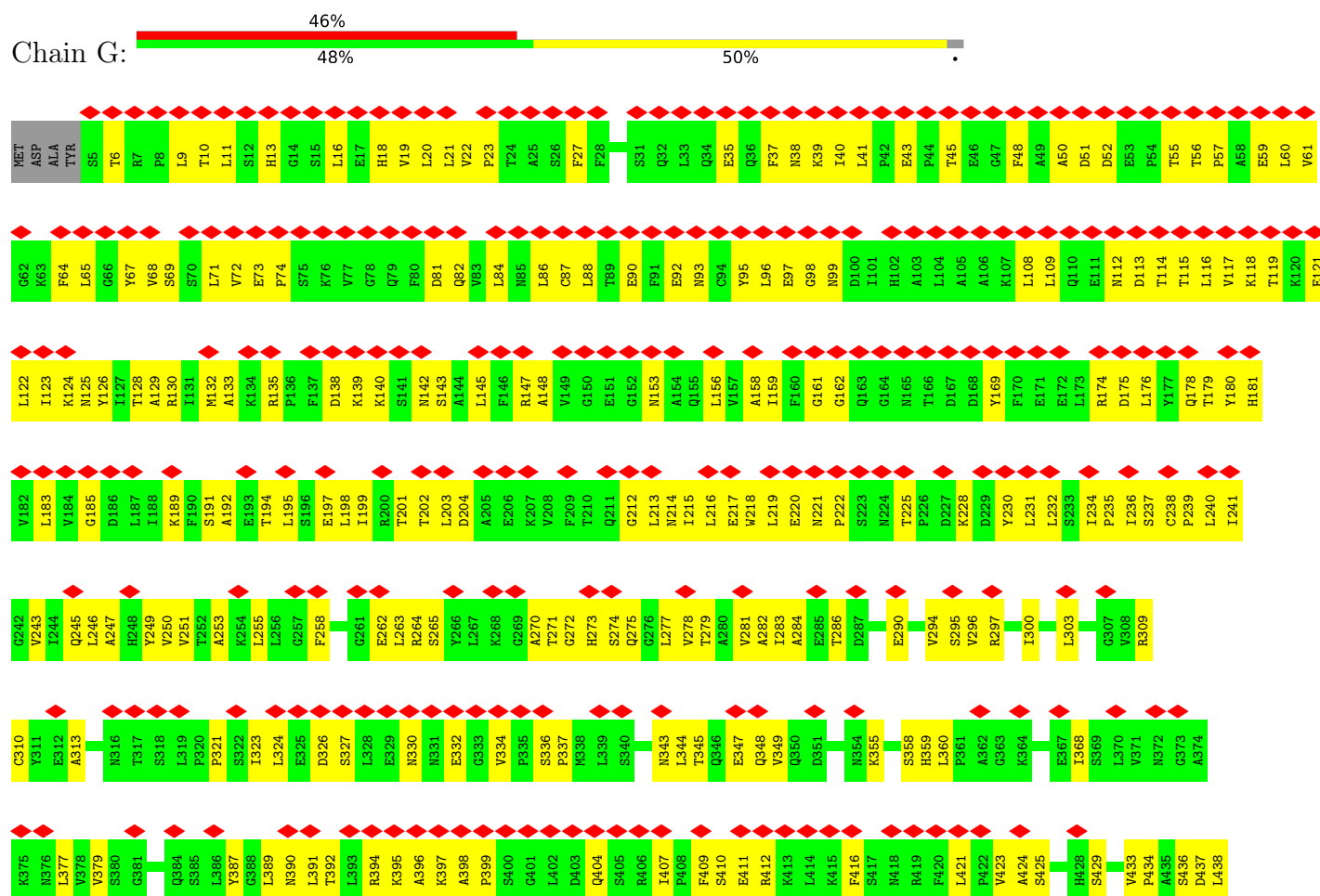


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	G	1	31	17	4	9	1	0





• Molecule 2: Fatty acid synthase subunit beta



A1303	I439	G508	G575	I649	A722	F501	H874	L951	E1026	I1097	V1166	N1243	A1303	I1327
V1304	M440	A509	E580	I652	H723	R804	L875	R952	K1030	P1098	S1167	N1244	G1305	V1328
G1306	K441	S510	T581	Y653	P724	V605	P876	R953	K1031	A1099	P1168	D1245	C1307	V1329
C1308	D442	G511	K582	V654	N725	M806	K877	E956	D1032	E1098	R1170	N1246	N1307	G1330
E1309	L443	L512	L586	F657	A729	A808	K878	R957	S1033	P1100	R1171	A1249	C1308	W1331
D1310	V444	G513	L587	M658	L730	K809	L880	R958	L1034	E1101	K1172	I1250	E1309	I1270
F1311	K445	V514	L515	L588	Q731	E910	V881	K960	W1036	P1107	V1174	I1251	C1309	I1271
V1312	M446	T516	G588	F657	L730	E910	P882	K963	D1037	V1109	K1175	S1252	D1310	D1272
R1313	M447	H517	P590	W661	G735	K812	T683	T963	E1038	ASP	P1176	E1253	F1311	E1273
R1314	W451	R518	L593	G662	R736	R816	L884	L966	H1039	VAL	S1177	E1254	V1312	E1274
R1315	A452	N519	V594	I663	G739	A817	E885	Q967	L1040	GLN	Q1178	M1255	R1314	R1269
D1316	K453	K520	P595	L665	H740	K818	R888	Q968	E1041	SER	G1179	E1256	P1315	N1260
P1317	D454	G524	G596	R657	S742	K819	D889	D974	A1042	VAL	M1180	D1257	D1316	R1261
C1318	I455	V525	M597	E668	F743	R820	Y890	K975	V1043	ASP	E1183	R1258	R1317	R1262
F1319	Q456	R526	T598	E669	E744	C520	L891	P976	V1044	SER	E1184	Q1259	T1318	Q1260
A1321	V459	R529	T599	R670	D745	R821	L892	E978	V1045	SER	M1186	D1261	M1319	R1261
P1322	Y460	A530	G600	G672	A746	G626	S893	E979	D1046	GLU	G1187	K1263	A1321	K1263
M1323	D461	G531	T601	G673	L751	D830	R894	I980	D1047	D1123	M1188	E1264	P1322	E1264
D1324	G465	T532	V602	Y674	Q752	K831	L895	E981	C1052	S1124	T1189	Y1266	M1323	M1265
I1327	S466	L533	D605	Q677	H750	D832	R896	K982	I1053	F1127	T1193	K1268	D1324	Y1267
V1328	D467	D534	F506	F678	L751	E833	A897	K983	I1054	K1128	L1197	K1269	V1328	K1269
G1330	L468	I535	V607	L679	Q752	Q834	D898	L985	H1055	F1127	S1198	W1270	V1329	W1270
W1331	R469	N536	G814	N612	N761	E834	P902	R896	G1056	K1127	L1199	I1271	G1330	I1271
A1333	V470	P537	G814	A883	N762	Q834	F904	K987	P1057	F1127	P1200	D1272	W1331	D1272
I1335	L471	D538	Y615	G684	N763	K837	Y907	A989	V1058	S1131	V1201	E1273	A1333	E1273
K1336	S472	D539	T619	Y615	N764	V844	N908	R991	A1059	S1132	Q1202	P1274	I1335	P1274
A1337	G473	D540	L619	T616	N766	T845	Y908	E992	K1064	T1133	L1197	F1275	I1336	F1275
I1338	S474	D540	E618	L617	N766	V846	G909	Q998	V1065	E1135	L1198	N1276	K1336	N1276
F1339	E477	F541	L619	E618	N766	R847	Q910	N996	V1066	E1136	L1205	K1277	A1337	K1277
P1340	R478	G542	L619	E618	N766	R848	R912	Q997	I1067	L1142	L1206	D1278	I1338	D1278
N1341	D481	K544	L619	E618	N766	S850	D913	D999	D1067	L1143	L1213	F1279	F1339	F1279
T1342	C482	Q545	L619	E618	N766	G851	L914	I1000	E1068	A1143	L1214	D1280	P1340	D1280
V1343	I483	E546	L619	E618	N766	E852	L915	D1001	P1069	G1144	K1215	P1281	N1341	P1281
D1344	I484	E547	L619	E618	N766	P853	T916	H1002	I1070	S1145	E1216	R1282	T1342	R1282
G1345	R485	I547	L619	E618	N766	H855	N917	F1003	K1071	E1146	L1217	V1284	V1343	D1283
L1346	L486	F548	L619	E618	N766	K856	V922	M1006	S1072	I1147	I1218	I1285	D1344	I1285
L1347	F487	D549	L619	E618	N766	R857	Y922	E1006	I1073	I1148	I1219	K1286	G1345	I1286
L1348	V488	V550	L619	E618	N766	A858	L926	N1009	M1074	N1148	Q1220	K1287	L1346	K1287
K1349	K489	T551	L619	E618	N766	T859	Y927	P1010	D1075	W1149	E1225	K1288	L1347	K1288
L1350	W490	S552	L619	E618	N766	R860	E928	M1011	H1078	H1151	E1226	D1289	L1348	D1289
V1351	E491	N553	L619	E618	N766	G861	E928	M1011	D1079	A1152	M1226	F1290	K1349	F1290
H1352	T494	G554	L619	E618	N766	V862	E928	K1013	D1080	S1153	R1227	E1291	L1350	E1291
L1353	Q495	L555	L619	E618	N766	L864	E928	V1018	H1081	L1155	M1229	I1292	D1344	I1292
S1354	Q496	K557	L619	E618	N766	R865	E928	P1019	L1085	C1156	D1230	T1293	G1345	T1293
Y1357	F496	N558	L619	E618	N766	E867	E928	V1020	L1086	S1157	G1231	K1295	L1353	K1295
I1360	K497	L562	L619	E618	N766	E868	E928	L1021	L1086	F1158	D1232	E1296	V1357	E1296
G1362	H500	Y565	L619	E618	N766	D869	E928	V1021	L1086	I1159	K1232	V1297	L1360	V1297
A1363	L502	L562	L619	E618	N766	E870	E928	L1022	L1086	D1162	L1236	I1298	T1361	I1298
L1366	D503	Y565	L619	E618	N766	T871	E928	D1023	L1086	K1163	L1237	F1299	G1362	F1299
	F504	K568	L619	E618	N766	S871	E928	R1024	L1086	D1162	L1238	F1300	A1363	F1300
	G505	L570	L619	E618	N766	S871	E928	R1024	L1086	D1162	L1239	H1302	L1366	H1302
	P506	K571	L619	E618	N766	S871	E928	R1024	L1086	D1162	L1239	H1302	L1366	H1302
	G507	K573	L619	E618	N766	S871	E928	R1024	L1086	D1162	L1239	H1302	L1366	H1302
		S574	L619	E618	N766	S871	E928	R1024	L1086	D1162	L1239	H1302	L1366	H1302

F2026	A1965	R1905	D1845	M1784	T1718	L1651	H1581	M1514	A1442	Q1367
Q2027	C1966	A1906	E1846	A1787	T1719	T1652	G1582	D1518	V1443	D1370
D2028	T1967	L1907	L1847	A1788	H1720	E1656	M1583	F1519	L1444	
V2029	P1968	D1908	G1848	F1789	F1721	I1657	F1584	L1520	S1446	T1378
V2030	L1969	T1909	R1849	E1790	R1728	E1658	R1590	K1521	K1447	E1379
D2031	V1970	V1910	S1850	D1791	I1729	P1659	A1591	R1522	E1448	S1380
L2032	G1971	T1911	M1851	L1792	R1730	P1660	L1592	M1523	V1449	V1381
T2033	I1972	N1912	Y1852	K1793	E1731	V1661	L1593	G1524	F1450	V1382
G2034	S1973	V1913	G1853	K1794		T1662	E1594	S1525	Q1451	M1383
S2035	V1974	L1914	M1854	K1795	S1734	T1663	M1595	D1453	L1452	Q1384
E2036	P1975	N1915	I1855	G1796	A1735	T1664	V1596	D1454	T1386	F1385
P2037	F1976	F1916	A1856	L1797	M1736	V1665	A1597	E1455	T1387	T1387
L2038	H1977	I1917	I1857	L1798	I1737	F1666	A1598	E1456	K1388	
K2039	S1978	K1918	P1799	P1799	E1738	T1667	D1599	F1457	I1389	
E2040	T1979	L1919	D1801	A1800	F1740	G1668	S1600	D1458	V1390	
L2041	Y1980	Q1920	T1802	T1803	I1741	Q1669	V1601	D1459	D1391	
D2042	M1982	K1921	V1862	F1804	V1742	G1670	R1604	L1460	V1392	
D2043	L1981	I1922	A1863	A1805	D1743	S1671	V1605	N1461	V1393	
N2044	M1983	D1923	A1864	G1806	G1744	Q1672	R1606	F1466	G1394	
V2045	G1984	I1924	S1865	H1807	K1745	E1673	G1607	E1467	T1395	
E2046	V1985	I1925	F1866	S1808	L1746	G1675	R1608	T1468	L1396	
K2047	K1986	I1926	S1867	L1809	K1747	M1676	Y1608	E1469	S1397	
Y2048	P1987	L1927	Q1868	L1810	T1748	G1677		T1470	G1400	
F1988	F1988	Q1928	E1869	G1811	E1749	M1678		E1471	K1401	
E2049	K1989	K1929	A1870	E1812	T1751	M1679		V1472		
Q2050	S1990	S1930	L1871	Y1813	F1752	D1679				
SER	F1991	L1931	Q1872	A1814	K1753	Y1681				
ASP	L1992	S1932	Y1873	L1815	E1754	K1682				
LYS	K1993	L1933	V1874	A1816	H1755	T1683				
ASP	K1994	E1934	V1875	S1817	H1756	T1620				
ASP	M1995	E1935	E1876	L1818	E1757	A1621				
GLY	I1997	V1936	E1877	A1819	H1758	L1622				
TYR	K1998	E1937	R1877	L1820	S1759	K1623				
LYS	E1999	G1938	V1878	V1821	Q1688	I1626				
ASP	N2000	H1939	K1879	M1822	D1689	Q1627				
ASP	V2001	L1940	R1880	S1823	V1690	H1628				
ASP	K2002	F1941	R1881	E1825	N1692					
ASP	V2003	E1942	T1882	S1826	R1693	M1631				
LYS	A2004	I1943	G1883	E1827	A1694	I1632				
ASP	R2005	I1944	W1884	V1828	D1695					
ASP		D1945	L1885	E1829	N1696					
ASP	G2008	E1946	V1886	L1829	H1697					
ASP	K2009	A1947	E1887	V1830	F1698					
ASP	Y2010	S1948	I1888	V1831	T1701					
ASP	I2011	K1949	V1889	F1832						
LYS	N2013	S1951	N1892	R1833	S1772					
ASP	L2014	A1952	M1893	R1834	A1773					
ASP	T2015	V1953	E1894	G1835	T1774					
LYS	A2016	K1954	T1837	M1836	Q1775					
ASP	K2017	P1955	M1838	T1837	F1776					
ASP	P2018	Q1956	M1839	Q1839	T1777					
ASP	F2019	F1957	N1895	V1840	Q1778					
ASP	Q2020	R1956	Q1897	A1841	P1779					
ASP	V2021	Y1998	Y1898	V1842	T1782					
ASP	T2022	L1958	V1899	P1843	L1783					
ASP	K2023	K1959	A1901	R1844						
ASP	E2024	L1960	G1902							
LYS	Y2025	E1961	D1903							
		G1963	L1904							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	637823	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	2.591	Depositor
Minimum map value	-1.261	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.696	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	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

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	0/12424	0.53	1/16819 (0.0%)
2	G	0.42	1/16360 (0.0%)	0.44	1/22198 (0.0%)
All	All	0.51	1/28784 (0.0%)	0.48	2/39017 (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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1721	PHE	CA-CB	-5.74	1.44	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1971	GLY	N-CA-C	-5.81	108.17	115.08
1	A	1150	ASP	N-CA-C	-5.51	105.85	112.58

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1294	SER	Peptide
1	A	702	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12202	0	11715	713	0
2	G	15995	0	15978	928	0
3	A	5	0	0	0	0
4	G	31	0	19	1	0
All	All	28233	0	27712	1601	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 29.

All (1601) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1335:PHE:HD1	1:A:1378:GLU:HG3	1.07	1.12
1:A:1343:PHE:CE2	1:A:1585:LYS:NZ	2.18	1.10
1:A:1333:ASP:OD2	1:A:1585:LYS:HB2	1.52	1.09
1:A:1584:PRO:HB2	1:A:1587:ALA:HB3	1.34	1.04
1:A:1335:PHE:HD1	1:A:1378:GLU:CG	1.71	1.02
1:A:1335:PHE:CD1	1:A:1378:GLU:HG3	1.97	0.99
1:A:1335:PHE:CD1	1:A:1378:GLU:CG	2.47	0.97
2:G:1180:MET:SD	2:G:1567:ARG:NH2	2.38	0.96
2:G:1750:LYS:O	2:G:1753:LYS:NZ	2.01	0.93
2:G:1951:SER:O	2:G:1954:LYS:NZ	2.02	0.92
2:G:556:LYS:NZ	2:G:558:ASN:OD1	2.02	0.92
2:G:1881:ARG:NH1	2:G:1948:SER:OG	2.02	0.92
1:A:36:LEU:O	1:A:76:ARG:NH2	2.02	0.92
2:G:1842:VAL:O	2:G:1844:ARG:NH1	2.04	0.90
2:G:966:LEU:O	2:G:982:LYS:NZ	2.06	0.89
2:G:1800:ALA:O	2:G:2009:LYS:NZ	2.03	0.89
1:A:1185:VAL:HB	1:A:1377:MET:HE1	1.54	0.89
1:A:1333:ASP:OD2	1:A:1584:PRO:O	1.92	0.88
2:G:1730:ARG:NH1	2:G:1759:SER:O	2.07	0.87
1:A:41:THR:O	1:A:76:ARG:NH1	2.08	0.87
1:A:872:THR:OG1	1:A:898:GLN:OE1	1.92	0.87
2:G:1791:ASP:OD1	2:G:1795:LYS:NZ	2.08	0.86
1:A:913:VAL:O	1:A:916:LEU:N	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1378:GLU:HB2	1:A:1585:LYS:HE2	1.54	0.86
1:A:1533:ILE:O	1:A:1566:ARG:NH1	2.09	0.86
2:G:2041:ILE:O	2:G:2045:TRP:N	2.10	0.85
1:A:458:THR:O	1:A:470:LYS:NZ	2.09	0.85
2:G:1991:PHE:O	2:G:1995:ASN:ND2	2.10	0.85
1:A:739:GLN:O	1:A:798:ASN:ND2	2.10	0.84
2:G:2047:LYS:O	2:G:2050:GLN:NE2	2.10	0.84
1:A:1186:ALA:O	1:A:1188:GLN:NE2	2.10	0.83
2:G:1695:ASP:OD2	2:G:1705:SER:OG	1.96	0.83
1:A:21:GLN:NE2	2:G:1811:GLU:OE2	2.11	0.83
1:A:517:GLU:N	1:A:517:GLU:OE1	2.12	0.83
1:A:661:ASP:OD1	1:A:662:GLY:N	2.12	0.82
1:A:1240:VAL:O	1:A:1295:SER:OG	1.98	0.82
2:G:1878:VAL:HG21	2:G:1910:VAL:HG22	1.61	0.82
2:G:1632:ILE:HD12	2:G:1637:LEU:HD13	1.59	0.82
1:A:42:GLU:OE1	2:G:1661:VAL:N	2.12	0.82
1:A:1616:LYS:NZ	1:A:1619:GLU:OE1	2.10	0.82
1:A:1343:PHE:HE2	1:A:1585:LYS:NZ	1.73	0.81
2:G:1431:TYR:OH	2:G:1521:LYS:NZ	2.11	0.81
2:G:2049:GLU:OE2	2:G:2049:GLU:N	2.13	0.81
1:A:384:GLU:OE2	1:A:384:GLU:N	2.13	0.81
1:A:1333:ASP:OD2	1:A:1585:LYS:CB	2.29	0.81
1:A:985:ARG:N	2:G:956:GLU:O	2.14	0.81
2:G:1839:GLN:O	2:G:1844:ARG:NH1	2.14	0.81
2:G:161:GLY:O	2:G:245:GLN:NE2	2.14	0.81
2:G:220:GLU:OE1	2:G:220:GLU:N	2.13	0.80
2:G:626:SER:O	2:G:630:MET:HE3	1.81	0.80
2:G:1917:ILE:O	2:G:1921:LYS:N	2.15	0.80
1:A:17:LEU:HD23	2:G:2014:LEU:HD23	1.63	0.80
1:A:1185:VAL:CB	1:A:1377:MET:HE1	2.12	0.80
1:A:442:ARG:NH1	1:A:726:GLY:O	2.13	0.80
1:A:81:TYR:OH	1:A:89:TYR:OH	1.98	0.80
2:G:1621:ALA:N	2:G:1645:GLU:OE2	2.15	0.80
2:G:491:GLU:N	2:G:491:GLU:OE1	2.15	0.79
2:G:1189:THR:O	2:G:1193:THR:OG1	1.99	0.79
2:G:121:GLU:OE2	2:G:125:ASN:ND2	2.15	0.79
2:G:1258:ARG:NH2	2:G:1572:TYR:OH	2.16	0.79
1:A:1351:ASN:OD1	1:A:1352:THR:N	2.15	0.79
2:G:264:ARG:NH1	2:G:286:THR:O	2.15	0.79
2:G:222:PRO:O	2:G:225:THR:OG1	2.01	0.79
1:A:652:ASP:OD1	1:A:653:ARG:N	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1734:SER:O	2:G:1750:LYS:NZ	2.12	0.79
2:G:297:ARG:NH1	2:G:447:ASN:OD1	2.16	0.79
2:G:1948:SER:O	2:G:1952:ALA:N	2.16	0.78
2:G:1236:LEU:HD22	2:G:1265:MET:HE3	1.64	0.78
1:A:764:ASP:OD2	1:A:818:ARG:NH1	2.17	0.77
2:G:1354:SER:HG	2:G:1409:SER:HG	1.10	0.77
1:A:931:GLN:OE1	1:A:931:GLN:N	2.16	0.77
2:G:1674:GLN:NE2	2:G:1710:VAL:O	2.18	0.77
2:G:1706:ILE:HG22	2:G:1710:VAL:HG13	1.67	0.77
2:G:326:ASP:OD1	2:G:327:SER:N	2.18	0.77
2:G:490:TRP:CZ2	2:G:512:LEU:HD21	2.20	0.77
2:G:1256:GLU:N	2:G:1256:GLU:OE2	2.18	0.76
1:A:347:ALA:O	1:A:351:LYS:N	2.16	0.76
2:G:35:GLU:O	2:G:39:LYS:NZ	2.17	0.76
2:G:175:ASP:O	2:G:179:THR:N	2.16	0.76
1:A:1151:LYS:HA	1:A:1168:LEU:HD22	1.66	0.76
2:G:821:ILE:HD11	2:G:1055:HIS:ND1	2.00	0.76
1:A:414:LEU:O	1:A:417:TYR:N	2.19	0.76
2:G:262:GLU:O	2:G:265:SER:OG	2.02	0.76
2:G:978:GLU:OE1	2:G:978:GLU:N	2.19	0.76
1:A:910:THR:O	1:A:914:VAL:HG23	1.86	0.76
2:G:264:ARG:NE	2:G:456:GLN:OE1	2.19	0.76
2:G:368:ILE:HA	2:G:379:VAL:HG12	1.68	0.75
2:G:1142:LEU:O	2:G:1150:ARG:NE	2.19	0.75
2:G:74:PRO:HD3	2:G:132:MET:HE3	1.66	0.75
2:G:1825:GLU:N	2:G:1825:GLU:OE2	2.19	0.75
2:G:1032:ASP:OD2	2:G:1035:TRP:NE1	2.19	0.75
2:G:996:ASN:OD1	2:G:998:GLN:N	2.19	0.75
2:G:139:LYS:NZ	2:G:140:LYS:O	2.19	0.74
2:G:933:ARG:NH2	2:G:977:ASP:OD2	2.20	0.74
1:A:957:VAL:HG23	2:G:1443:VAL:HG12	1.69	0.74
2:G:50:ALA:O	2:G:118:LYS:NZ	2.17	0.74
2:G:290:GLU:N	2:G:290:GLU:OE1	2.20	0.74
2:G:716:VAL:HG21	2:G:730:LEU:HD21	1.69	0.74
2:G:649:ILE:HD13	2:G:666:ILE:HD11	1.70	0.74
2:G:1903:ASP:OD2	2:G:1906:ALA:N	2.20	0.74
1:A:46:GLU:OE2	1:A:53:LEU:N	2.21	0.73
1:A:520:ARG:N	1:A:524:GLN:OE1	2.21	0.73
2:G:1614:ASP:OD1	2:G:1650:VAL:HG12	1.88	0.73
2:G:1890:ASN:HB2	2:G:1899:VAL:HG22	1.71	0.73
2:G:670:ARG:NH1	2:G:674:TYR:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1905:ARG:NH1	2:G:1954:LYS:O	2.21	0.73
1:A:1256:ALA:O	1:A:1259:GLY:N	2.21	0.73
1:A:986:ALA:O	2:G:957:ARG:NH1	2.22	0.73
2:G:67:TYR:CZ	2:G:71:LEU:HD11	2.23	0.73
1:A:1505:GLN:O	1:A:1509:GLY:N	2.22	0.73
1:A:1185:VAL:CG2	1:A:1377:MET:HE1	2.18	0.72
1:A:1288:ASN:OD1	1:A:1293:SER:N	2.21	0.72
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.54	0.72
1:A:1034:ARG:NH2	1:A:1052:GLU:OE2	2.22	0.72
1:A:1245:ASN:ND2	1:A:1284:SER:OG	2.21	0.72
2:G:668:GLU:N	2:G:668:GLU:OE1	2.22	0.72
1:A:513:GLU:OE2	1:A:873:ARG:NH1	2.23	0.72
2:G:857:ILE:O	2:G:862:VAL:HG11	1.89	0.72
2:G:1741:ILE:HD12	2:G:1983:ASN:HA	1.70	0.72
1:A:1307:THR:O	1:A:1311:SER:OG	2.05	0.72
1:A:53:LEU:O	1:A:57:ALA:N	2.22	0.72
2:G:270:ALA:O	2:G:271:THR:OG1	2.08	0.72
1:A:475:GLN:NE2	1:A:610:THR:O	2.22	0.72
1:A:715:THR:O	1:A:719:GLN:N	2.23	0.72
2:G:1754:GLU:OE1	2:G:1754:GLU:N	2.23	0.72
2:G:1154:PHE:O	2:G:1171:ARG:NE	2.23	0.71
2:G:1550:ASN:ND2	2:G:1579:ILE:O	2.23	0.71
1:A:1450:ARG:O	1:A:1454:THR:OG1	2.07	0.71
2:G:1874:VAL:HG23	2:G:1877:ARG:HH21	1.54	0.71
1:A:953:VAL:HG12	2:G:1439:LYS:HB2	1.70	0.71
1:A:1305:CYS:HA	1:A:1585:LYS:O	1.90	0.71
1:A:528:GLU:OE2	1:A:894:ARG:NH1	2.23	0.71
1:A:26:VAL:HG13	2:G:2013:ASN:HB3	1.72	0.71
2:G:736:ARG:NE	2:G:769:SER:O	2.23	0.71
1:A:21:GLN:O	2:G:1977:HIS:NE2	2.23	0.71
2:G:1767:GLU:N	2:G:1767:GLU:OE1	2.22	0.71
1:A:1130:ASP:OD2	1:A:1167:LEU:N	2.23	0.71
2:G:1773:ALA:O	2:G:1777:THR:HG23	1.91	0.71
1:A:727:ALA:O	1:A:730:SER:OG	2.05	0.70
2:G:739:GLY:HA2	2:G:1054:LEU:HD13	1.71	0.70
1:A:472:LEU:O	1:A:475:GLN:N	2.25	0.70
2:G:996:ASN:OD1	2:G:997:ALA:N	2.24	0.70
1:A:1584:PRO:CB	1:A:1587:ALA:HB3	2.19	0.70
2:G:1236:LEU:HD22	2:G:1265:MET:CE	2.21	0.70
2:G:1350:LEU:HD12	2:G:1351:VAL:H	1.55	0.70
1:A:504:ASP:OD2	1:A:506:ASN:ND2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:72:VAL:HB	2:G:132:MET:HE2	1.73	0.70
1:A:1077:ASP:OD2	1:A:1079:LYS:N	2.25	0.70
2:G:109:LEU:O	2:G:114:THR:OG1	2.10	0.70
2:G:1893:VAL:HG22	2:G:1897:GLN:CB	2.21	0.70
1:A:1186:ALA:HB1	1:A:1378:GLU:O	1.91	0.70
2:G:456:GLN:O	2:G:469:ARG:NH2	2.24	0.70
1:A:827:SER:O	1:A:830:HIS:NE2	2.25	0.69
1:A:1334:ASP:OD1	1:A:1335:PHE:N	2.24	0.69
2:G:850:MET:HE2	2:G:850:MET:HA	1.74	0.69
1:A:915:GLU:N	1:A:915:GLU:OE1	2.25	0.69
2:G:347:GLU:N	2:G:347:GLU:OE1	2.26	0.69
1:A:78:ILE:C	1:A:79:LEU:HD12	2.18	0.69
1:A:1046:SER:OG	1:A:1048:GLU:OE1	2.08	0.69
1:A:69:ASP:OD1	1:A:70:ALA:N	2.25	0.69
2:G:857:ILE:HD12	2:G:1053:ILE:CD1	2.22	0.69
1:A:905:LEU:HD12	1:A:905:LEU:H	1.58	0.69
1:A:856:GLU:OE1	1:A:858:TRP:NE1	2.25	0.68
2:G:907:VAL:O	2:G:910:GLN:N	2.25	0.68
2:G:1885:LEU:O	2:G:1903:ASP:N	2.26	0.68
2:G:1452:LEU:HD22	2:G:1501:ILE:HG22	1.74	0.68
2:G:582:LYS:NZ	2:G:761:PRO:O	2.26	0.68
1:A:431:GLU:O	1:A:435:GLU:N	2.25	0.68
1:A:538:GLU:N	1:A:633:GLU:O	2.27	0.68
1:A:727:ALA:N	1:A:730:SER:OG	2.26	0.68
1:A:957:VAL:CG2	2:G:1443:VAL:HG12	2.24	0.68
2:G:246:LEU:O	2:G:250:VAL:HG13	1.94	0.68
2:G:1841:ALA:O	2:G:1980:TYR:OH	2.11	0.68
1:A:527:GLN:O	1:A:530:ALA:N	2.26	0.68
1:A:655:LEU:C	1:A:655:LEU:HD23	2.19	0.68
1:A:18:LEU:HD22	2:G:1812:TYR:CE2	2.29	0.68
2:G:1853:GLY:HA3	2:G:1904:LEU:HD21	1.76	0.68
2:G:857:ILE:HD12	2:G:1053:ILE:HD12	1.75	0.68
1:A:777:GLN:N	1:A:777:GLN:OE1	2.27	0.67
1:A:865:CYS:HB3	1:A:908:LEU:HD21	1.77	0.67
1:A:501:THR:HG21	1:A:883:ILE:O	1.93	0.67
1:A:748:LEU:HD23	1:A:748:LEU:C	2.20	0.67
2:G:1812:TYR:HA	2:G:1815:LEU:HD12	1.74	0.67
1:A:516:ARG:NH2	1:A:889:GLU:OE2	2.27	0.67
1:A:1104:ARG:NE	1:A:1107:GLU:OE2	2.28	0.67
2:G:914:LEU:HD23	2:G:1000:ILE:HG23	1.76	0.67
1:A:1:MET:HE1	2:G:2048:TYR:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:CYS:CB	1:A:908:LEU:HD21	2.23	0.67
1:A:1343:PHE:CD2	1:A:1585:LYS:NZ	2.62	0.67
2:G:696:GLU:N	2:G:696:GLU:OE1	2.28	0.67
1:A:1130:ASP:OD2	1:A:1168:LEU:N	2.28	0.67
1:A:1185:VAL:HG23	1:A:1377:MET:SD	2.35	0.67
2:G:690:VAL:HG22	2:G:694:TYR:HE2	1.59	0.67
2:G:1367:GLN:N	2:G:1370:ASP:OD2	2.27	0.67
2:G:1926:GLU:O	2:G:1930:SER:OG	2.11	0.67
2:G:1836:MET:O	2:G:1839:GLN:N	2.28	0.66
2:G:279:THR:O	2:G:282:ALA:HB3	1.95	0.66
2:G:2046:GLU:N	2:G:2046:GLU:OE1	2.28	0.66
2:G:239:PRO:O	2:G:243:VAL:HG13	1.96	0.66
2:G:1311:PHE:O	2:G:1319:MET:HE3	1.95	0.66
1:A:695:GLY:O	1:A:698:GLN:N	2.27	0.66
2:G:1173:VAL:O	2:G:1567:ARG:NH1	2.29	0.66
1:A:1203:ASP:OD1	1:A:1204:ILE:N	2.29	0.66
2:G:1213:LEU:C	2:G:1214:LEU:HD22	2.21	0.66
1:A:57:ALA:O	1:A:58:GLN:NE2	2.29	0.66
2:G:1500:GLU:OE1	2:G:1500:GLU:N	2.29	0.66
2:G:860:ARG:NH2	2:G:1047:ASP:OD2	2.29	0.65
1:A:1521:PRO:O	1:A:1525:ALA:N	2.29	0.65
2:G:509:ALA:O	2:G:514:VAL:HG21	1.95	0.65
2:G:1440:ASP:OD1	2:G:1441:ILE:N	2.29	0.65
1:A:46:GLU:OE2	1:A:52:THR:N	2.29	0.65
2:G:688:LEU:HD13	2:G:719:ILE:HD13	1.78	0.65
2:G:228:LYS:O	2:G:232:LEU:N	2.26	0.65
2:G:605:ASP:OD2	2:G:812:LYS:NZ	2.28	0.65
2:G:860:ARG:NH1	2:G:898:ASP:OD1	2.29	0.65
1:A:1184:LEU:HD12	1:A:1184:LEU:O	1.97	0.65
2:G:981:GLU:O	2:G:985:ASN:ND2	2.29	0.65
1:A:826:MET:O	1:A:827:SER:OG	2.13	0.65
2:G:512:LEU:O	2:G:516:THR:HG23	1.97	0.65
2:G:1197:LEU:HD12	2:G:1198:SER:N	2.12	0.65
2:G:1354:SER:OG	2:G:1409:SER:OG	1.94	0.65
2:G:1530:LYS:CG	2:G:1632:ILE:HD11	2.27	0.65
2:G:1877:ARG:NH2	2:G:1913:VAL:HG21	2.11	0.65
2:G:1893:VAL:HG22	2:G:1897:GLN:HB3	1.78	0.65
2:G:2030:TYR:O	2:G:2034:GLY:N	2.27	0.65
2:G:1855:ILE:HB	2:G:1907:LEU:HD21	1.79	0.65
2:G:1054:LEU:HD12	4:G:3051:FMN:HM72	1.77	0.65
1:A:27:ARG:NH1	2:G:2014:LEU:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:VAL:HG11	1:A:894:ARG:HH12	1.63	0.64
2:G:1151:HIS:CD2	2:G:1155:LEU:HD12	2.33	0.64
2:G:1673:GLU:N	2:G:1673:GLU:OE1	2.31	0.64
1:A:1033:ALA:O	1:A:1598:GLN:NE2	2.30	0.64
2:G:1452:LEU:HD23	2:G:1502:GLY:HA3	1.78	0.64
2:G:130:ARG:NE	2:G:135:ARG:O	2.31	0.64
1:A:1302:VAL:HG13	1:A:1302:VAL:O	1.97	0.64
2:G:1318:THR:O	2:G:1318:THR:HG23	1.96	0.64
1:A:471:THR:HG23	1:A:472:LEU:N	2.13	0.64
1:A:660:LEU:N	1:A:660:LEU:HD12	2.12	0.64
1:A:430:ARG:NE	1:A:606:ASP:OD1	2.31	0.64
2:G:142:ASN:C	2:G:550:VAL:HG12	2.23	0.64
2:G:864:LEU:HD11	2:G:868:PHE:CZ	2.33	0.64
2:G:217:GLU:N	2:G:217:GLU:OE1	2.30	0.63
2:G:1293:THR:HG23	2:G:1296:GLU:H	1.63	0.63
1:A:1486:LEU:O	1:A:1490:THR:N	2.30	0.63
1:A:1538:VAL:HG12	1:A:1539:ALA:H	1.62	0.63
2:G:6:THR:HG21	2:G:21:LEU:HD21	1.80	0.63
2:G:59:GLU:HA	2:G:122:LEU:HD11	1.80	0.63
1:A:1333:ASP:CG	1:A:1584:PRO:O	2.42	0.63
1:A:1501:LEU:HD23	1:A:1502:ARG:N	2.13	0.63
2:G:848:SER:N	2:G:852:GLU:O	2.30	0.63
2:G:1771:LEU:O	2:G:1777:THR:HG22	1.97	0.63
1:A:495:LYS:O	1:A:497:THR:HG23	1.98	0.63
1:A:1183:ARG:NH1	1:A:1349:THR:OG1	2.31	0.63
1:A:483:VAL:O	1:A:486:VAL:N	2.30	0.63
1:A:1309:VAL:O	1:A:1312:VAL:N	2.32	0.63
2:G:751:LEU:HD21	2:G:791:TYR:CZ	2.33	0.63
2:G:952:ARG:NH2	2:G:967:ILE:O	2.31	0.63
2:G:1086:LEU:HD23	2:G:1090:TYR:HB2	1.81	0.63
2:G:1243:ASN:N	2:G:1250:PRO:O	2.30	0.63
1:A:353:ASP:OD1	1:A:355:ASP:N	2.28	0.63
2:G:1159:ILE:HD12	2:G:1251:ILE:CG2	2.28	0.63
2:G:1443:VAL:O	2:G:1446:SER:OG	2.10	0.63
2:G:96:LEU:HD21	2:G:99:ASN:O	1.99	0.63
2:G:129:ALA:O	2:G:133:ALA:N	2.29	0.63
2:G:1731:GLU:O	2:G:1735:ALA:N	2.30	0.63
1:A:372:GLN:O	1:A:375:LEU:N	2.32	0.63
2:G:271:THR:HG22	2:G:272:GLY:H	1.64	0.63
2:G:1381:VAL:HG23	2:G:1381:VAL:O	1.99	0.62
1:A:529:MET:HE2	1:A:637:PHE:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1323:MET:HE3	2:G:1357:TYR:CD2	2.34	0.62
2:G:1342:THR:O	2:G:1421:ASN:ND2	2.31	0.62
2:G:1888:ILE:HD13	2:G:1900:ALA:HB2	1.79	0.62
1:A:1335:PHE:CE1	1:A:1378:GLU:CD	2.77	0.62
2:G:228:LYS:O	2:G:231:LEU:N	2.32	0.62
2:G:1893:VAL:HG23	2:G:1896:GLN:HB3	1.80	0.62
1:A:1026:GLU:OE1	1:A:1036:ARG:NH1	2.32	0.62
1:A:1590:ALA:O	1:A:1594:ASN:N	2.32	0.62
2:G:1320:LEU:H	2:G:1320:LEU:HD23	1.65	0.62
1:A:1475:GLU:OE1	1:A:1482:GLN:NE2	2.32	0.62
1:A:1377:MET:O	1:A:1583:HIS:N	2.30	0.62
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	1.81	0.62
1:A:1249:SER:OG	1:A:1250:GLY:N	2.30	0.62
1:A:1538:VAL:HG12	1:A:1539:ALA:N	2.15	0.62
2:G:72:VAL:HG12	2:G:73:GLU:N	2.15	0.62
1:A:17:LEU:CD2	2:G:2014:LEU:HD23	2.30	0.61
1:A:1047:LEU:H	1:A:1047:LEU:HD23	1.65	0.61
1:A:1558:ASN:O	1:A:1562:LYS:N	2.31	0.61
2:G:1350:LEU:HD13	2:G:1412:TYR:CD2	2.35	0.61
1:A:1360:ARG:CZ	1:A:1367:ARG:HE	2.13	0.61
2:G:834:GLN:OE1	2:G:837:LYS:NZ	2.20	0.61
2:G:1939:HIS:CE1	2:G:1943:ILE:HD11	2.35	0.61
1:A:845:SER:O	1:A:846:LEU:HD12	1.99	0.61
2:G:765:LEU:HD23	2:G:796:PHE:CD1	2.35	0.61
2:G:1100:VAL:HG13	2:G:1147:ILE:HG21	1.82	0.61
2:G:1378:ILE:HD13	2:G:1392:VAL:HG22	1.82	0.61
2:G:1246:ASN:OD1	2:G:1249:ALA:N	2.33	0.61
2:G:1714:PRO:O	2:G:1770:LEU:HD12	2.00	0.61
1:A:822:VAL:HG12	1:A:824:LEU:CD2	2.31	0.61
2:G:1679:ASP:OD1	2:G:1680:LEU:N	2.32	0.61
1:A:1354:GLU:OE2	1:A:1374:ASN:ND2	2.30	0.61
2:G:1267:TRP:O	2:G:1271:ILE:N	2.29	0.61
2:G:1300:PHE:O	2:G:1304:VAL:HG23	2.00	0.61
2:G:1442:ALA:O	2:G:1446:SER:N	2.29	0.61
2:G:1491:VAL:HG12	2:G:1501:ILE:HD11	1.83	0.61
1:A:1245:ASN:OD1	1:A:1247:SER:N	2.29	0.61
2:G:1153:SER:O	2:G:1168:ASN:ND2	2.32	0.61
2:G:1378:ILE:HD12	2:G:1391:ASP:O	2.01	0.61
2:G:437:ASP:OD1	2:G:438:LEU:N	2.33	0.61
2:G:1339:PHE:N	2:G:1340:PRO:HD2	2.15	0.61
2:G:1267:TRP:CZ3	2:G:1271:ILE:HG21	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1475:LYS:O	2:G:1476:ASN:ND2	2.34	0.61
1:A:1089:VAL:HG13	1:A:1090:LYS:N	2.16	0.60
2:G:251:VAL:O	2:G:255:LEU:HD13	2.01	0.60
2:G:742:SER:OG	2:G:744:GLU:OE1	2.19	0.60
1:A:409:ALA:HB1	1:A:447:LEU:HD11	1.84	0.60
1:A:439:ILE:O	1:A:442:ARG:N	2.33	0.60
2:G:887:LYS:O	2:G:891:ILE:HG23	2.02	0.60
1:A:750:GLU:OE1	1:A:750:GLU:N	2.32	0.60
1:A:213:PHE:O	1:A:217:PHE:N	2.32	0.60
2:G:1710:VAL:HA	2:G:1771:LEU:HD21	1.84	0.60
1:A:1107:GLU:OE1	1:A:1191:THR:OG1	2.11	0.60
1:A:1677:VAL:O	1:A:1680:ARG:N	2.34	0.60
2:G:13:HIS:CE1	2:G:60:LEU:HD21	2.37	0.60
2:G:902:PRO:O	2:G:1018:VAL:N	2.35	0.60
2:G:1011:MET:O	2:G:1012:GLN:NE2	2.35	0.60
1:A:337:VAL:O	1:A:341:GLN:N	2.35	0.60
2:G:429:SER:N	2:G:484:ILE:O	2.32	0.60
2:G:910:GLN:OE1	2:G:912:ARG:NH2	2.35	0.60
2:G:1363:ALA:O	2:G:1606:ARG:NH1	2.33	0.60
2:G:615:TYR:OH	2:G:1075:ASP:OD2	2.20	0.60
1:A:1624:VAL:O	1:A:1625:LEU:HD23	2.02	0.59
1:A:713:GLN:OE1	1:A:713:GLN:N	2.32	0.59
2:G:540:ASP:O	2:G:558:ASN:ND2	2.36	0.59
2:G:1045:ASP:OD1	2:G:1050:ARG:NH1	2.35	0.59
1:A:529:MET:HE2	1:A:637:PHE:HD2	1.67	0.59
2:G:278:VAL:HG21	2:G:303:LEU:HD21	1.82	0.59
2:G:678:PHE:HA	2:G:700:LEU:HD22	1.83	0.59
1:A:1533:ILE:HD11	1:A:1561:MET:SD	2.42	0.59
2:G:38:ASN:HA	2:G:41:LEU:HD21	1.85	0.59
2:G:1806:GLY:O	2:G:2013:ASN:ND2	2.33	0.59
1:A:483:VAL:O	1:A:486:VAL:HG12	2.02	0.59
1:A:1370:THR:HG22	1:A:1372:THR:H	1.67	0.59
2:G:175:ASP:OD1	2:G:176:LEU:N	2.36	0.59
2:G:1804:PHE:HD2	2:G:1814:ALA:HB1	1.68	0.59
1:A:451:MET:O	1:A:454:HIS:N	2.35	0.59
1:A:473:GLY:O	1:A:477:ILE:HG23	2.03	0.59
2:G:1034:LEU:HD12	2:G:1034:LEU:N	2.16	0.59
2:G:1828:VAL:HA	2:G:1831:VAL:HG12	1.85	0.59
2:G:1896:GLN:O	2:G:1896:GLN:NE2	2.35	0.59
2:G:1923:ASP:O	2:G:1926:GLU:HG3	2.03	0.59
2:G:2017:LYS:O	2:G:2025:TYR:OH	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:216:LEU:HD12	2:G:216:LEU:H	1.68	0.59
2:G:344:LEU:HD23	2:G:349:VAL:CG1	2.32	0.59
1:A:1245:ASN:OD1	1:A:1246:CYS:N	2.35	0.59
1:A:1391:ASP:OD1	1:A:1392:LEU:N	2.36	0.59
2:G:1351:VAL:HG21	2:G:1413:ARG:HH21	1.68	0.59
1:A:737:PHE:CZ	1:A:745:VAL:HG22	2.37	0.59
1:A:1335:PHE:CD1	1:A:1378:GLU:HG2	2.35	0.59
2:G:875:LEU:HD21	2:G:879:LYS:HB2	1.85	0.59
2:G:1130:THR:N	2:G:1133:THR:OG1	2.35	0.59
1:A:1343:PHE:HE2	1:A:1585:LYS:HZ2	1.35	0.59
2:G:20:LEU:HD12	2:G:90:GLU:OE1	2.03	0.58
2:G:115:THR:O	2:G:115:THR:HG23	2.03	0.58
2:G:1323:MET:HE1	2:G:1608:TYR:HB3	1.85	0.58
1:A:429:ASP:OD1	1:A:430:ARG:N	2.34	0.58
2:G:740:HIS:HA	2:G:854:ILE:HD13	1.83	0.58
1:A:390:VAL:HG23	1:A:740:GLY:O	2.03	0.58
1:A:824:LEU:HD12	1:A:846:LEU:HD23	1.84	0.58
2:G:284:ALA:HB3	2:G:455:ILE:HG22	1.86	0.58
2:G:568:LYS:C	2:G:569:LEU:HD22	2.29	0.58
2:G:946:PHE:CE1	2:G:1006:MET:HE2	2.38	0.58
2:G:1033:SER:C	2:G:1034:LEU:HD12	2.28	0.58
2:G:1167:SER:OG	2:G:1172:LYS:NZ	2.32	0.58
1:A:1012:LEU:O	1:A:1013:LEU:HD12	2.04	0.58
1:A:1445:MET:O	1:A:1448:ARG:N	2.36	0.58
2:G:1598:ALA:O	2:G:1601:VAL:HG12	2.02	0.58
2:G:1845:ASP:N	2:G:1849:ARG:O	2.36	0.58
2:G:9:LEU:HD23	2:G:9:LEU:C	2.29	0.58
2:G:56:THR:HG21	2:G:108:LEU:HD11	1.86	0.58
2:G:1730:ARG:NH2	2:G:1757:GLU:O	2.37	0.58
1:A:884:ILE:HD12	1:A:940:THR:HG23	1.86	0.58
2:G:1001:ASP:OD1	2:G:1001:ASP:N	2.37	0.58
2:G:1301:THR:HG23	2:G:1306:ASN:HB3	1.84	0.58
2:G:1956:ARG:NE	2:G:1956:ARG:O	2.36	0.58
1:A:768:ILE:HG22	1:A:770:PRO:HD3	1.85	0.58
1:A:71:ALA:O	1:A:72:LEU:HD23	2.04	0.58
1:A:468:LEU:O	1:A:472:LEU:HD23	2.03	0.58
2:G:626:SER:OG	2:G:627:ALA:N	2.34	0.58
2:G:20:LEU:HD12	2:G:90:GLU:CD	2.29	0.58
2:G:1277:LEU:HD12	2:G:1277:LEU:N	2.18	0.58
2:G:1756:ASN:OD1	2:G:1759:SER:N	2.37	0.58
1:A:1452:LEU:HD21	1:A:1505:GLN:OE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1501:LEU:O	1:A:1504:ALA:N	2.35	0.57
2:G:800:LEU:C	2:G:800:LEU:HD12	2.28	0.57
2:G:1224:ILE:O	2:G:1568:HIS:NE2	2.36	0.57
1:A:442:ARG:HD3	1:A:726:GLY:O	2.04	0.57
2:G:555:LEU:O	2:G:555:LEU:HD23	2.04	0.57
2:G:1041:GLU:OE1	2:G:1041:GLU:N	2.33	0.57
2:G:1350:LEU:HD13	2:G:1412:TYR:CE2	2.39	0.57
1:A:748:LEU:O	1:A:751:PHE:N	2.37	0.57
1:A:1095:THR:HG23	1:A:1096:SER:N	2.18	0.57
1:A:1019:ILE:HG22	1:A:1020:VAL:N	2.19	0.57
2:G:598:THR:HA	2:G:620:ALA:HB1	1.86	0.57
2:G:1152:ALA:O	2:G:1156:CYS:N	2.32	0.57
2:G:1448:GLU:OE1	2:G:1448:GLU:N	2.37	0.57
1:A:981:GLU:OE2	2:G:963:THR:N	2.37	0.57
2:G:96:LEU:HD23	2:G:97:GLU:N	2.20	0.57
2:G:212:GLY:O	2:G:230:TYR:OH	2.14	0.57
2:G:296:VAL:O	2:G:300:ILE:HG22	2.04	0.57
2:G:1435:ILE:HG21	2:G:1459:LEU:O	2.05	0.57
2:G:1874:VAL:HG23	2:G:1877:ARG:NH2	2.19	0.57
2:G:916:THR:O	2:G:916:THR:HG22	2.04	0.57
2:G:1386:THR:HG23	2:G:1411:PHE:HZ	1.70	0.57
2:G:1868:GLN:OE1	2:G:1895:ASN:N	2.38	0.57
1:A:491:LYS:NZ	1:A:616:LEU:O	2.38	0.57
2:G:983:VAL:O	2:G:986:ALA:N	2.38	0.57
2:G:1519:PHE:O	2:G:1523:ASN:ND2	2.37	0.57
1:A:333:LYS:O	1:A:337:VAL:HG13	2.04	0.57
1:A:662:GLY:O	1:A:666:ALA:N	2.36	0.57
1:A:1030:TRP:CH2	1:A:1039:MET:HE2	2.40	0.57
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.35	0.57
1:A:1340:SER:O	1:A:1343:PHE:N	2.38	0.57
2:G:1427:VAL:HG22	2:G:1469:GLU:HG2	1.87	0.57
2:G:1695:ASP:OD1	2:G:1706:ILE:HD12	2.03	0.57
2:G:2026:PHE:HB3	2:G:2038:ILE:HG23	1.87	0.57
2:G:239:PRO:HA	2:G:303:LEU:HD12	1.86	0.57
2:G:377:LEU:N	2:G:377:LEU:HD12	2.19	0.57
2:G:878:ASN:OD1	2:G:879:LYS:N	2.36	0.57
2:G:1666:PHE:CD1	2:G:1814:ALA:HB2	2.40	0.57
2:G:1824:ILE:HD12	2:G:1824:ILE:H	1.68	0.57
1:A:893:VAL:HG12	1:A:894:ARG:N	2.18	0.56
1:A:1333:ASP:OD2	1:A:1586:GLY:N	2.32	0.56
2:G:784:GLU:O	2:G:787:THR:OG1	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1366:LEU:HD23	2:G:1366:LEU:H	1.68	0.56
2:G:1985:VAL:O	2:G:1989:LYS:N	2.34	0.56
2:G:1906:ALA:O	2:G:1910:VAL:HG23	2.04	0.56
1:A:1559:GLU:O	1:A:1562:LYS:N	2.38	0.56
2:G:875:LEU:HD21	2:G:879:LYS:CB	2.35	0.56
2:G:1507:GLU:OE1	2:G:1507:GLU:N	2.38	0.56
2:G:1795:LYS:HB2	2:G:1797:LEU:HD13	1.86	0.56
1:A:737:PHE:HZ	1:A:745:VAL:HG22	1.69	0.56
1:A:755:THR:O	1:A:760:GLY:N	2.35	0.56
1:A:1106:ILE:HD12	1:A:1184:LEU:C	2.30	0.56
2:G:1540:ALA:HB1	2:G:1542:LEU:HD21	1.87	0.56
1:A:13:LEU:HD22	2:G:2026:PHE:CE1	2.40	0.56
1:A:807:LYS:O	1:A:810:LYS:N	2.36	0.56
2:G:1893:VAL:HG22	2:G:1897:GLN:HB2	1.87	0.56
1:A:1426:LEU:O	1:A:1426:LEU:HD23	2.06	0.56
1:A:1544:THR:O	1:A:1545:SER:HB3	2.06	0.56
2:G:830:ASP:OD1	2:G:831:LYS:N	2.39	0.56
1:A:1474:ALA:O	1:A:1482:GLN:NE2	2.35	0.56
2:G:234:ILE:HG21	2:G:425:SER:OG	2.06	0.56
2:G:1862:VAL:O	2:G:1921:LYS:NZ	2.39	0.56
2:G:2030:TYR:HB2	2:G:2038:ILE:HG21	1.88	0.55
1:A:30:GLU:HB2	2:G:2016:ALA:CB	2.36	0.55
1:A:1264:ARG:NH2	1:A:1271:GLN:O	2.40	0.55
1:A:1556:THR:HG23	1:A:1557:ILE:N	2.21	0.55
2:G:436:SER:O	2:G:440:ASN:ND2	2.40	0.55
2:G:1094:GLU:O	2:G:1097:ILE:HG22	2.06	0.55
2:G:1123:ASP:OD1	2:G:1124:SER:N	2.40	0.55
2:G:1550:ASN:ND2	2:G:1564:HIS:O	2.35	0.55
2:G:1850:SER:OG	2:G:1851:ASN:N	2.37	0.55
2:G:470:VAL:HG23	2:G:470:VAL:O	2.07	0.55
2:G:975:LYS:NZ	2:G:978:GLU:OE1	2.27	0.55
2:G:1428:GLU:OE2	2:G:1470:THR:OG1	2.16	0.55
2:G:1677:GLY:O	2:G:1680:LEU:N	2.37	0.55
1:A:492:ASP:OD2	1:A:493:VAL:N	2.39	0.55
1:A:519:VAL:HG13	1:A:519:VAL:O	2.07	0.55
1:A:1703:HIS:O	1:A:1703:HIS:ND1	2.39	0.55
2:G:1159:ILE:HD12	2:G:1251:ILE:HG22	1.88	0.55
1:A:433:VAL:HG21	1:A:493:VAL:HG11	1.88	0.55
1:A:1219:VAL:HA	1:A:1384:ILE:HD11	1.88	0.55
1:A:1523:ARG:NH1	1:A:1564:LEU:O	2.40	0.55
2:G:142:ASN:OD1	2:G:147:ARG:NE	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:745:ASP:OD1	2:G:746:ALA:N	2.39	0.55
2:G:751:LEU:HD21	2:G:791:TYR:CE2	2.41	0.55
2:G:890:TYR:O	2:G:893:SER:OG	2.21	0.55
2:G:1430:VAL:HG13	2:G:1527:LEU:HB3	1.88	0.55
1:A:1479:SER:OG	1:A:1480:GLU:N	2.39	0.55
1:A:824:LEU:HD12	1:A:846:LEU:CD2	2.37	0.55
1:A:14:LEU:C	1:A:14:LEU:HD23	2.32	0.54
2:G:1384:GLN:NE2	2:G:1389:ILE:HD12	2.22	0.54
2:G:1738:PHE:N	2:G:1749:GLU:O	2.29	0.54
1:A:34:VAL:HG13	1:A:35:PHE:N	2.22	0.54
1:A:908:LEU:O	1:A:908:LEU:HD23	2.07	0.54
2:G:602:VAL:HG23	2:G:624:TYR:CE1	2.41	0.54
2:G:695:ILE:HD11	2:G:723:HIS:CG	2.42	0.54
1:A:1559:GLU:O	1:A:1563:HIS:N	2.39	0.54
2:G:195:LEU:CD2	2:G:213:LEU:HD21	2.37	0.54
2:G:627:ALA:O	2:G:631:THR:OG1	2.25	0.54
2:G:1350:LEU:HD12	2:G:1351:VAL:N	2.23	0.54
1:A:509:ILE:HG23	1:A:509:ILE:O	2.07	0.54
1:A:1655:VAL:HG12	1:A:1656:VAL:N	2.22	0.54
1:A:770:PRO:HB2	1:A:799:ILE:HD11	1.88	0.54
1:A:949:GLU:O	1:A:953:VAL:HG13	2.08	0.54
2:G:1546:THR:OG1	2:G:1620:THR:N	2.38	0.54
2:G:1324:ASP:O	2:G:1327:ILE:HG22	2.07	0.54
2:G:215:ILE:HD12	2:G:240:LEU:HD21	1.89	0.54
2:G:593:LEU:N	2:G:593:LEU:HD23	2.22	0.54
2:G:710:ILE:HD11	2:G:752:GLN:NE2	2.22	0.54
2:G:271:THR:HG22	2:G:272:GLY:N	2.22	0.54
2:G:1440:ASP:OD1	2:G:1441:ILE:HG23	2.08	0.54
2:G:1854:MET:HB3	2:G:1901:ALA:HB2	1.90	0.54
1:A:71:ALA:C	1:A:72:LEU:HD23	2.32	0.54
1:A:1144:PHE:O	1:A:1148:HIS:N	2.30	0.54
2:G:236:ILE:O	2:G:240:LEU:HD13	2.08	0.54
2:G:662:GLY:O	2:G:666:ILE:N	2.27	0.54
2:G:1263:LYS:HG2	2:G:1347:LEU:HD11	1.90	0.54
2:G:1693:ARG:HD2	2:G:1824:ILE:HD13	1.90	0.54
2:G:1778:GLN:HA	2:G:1809:LEU:HD11	1.89	0.54
2:G:1923:ASP:O	2:G:1926:GLU:N	2.40	0.54
1:A:1719:LEU:HD12	1:A:1744:TYR:HA	1.89	0.54
1:A:1725:ASP:O	1:A:1729:GLY:N	2.30	0.54
1:A:1019:ILE:HG22	1:A:1020:VAL:H	1.73	0.53
2:G:115:THR:HG21	2:G:118:LYS:HZ3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1351:VAL:HG21	2:G:1413:ARG:NH2	2.23	0.53
2:G:1458:ASP:C	2:G:1459:LEU:HD12	2.34	0.53
2:G:1737:ILE:HG21	2:G:1748:THR:HG23	1.90	0.53
2:G:2030:TYR:CB	2:G:2038:ILE:HG21	2.38	0.53
1:A:44:VAL:HG12	2:G:1663:THR:HB	1.90	0.53
1:A:732:LEU:C	1:A:733:ILE:HD12	2.34	0.53
1:A:960:GLU:OE2	1:A:961:THR:HG23	2.08	0.53
1:A:1020:VAL:CG2	1:A:1400:ILE:HG23	2.39	0.53
1:A:1021:VAL:HG22	1:A:1387:ILE:HG22	1.89	0.53
1:A:1355:GLU:OE2	1:A:1360:ARG:NH1	2.41	0.53
1:A:492:ASP:OD2	1:A:494:ALA:N	2.34	0.53
1:A:1476:GLU:OE2	1:A:1476:GLU:N	2.40	0.53
2:G:1213:LEU:O	2:G:1214:LEU:HD22	2.08	0.53
1:A:707:THR:O	1:A:737:PHE:N	2.41	0.53
1:A:904:ASN:HB3	1:A:926:LEU:HD13	1.91	0.53
1:A:1456:GLU:O	1:A:1460:LYS:N	2.41	0.53
1:A:1584:PRO:HG3	1:A:1591:TRP:CE3	2.43	0.53
2:G:529:VAL:HG11	2:G:532:THR:OG1	2.07	0.53
2:G:1384:GLN:N	2:G:1384:GLN:OE1	2.41	0.53
1:A:459:ASP:OD1	1:A:461:THR:HG22	2.08	0.53
1:A:1132:GLU:N	1:A:1133:PRO:HD3	2.24	0.53
2:G:43:GLU:O	2:G:45:THR:HG23	2.08	0.53
2:G:117:VAL:HG23	2:G:118:LYS:N	2.24	0.53
2:G:607:VAL:HG23	2:G:617:ILE:HG21	1.90	0.53
1:A:1600:LEU:HD11	1:A:1655:VAL:CG1	2.39	0.53
2:G:787:THR:O	2:G:790:ASP:N	2.36	0.53
2:G:1388:LYS:NZ	2:G:1418:ASP:OD2	2.42	0.53
2:G:1924:ILE:HA	2:G:1927:LEU:HD12	1.89	0.53
1:A:1185:VAL:HG23	1:A:1377:MET:HE1	1.88	0.53
2:G:1032:ASP:O	2:G:1036:GLN:NE2	2.39	0.53
1:A:1625:LEU:C	1:A:1626:TYR:CD2	2.87	0.53
2:G:709:SER:OG	2:G:710:ILE:N	2.42	0.53
1:A:1029:PRO:HA	1:A:1189:ILE:HA	1.91	0.53
2:G:237:SER:O	2:G:240:LEU:N	2.41	0.53
2:G:621:GLY:HA3	2:G:658:MET:HE1	1.91	0.53
2:G:2032:LEU:HD12	2:G:2033:THR:N	2.24	0.53
1:A:403:ASP:OD1	1:A:1613:ASN:ND2	2.38	0.53
1:A:658:LEU:C	1:A:658:LEU:HD12	2.33	0.53
1:A:1119:LYS:N	1:A:1178:ALA:O	2.41	0.52
2:G:1741:ILE:HD11	2:G:1985:VAL:HG22	1.90	0.52
1:A:1019:ILE:HG13	1:A:1316:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:PRO:HA	1:A:1213:LEU:HD23	1.91	0.52
1:A:1227:GLY:O	1:A:1680:ARG:NH2	2.42	0.52
1:A:1008:GLU:OE1	1:A:1008:GLU:N	2.37	0.52
1:A:1115:ASN:O	1:A:1118:LYS:N	2.41	0.52
2:G:355:LYS:O	2:G:358:SER:OG	2.17	0.52
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.91	0.52
2:G:735:GLY:O	2:G:741:HIS:ND1	2.37	0.52
2:G:1149:TRP:NE1	2:G:1213:LEU:HD11	2.23	0.52
1:A:332:THR:O	1:A:335:HIS:N	2.42	0.52
1:A:1533:ILE:HD11	1:A:1561:MET:HE1	1.91	0.52
1:A:1630:THR:HG22	1:A:1631:LEU:N	2.24	0.52
2:G:45:THR:O	2:G:48:PHE:N	2.42	0.52
2:G:64:PHE:O	2:G:68:VAL:HG12	2.10	0.52
2:G:2037:PRO:O	2:G:2041:ILE:HD12	2.09	0.52
2:G:96:LEU:HD23	2:G:98:GLY:N	2.24	0.52
2:G:409:PHE:N	2:G:833:GLU:OE2	2.39	0.52
2:G:601:THR:OG1	2:G:620:ALA:HB2	2.09	0.52
2:G:770:GLY:HA2	2:G:1058:VAL:HG13	1.92	0.52
2:G:1225:GLU:OE2	2:G:1227:ARG:N	2.42	0.52
2:G:1593:ILE:O	2:G:1596:TRP:N	2.39	0.52
2:G:194:THR:O	2:G:198:LEU:HD23	2.10	0.52
2:G:222:PRO:HA	2:G:225:THR:HG23	1.92	0.52
2:G:649:ILE:CD1	2:G:666:ILE:HD11	2.39	0.52
2:G:1906:ALA:O	2:G:1909:THR:OG1	2.24	0.52
1:A:904:ASN:CB	1:A:926:LEU:HD13	2.40	0.52
1:A:1639:VAL:HG12	1:A:1640:SER:N	2.24	0.52
2:G:1924:ILE:O	2:G:1928:GLN:NE2	2.42	0.52
1:A:791:ALA:O	1:A:794:ILE:N	2.42	0.52
1:A:823:ILE:HD12	1:A:908:LEU:CD2	2.40	0.52
1:A:1089:VAL:HG13	1:A:1090:LYS:H	1.75	0.52
1:A:1185:VAL:HG23	1:A:1377:MET:CE	2.40	0.52
1:A:1316:VAL:O	1:A:1319:ILE:N	2.38	0.52
1:A:1480:GLU:N	1:A:1480:GLU:OE1	2.43	0.52
2:G:21:LEU:C	2:G:21:LEU:HD23	2.35	0.52
2:G:272:GLY:H	2:G:277:LEU:HD12	1.74	0.52
2:G:879:LYS:O	2:G:883:THR:HG22	2.10	0.52
1:A:1035:THR:HG23	1:A:1036:ARG:N	2.25	0.52
2:G:774:ALA:HB1	2:G:1081:HIS:HD2	1.74	0.52
2:G:1149:TRP:CD1	2:G:1213:LEU:HD11	2.45	0.52
2:G:1827:LEU:O	2:G:1830:VAL:HG22	2.10	0.52
1:A:31:THR:HA	1:A:34:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:O	1:A:368:VAL:HG23	2.09	0.51
1:A:823:ILE:HD12	1:A:908:LEU:HD22	1.91	0.51
1:A:1077:ASP:OD2	1:A:1080:THR:N	2.38	0.51
2:G:59:GLU:N	2:G:59:GLU:OE1	2.42	0.51
2:G:116:LEU:HA	2:G:119:THR:HG22	1.92	0.51
2:G:359:HIS:C	2:G:360:LEU:HD12	2.34	0.51
2:G:1459:LEU:HD12	2:G:1459:LEU:N	2.25	0.51
2:G:1855:ILE:HD12	2:G:1968:PRO:HA	1.92	0.51
1:A:331:ILE:HG23	1:A:332:THR:HG23	1.92	0.51
2:G:766:ILE:HG23	2:G:798:GLY:C	2.35	0.51
2:G:1316:ASP:OD1	2:G:1316:ASP:C	2.53	0.51
1:A:420:ILE:HG21	1:A:469:VAL:HG13	1.92	0.51
1:A:1335:PHE:HE1	1:A:1378:GLU:CD	2.19	0.51
1:A:1648:GLN:O	1:A:1650:GLY:N	2.43	0.51
2:G:1796:GLY:C	2:G:1797:LEU:HD12	2.35	0.51
1:A:400:ARG:HE	1:A:710:PHE:HZ	1.58	0.51
1:A:1370:THR:O	1:A:1373:ARG:NE	2.44	0.51
1:A:1376:PHE:HB3	1:A:1544:THR:O	2.11	0.51
1:A:1062:TYR:CG	1:A:1693:ILE:HG23	2.45	0.51
1:A:1418:VAL:N	1:A:1419:PRO:HD3	2.26	0.51
2:G:218:TRP:HB3	2:G:225:THR:HG22	1.93	0.51
2:G:310:CYS:O	2:G:313:ALA:N	2.43	0.51
1:A:410:LYS:HB3	1:A:450:PHE:CE2	2.45	0.51
1:A:988:ILE:HG22	1:A:989:GLN:N	2.25	0.51
1:A:1445:MET:HE3	1:A:1530:GLY:N	2.26	0.51
1:A:1528:THR:HG23	1:A:1529:TYR:CD2	2.45	0.51
2:G:61:VAL:O	2:G:65:LEU:HD23	2.10	0.51
2:G:1530:LYS:HG3	2:G:1632:ILE:HD11	1.93	0.51
2:G:1737:ILE:C	2:G:1751:ILE:HD11	2.35	0.51
2:G:1739:GLU:HB2	2:G:1987:PRO:HB3	1.91	0.51
2:G:1997:ILE:HG22	2:G:1999:GLU:H	1.75	0.51
1:A:433:VAL:HG23	1:A:434:SER:N	2.25	0.51
1:A:893:VAL:HG11	1:A:930:LEU:HD21	1.92	0.51
1:A:1423:LYS:O	1:A:1425:ILE:N	2.44	0.51
2:G:984:PHE:O	2:G:991:ARG:NE	2.44	0.51
1:A:420:ILE:HD13	1:A:469:VAL:HG12	1.93	0.51
1:A:1075:TRP:C	1:A:1076:VAL:HG23	2.36	0.51
1:A:1424:GLY:O	1:A:1427:THR:HG22	2.10	0.51
2:G:410:SER:OG	2:G:411:GLU:OE2	2.28	0.51
2:G:1666:PHE:HD1	2:G:1814:ALA:HB2	1.74	0.51
2:G:1762:TYR:CD2	2:G:1763:THR:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1636:VAL:HG12	1:A:1637:ARG:N	2.24	0.51
2:G:847:ARG:NH2	2:G:869:ASP:O	2.44	0.51
2:G:1607:GLY:O	2:G:1656:GLU:N	2.41	0.51
2:G:1741:ILE:HD12	2:G:1982:MET:O	2.11	0.51
1:A:400:ARG:HH12	1:A:1367:ARG:NH2	2.09	0.51
1:A:1542:HIS:O	1:A:1578:LYS:NZ	2.37	0.51
2:G:740:HIS:CE1	2:G:854:ILE:HD11	2.46	0.51
2:G:1737:ILE:O	2:G:1833:TYR:OH	2.25	0.51
2:G:611:THR:HB	2:G:617:ILE:HD12	1.92	0.50
2:G:1199:GLU:OE2	2:G:1567:ARG:NH2	2.45	0.50
2:G:1576:PRO:HB2	2:G:1617:LEU:HD21	1.91	0.50
1:A:842:SER:O	1:A:846:LEU:HD13	2.11	0.50
1:A:1501:LEU:HD23	1:A:1501:LEU:C	2.36	0.50
2:G:84:LEU:HD23	2:G:133:ALA:HA	1.92	0.50
2:G:192:ALA:CB	2:G:216:LEU:HD11	2.41	0.50
2:G:389:LEU:HA	2:G:392:THR:HG22	1.94	0.50
2:G:485:ARG:NH1	2:G:486:LEU:HD21	2.26	0.50
2:G:1539:ILE:HD11	2:G:1628:HIS:HB2	1.92	0.50
2:G:1973:SER:O	2:G:1973:SER:OG	2.29	0.50
2:G:123:ILE:HD12	2:G:123:ILE:H	1.76	0.50
2:G:1022:ASP:OD2	2:G:1024:ARG:NH2	2.43	0.50
1:A:873:ARG:NH2	1:A:895:THR:O	2.38	0.50
1:A:1095:THR:HG23	1:A:1096:SER:H	1.76	0.50
1:A:1352:THR:HG23	1:A:1365:MET:HE1	1.93	0.50
1:A:1431:GLU:HA	1:A:1517:PRO:O	2.10	0.50
2:G:86:LEU:HD23	2:G:87:CYS:N	2.27	0.50
2:G:148:ALA:O	2:G:153:ASN:N	2.45	0.50
2:G:996:ASN:OD1	2:G:996:ASN:C	2.54	0.50
2:G:1884:TRP:HB2	2:G:1906:ALA:HB2	1.92	0.50
1:A:1403:ILE:HG22	1:A:1404:VAL:N	2.25	0.50
2:G:56:THR:OG1	2:G:59:GLU:OE1	2.28	0.50
1:A:80:CYS:N	1:A:84:ASP:OD2	2.41	0.50
2:G:1101:GLU:HB3	2:G:1147:ILE:HG22	1.93	0.50
2:G:1543:ASP:OD1	2:G:1544:SER:N	2.45	0.50
1:A:464:GLU:OE2	1:A:465:ASN:ND2	2.45	0.50
1:A:1600:LEU:HD11	1:A:1655:VAL:HG12	1.93	0.50
2:G:811:VAL:HG22	2:G:812:LYS:H	1.77	0.50
2:G:997:ALA:O	2:G:1000:ILE:N	2.39	0.50
2:G:1569:PHE:O	2:G:1572:TYR:N	2.44	0.50
2:G:1822:MET:HE3	2:G:1827:LEU:HD13	1.93	0.50
1:A:608:ASP:OD2	1:A:611:LYS:NZ	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:LEU:HD12	1:A:1184:LEU:C	2.36	0.50
2:G:195:LEU:HD13	2:G:300:ILE:HD11	1.93	0.50
2:G:253:ALA:O	2:G:258:PHE:N	2.45	0.50
2:G:525:VAL:C	2:G:526:ARG:HD3	2.37	0.50
2:G:174:ARG:NH2	2:G:219:LEU:HA	2.27	0.50
2:G:806:MET:HE1	2:G:1054:LEU:O	2.12	0.50
2:G:1044:VAL:HG23	2:G:1045:ASP:N	2.27	0.50
2:G:1270:TRP:CB	2:G:1271:ILE:HD12	2.42	0.50
2:G:1539:ILE:HD12	2:G:1539:ILE:N	2.27	0.50
1:A:779:ILE:N	1:A:779:ILE:HD12	2.27	0.49
1:A:1455:ARG:O	1:A:1459:ILE:N	2.37	0.49
2:G:159:ILE:HD11	2:G:490:TRP:CH2	2.47	0.49
2:G:1456:ASP:OD1	2:G:1457:PHE:N	2.44	0.49
2:G:1741:ILE:HB	2:G:1983:ASN:HA	1.94	0.49
2:G:1889:VAL:O	2:G:1890:ASN:ND2	2.43	0.49
1:A:1425:ILE:HD11	1:A:1651:GLY:N	2.27	0.49
2:G:1297:VAL:HG21	2:G:1319:MET:HE2	1.93	0.49
1:A:933:VAL:HG13	1:A:933:VAL:O	2.10	0.49
1:A:660:LEU:N	1:A:660:LEU:CD1	2.76	0.49
1:A:697:LEU:HD12	1:A:721:ILE:HG22	1.94	0.49
1:A:745:VAL:C	1:A:747:ALA:H	2.20	0.49
1:A:905:LEU:HD12	1:A:905:LEU:N	2.24	0.49
1:A:1329:VAL:HG22	1:A:1385:GLN:O	2.12	0.49
2:G:18:HIS:ND1	2:G:95:TYR:OH	2.32	0.49
2:G:230:TYR:O	2:G:236:ILE:HD13	2.12	0.49
1:A:1012:LEU:C	1:A:1013:LEU:HD12	2.38	0.49
1:A:1245:ASN:OD1	1:A:1245:ASN:C	2.56	0.49
1:A:1403:ILE:CG2	1:A:1404:VAL:N	2.75	0.49
1:A:1555:ALA:O	1:A:1558:ASN:N	2.44	0.49
1:A:1624:VAL:C	1:A:1625:LEU:HD23	2.38	0.49
1:A:1714:VAL:HG13	1:A:1720:ALA:CB	2.42	0.49
2:G:72:VAL:HG12	2:G:73:GLU:H	1.76	0.49
2:G:326:ASP:OD2	2:G:387:TYR:OH	2.26	0.49
2:G:992:GLU:N	2:G:992:GLU:OE1	2.45	0.49
2:G:1739:GLU:HA	2:G:1747:LYS:O	2.12	0.49
1:A:44:VAL:CG2	1:A:78:ILE:HG22	2.43	0.49
1:A:178:GLY:O	1:A:180:SER:N	2.45	0.49
1:A:1658:PRO:O	1:A:1661:LEU:N	2.42	0.49
2:G:174:ARG:O	2:G:178:GLN:N	2.44	0.49
2:G:330:ASN:HB3	2:G:394:ARG:CZ	2.42	0.49
2:G:672:LYS:HZ3	2:G:1164:MET:CG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1013:LYS:NZ	2:G:1032:ASP:OD2	2.29	0.49
2:G:1173:VAL:HG13	2:G:1174:PHE:N	2.26	0.49
2:G:1838:MET:HE3	2:G:1976:PHE:CD1	2.47	0.49
2:G:1954:LYS:HE3	2:G:1958:LEU:HD11	1.95	0.49
1:A:393:SER:O	1:A:736:PRO:HB2	2.13	0.49
1:A:873:ARG:O	1:A:898:GLN:NE2	2.46	0.49
2:G:926:LEU:HD21	2:G:946:PHE:HE2	1.78	0.49
2:G:976:PRO:O	2:G:979:ALA:N	2.46	0.49
2:G:1632:ILE:O	2:G:1635:ARG:HG2	2.11	0.49
2:G:1878:VAL:HG22	2:G:1944:ILE:CG1	2.42	0.49
2:G:2015:THR:OG1	2:G:2029:VAL:HG12	2.13	0.49
1:A:625:THR:HG22	1:A:627:SER:H	1.78	0.49
2:G:294:VAL:HG13	2:G:295:SER:N	2.28	0.49
2:G:1551:GLU:N	2:G:1552:PRO:CD	2.76	0.49
2:G:1566:SER:O	2:G:1578:THR:HG22	2.11	0.49
1:A:346:LEU:O	1:A:349:TYR:N	2.44	0.49
1:A:1570:ASN:N	1:A:1571:PRO:HD3	2.28	0.49
2:G:1741:ILE:HD12	2:G:1983:ASN:CA	2.41	0.49
1:A:484:LEU:HD23	1:A:485:ASP:N	2.27	0.49
1:A:1238:VAL:HG22	1:A:1239:HIS:N	2.28	0.49
2:G:197:GLU:O	2:G:201:THR:HG22	2.12	0.49
2:G:394:ARG:HA	2:G:397:LYS:HG2	1.94	0.49
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.48	0.49
1:A:1320:LEU:HD23	1:A:1320:LEU:H	1.78	0.48
1:A:1656:VAL:HG12	1:A:1657:HIS:N	2.28	0.48
2:G:156:LEU:HD23	2:G:500:HIS:HB2	1.95	0.48
2:G:665:LEU:HD21	2:G:669:LEU:HD11	1.94	0.48
2:G:1350:LEU:HD11	2:G:1410:PHE:HB3	1.95	0.48
2:G:1770:LEU:HD12	2:G:1770:LEU:H	1.78	0.48
2:G:1985:VAL:HG23	2:G:1986:LYS:N	2.28	0.48
1:A:15:THR:HG21	2:G:1993:LYS:NZ	2.28	0.48
1:A:605:LEU:HD23	1:A:612:GLU:OE2	2.13	0.48
1:A:1376:PHE:CB	1:A:1544:THR:O	2.62	0.48
2:G:55:THR:HG23	2:G:56:THR:HG23	1.95	0.48
2:G:126:TYR:C	2:G:126:TYR:CD2	2.91	0.48
2:G:1321:ALA:HB1	2:G:1322:PRO:HD2	1.95	0.48
2:G:1395:THR:C	2:G:1396:LEU:HD12	2.38	0.48
1:A:402:PHE:HB2	1:A:732:LEU:CD2	2.43	0.48
1:A:697:LEU:HB3	1:A:726:GLY:HA2	1.96	0.48
1:A:850:PHE:CD1	1:A:921:PRO:HB2	2.48	0.48
1:A:998:TYR:OH	1:A:1665:ILE:O	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:LEU:HD12	1:A:1110:LEU:N	2.28	0.48
1:A:1581:THR:OG1	1:A:1582:GLY:N	2.45	0.48
2:G:72:VAL:C	2:G:132:MET:HE2	2.38	0.48
2:G:86:LEU:HD23	2:G:86:LEU:C	2.38	0.48
2:G:270:ALA:O	2:G:459:VAL:HA	2.14	0.48
2:G:844:VAL:CG1	2:G:845:THR:N	2.76	0.48
1:A:660:LEU:HA	1:A:663:LEU:HG	1.95	0.48
1:A:663:LEU:O	1:A:666:ALA:N	2.46	0.48
1:A:1548:ALA:O	1:A:1551:LYS:N	2.47	0.48
2:G:1854:MET:HG3	2:G:1969:LEU:HD12	1.94	0.48
1:A:507:GLY:HA3	1:A:955:LYS:HZ2	1.79	0.48
1:A:822:VAL:N	1:A:863:THR:O	2.43	0.48
1:A:1584:PRO:O	1:A:1586:GLY:N	2.47	0.48
2:G:1484:LYS:HZ3	2:G:1507:GLU:HB3	1.79	0.48
2:G:1646:ASP:OD1	2:G:1648:VAL:HG12	2.14	0.48
2:G:1828:VAL:O	2:G:1831:VAL:HG12	2.14	0.48
2:G:1884:TRP:CB	2:G:1906:ALA:HB2	2.43	0.48
1:A:436:ALA:HA	1:A:439:ILE:HD12	1.96	0.48
1:A:1137:SER:O	1:A:1138:LYS:HB3	2.14	0.48
1:A:1208:VAL:CG1	1:A:1209:ASP:N	2.76	0.48
2:G:278:VAL:O	2:G:281:VAL:HG12	2.12	0.48
2:G:927:VAL:HG13	2:G:928:GLU:N	2.28	0.48
2:G:1167:SER:CB	2:G:1172:LYS:HZ2	2.26	0.48
2:G:1877:ARG:CZ	2:G:1944:ILE:HD13	2.44	0.48
1:A:1615:ASP:OD2	1:A:1617:ILE:HG22	2.14	0.48
2:G:610:THR:HB	2:G:617:ILE:HD11	1.95	0.48
2:G:1069:PRO:O	2:G:1072:SER:OG	2.27	0.48
2:G:1739:GLU:OE1	2:G:1739:GLU:N	2.41	0.48
1:A:31:THR:HG22	2:G:2011:ILE:CG2	2.44	0.48
1:A:1463:VAL:HG23	1:A:1464:GLU:N	2.27	0.48
2:G:234:ILE:HG12	2:G:235:PRO:HD3	1.95	0.48
2:G:234:ILE:N	2:G:235:PRO:CD	2.77	0.48
2:G:278:VAL:HG23	2:G:279:THR:N	2.29	0.48
2:G:1267:TRP:HA	2:G:1271:ILE:HD13	1.94	0.48
2:G:1459:LEU:O	2:G:1460:LEU:HD22	2.14	0.48
2:G:1830:VAL:HG12	2:G:1991:PHE:CE2	2.49	0.48
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.28	0.48
1:A:753:TYR:CE1	1:A:764:ASP:HA	2.48	0.48
1:A:851:ASN:OD1	1:A:851:ASN:O	2.32	0.48
1:A:1548:ALA:O	1:A:1552:ASN:N	2.42	0.48
1:A:1707:THR:O	1:A:1710:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:423:VAL:HG12	2:G:424:ALA:H	1.79	0.48
2:G:619:LEU:H	2:G:649:ILE:HA	1.78	0.48
2:G:857:ILE:HD12	2:G:1053:ILE:HG13	1.96	0.48
2:G:953:ARG:HE	2:G:1002:HIS:CE1	2.32	0.48
2:G:1227:ARG:NE	2:G:1551:GLU:OE2	2.47	0.48
2:G:1691:TRP:CZ3	2:G:1783:LEU:HD12	2.49	0.48
1:A:31:THR:HG22	2:G:2011:ILE:HG21	1.95	0.47
1:A:823:ILE:HD13	1:A:865:CYS:HB2	1.95	0.47
1:A:878:MET:O	1:A:881:ASN:N	2.44	0.47
1:A:963:LEU:HD23	2:G:1522:ARG:NH2	2.28	0.47
1:A:1234:MET:O	1:A:1238:VAL:HG12	2.14	0.47
2:G:490:TRP:O	2:G:494:THR:OG1	2.17	0.47
2:G:894:ARG:O	2:G:897:ALA:N	2.45	0.47
2:G:1491:VAL:CG1	2:G:1501:ILE:HD11	2.43	0.47
2:G:2041:ILE:HG23	2:G:2047:LYS:HZ1	1.79	0.47
2:G:569:LEU:HD21	2:G:1085:LEU:HD13	1.95	0.47
2:G:2023:LYS:HD2	2:G:2045:TRP:CD2	2.48	0.47
1:A:773:ALA:HB1	1:A:795:MET:HE2	1.96	0.47
2:G:670:ARG:O	2:G:673:GLY:N	2.47	0.47
2:G:857:ILE:HD12	2:G:1053:ILE:CG1	2.44	0.47
2:G:980:ILE:HG13	2:G:981:GLU:N	2.28	0.47
2:G:1710:VAL:HG23	2:G:1711:ILE:N	2.29	0.47
1:A:395:SER:OG	1:A:398:LYS:HG3	2.14	0.47
1:A:871:TRP:HB3	1:A:895:THR:HG22	1.96	0.47
2:G:115:THR:HG21	2:G:118:LYS:NZ	2.29	0.47
2:G:336:SER:OG	2:G:423:VAL:O	2.32	0.47
2:G:922:VAL:HG11	2:G:950:PHE:CZ	2.49	0.47
2:G:1714:PRO:O	2:G:1769:GLY:HA2	2.14	0.47
2:G:615:TYR:CE2	2:G:1074:MET:HB3	2.49	0.47
2:G:690:VAL:HG22	2:G:694:TYR:CE2	2.45	0.47
2:G:1201:VAL:HG13	2:G:1204:GLU:HG3	1.97	0.47
2:G:2021:VAL:O	2:G:2021:VAL:HG23	2.14	0.47
1:A:15:THR:HG21	2:G:1993:LYS:HZ3	1.78	0.47
1:A:753:TYR:O	1:A:813:ARG:NH2	2.47	0.47
2:G:807:ILE:HD13	2:G:1065:VAL:O	2.14	0.47
1:A:471:THR:CG2	1:A:472:LEU:N	2.78	0.47
1:A:521:LYS:HG2	1:A:522:LEU:H	1.80	0.47
1:A:1132:GLU:N	1:A:1133:PRO:CD	2.78	0.47
1:A:1335:PHE:CD1	1:A:1378:GLU:CD	2.92	0.47
1:A:1590:ALA:O	1:A:1593:MET:N	2.47	0.47
2:G:586:LEU:HD21	2:G:1107:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:595:PRO:O	2:G:601:THR:HG21	2.14	0.47
2:G:1201:VAL:HG13	2:G:1201:VAL:O	2.15	0.47
2:G:1715:VAL:HG23	2:G:1766:SER:O	2.14	0.47
2:G:1887:GLU:O	2:G:1889:VAL:HG13	2.15	0.47
2:G:1988:PHE:O	2:G:1992:LEU:HD23	2.15	0.47
1:A:79:LEU:HD21	1:A:87:GLU:CB	2.44	0.47
1:A:402:PHE:HB2	1:A:732:LEU:HD23	1.95	0.47
1:A:501:THR:N	1:A:886:GLU:OE1	2.39	0.47
1:A:971:ASN:O	1:A:975:ALA:N	2.46	0.47
1:A:1001:VAL:HG23	1:A:1002:LYS:N	2.30	0.47
1:A:1067:LEU:HB3	1:A:1072:TYR:CD2	2.49	0.47
1:A:1185:VAL:CG2	1:A:1377:MET:SD	3.03	0.47
1:A:1211:ILE:HD11	1:A:1332:TYR:HD2	1.80	0.47
1:A:1220:VAL:O	1:A:1224:ILE:HG12	2.14	0.47
2:G:96:LEU:HD23	2:G:98:GLY:H	1.80	0.47
2:G:1228:THR:HG22	2:G:1229:MET:N	2.29	0.47
2:G:1447:LYS:HB3	2:G:1450:PHE:HB3	1.97	0.47
2:G:1709:ILE:HG22	2:G:1771:LEU:HD11	1.97	0.47
1:A:486:VAL:HG22	1:A:487:ASP:H	1.80	0.47
1:A:522:LEU:N	1:A:522:LEU:HD22	2.29	0.47
1:A:803:MET:C	1:A:805:CYS:H	2.23	0.47
1:A:953:VAL:HG23	1:A:954:ARG:N	2.29	0.47
1:A:1186:ALA:HB2	1:A:1378:GLU:OE1	2.14	0.47
1:A:1303:GLY:O	1:A:1304:ALA:C	2.58	0.47
2:G:273:HIS:O	2:G:274:SER:C	2.58	0.47
2:G:387:TYR:CE2	2:G:391:LEU:HD11	2.49	0.47
2:G:1742:VAL:O	2:G:1745:LYS:N	2.42	0.47
1:A:81:TYR:HE1	2:G:1792:LEU:HD21	1.79	0.47
1:A:754:ASP:O	1:A:762:GLY:N	2.47	0.47
1:A:968:VAL:O	2:G:1512:HIS:ND1	2.48	0.47
1:A:1214:PHE:N	1:A:1214:PHE:CD1	2.83	0.47
2:G:16:LEU:HD11	2:G:56:THR:HA	1.97	0.47
2:G:572:ASN:O	2:G:575:GLY:N	2.38	0.47
2:G:831:LYS:O	2:G:831:LYS:HD3	2.15	0.47
2:G:1979:THR:HA	2:G:1982:MET:HG2	1.97	0.47
1:A:727:ALA:O	1:A:730:SER:N	2.40	0.46
1:A:1308:SER:OG	1:A:1586:GLY:O	2.33	0.46
1:A:1337:GLU:OE1	1:A:1337:GLU:N	2.38	0.46
2:G:617:ILE:HG22	2:G:618:GLU:N	2.31	0.46
2:G:1530:LYS:HG2	2:G:1632:ILE:HD11	1.95	0.46
2:G:1698:PHE:HZ	2:G:1828:VAL:HG22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASN:ND2	1:A:608:ASP:OD1	2.48	0.46
1:A:451:MET:O	1:A:452:GLU:C	2.57	0.46
1:A:1279:PHE:HB2	1:A:1282:THR:CG2	2.45	0.46
1:A:1353:LEU:O	1:A:1356:PHE:N	2.48	0.46
2:G:21:LEU:HD23	2:G:21:LEU:O	2.15	0.46
2:G:22:VAL:HG11	2:G:27:PHE:HA	1.98	0.46
2:G:1485:CYS:SG	2:G:1514:ASN:ND2	2.78	0.46
2:G:1889:VAL:HG12	2:G:1977:HIS:O	2.14	0.46
1:A:32:GLN:HA	1:A:35:PHE:CE1	2.51	0.46
1:A:1556:THR:HG23	1:A:1557:ILE:H	1.80	0.46
2:G:145:LEU:N	2:G:145:LEU:HD23	2.30	0.46
2:G:198:LEU:HA	2:G:201:THR:HG22	1.98	0.46
2:G:433:VAL:N	2:G:434:PRO:CD	2.78	0.46
2:G:1424:GLN:HE22	2:G:1426:THR:HG22	1.81	0.46
2:G:1564:HIS:ND1	2:G:1580:THR:O	2.48	0.46
2:G:1593:ILE:O	2:G:1594:GLU:C	2.58	0.46
1:A:1312:VAL:O	1:A:1316:VAL:HG12	2.16	0.46
1:A:1622:GLU:OE1	1:A:1622:GLU:N	2.34	0.46
1:A:1677:VAL:O	1:A:1678:SER:C	2.57	0.46
2:G:1300:PHE:CE1	2:G:1304:VAL:HG21	2.50	0.46
1:A:447:LEU:O	1:A:450:PHE:HB3	2.15	0.46
1:A:1130:ASP:O	1:A:1131:LEU:HG	2.16	0.46
1:A:1303:GLY:O	1:A:1307:THR:N	2.46	0.46
1:A:1604:ILE:CG2	1:A:1605:ILE:N	2.79	0.46
2:G:60:LEU:C	2:G:60:LEU:HD23	2.41	0.46
2:G:247:ALA:HA	2:G:250:VAL:HG22	1.97	0.46
2:G:868:PHE:HB3	2:G:873:PHE:CE2	2.50	0.46
2:G:1454:ASP:OD1	2:G:1454:ASP:N	2.48	0.46
2:G:1918:LYS:HD3	2:G:1964:PHE:HB3	1.97	0.46
1:A:806:VAL:HG23	1:A:807:LYS:N	2.30	0.46
1:A:1040:GLU:HA	1:A:1580:LEU:HD11	1.97	0.46
1:A:1115:ASN:O	1:A:1117:GLU:N	2.49	0.46
1:A:1326:ILE:CG2	1:A:1327:CYS:N	2.79	0.46
2:G:97:GLU:N	2:G:97:GLU:OE1	2.48	0.46
2:G:569:LEU:HD23	2:G:1090:TYR:CE1	2.51	0.46
2:G:766:ILE:HG23	2:G:799:PHE:N	2.31	0.46
1:A:339:ALA:HA	1:A:342:GLN:HG3	1.96	0.46
1:A:451:MET:O	1:A:455:ILE:N	2.44	0.46
1:A:1560:MET:O	1:A:1564:LEU:HD12	2.16	0.46
2:G:124:LYS:O	2:G:128:THR:HG23	2.16	0.46
2:G:203:LEU:HD23	2:G:203:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:423:VAL:HG12	2:G:424:ALA:N	2.31	0.46
2:G:569:LEU:HB3	2:G:1097:ILE:CD1	2.45	0.46
2:G:859:THR:OG1	2:G:862:VAL:HG12	2.15	0.46
2:G:1878:VAL:CG2	2:G:1910:VAL:HG22	2.41	0.46
2:G:2036:GLU:N	2:G:2037:PRO:CD	2.78	0.46
1:A:521:LYS:HG2	1:A:522:LEU:N	2.31	0.46
1:A:622:ILE:HD13	1:A:664:GLU:OE1	2.15	0.46
1:A:1477:ILE:HB	1:A:1478:PRO:HD3	1.98	0.46
1:A:1599:ILE:HG23	1:A:1604:ILE:O	2.15	0.46
2:G:467:ASP:OD1	2:G:468:LEU:N	2.48	0.46
2:G:646:THR:HG23	2:G:677:GLN:OE1	2.16	0.46
2:G:1332:ARG:O	2:G:1336:LYS:NZ	2.34	0.46
2:G:1890:ASN:CB	2:G:1899:VAL:HG22	2.42	0.46
1:A:1104:ARG:NH2	1:A:1189:ILE:O	2.49	0.46
1:A:1152:VAL:HG21	1:A:1165:VAL:HB	1.98	0.46
2:G:81:ASP:OD1	2:G:82:GLN:N	2.49	0.46
2:G:243:VAL:HA	2:G:246:LEU:HD12	1.98	0.46
2:G:562:LEU:HD12	2:G:562:LEU:O	2.16	0.46
2:G:844:VAL:HG12	2:G:845:THR:N	2.31	0.46
2:G:1267:TRP:HZ3	2:G:1271:ILE:HG21	1.81	0.46
2:G:1822:MET:HE3	2:G:1827:LEU:CD1	2.46	0.46
1:A:420:ILE:HD13	1:A:469:VAL:CG1	2.45	0.46
1:A:1513:TYR:CE2	1:A:1521:PRO:HA	2.51	0.46
2:G:619:LEU:N	2:G:648:GLY:O	2.49	0.46
2:G:646:THR:CG2	2:G:647:PHE:N	2.79	0.46
2:G:1070:ILE:HG23	2:G:1071:LYS:N	2.31	0.46
1:A:807:LYS:HD2	1:A:858:TRP:HB3	1.97	0.45
2:G:51:ASP:OD1	2:G:52:ASP:N	2.49	0.45
2:G:159:ILE:HD11	2:G:490:TRP:HH2	1.79	0.45
2:G:665:LEU:HD23	2:G:665:LEU:C	2.40	0.45
2:G:861:GLY:HA2	2:G:898:ASP:O	2.16	0.45
2:G:1170:ILE:HA	2:G:1173:VAL:HG12	1.99	0.45
2:G:1678:MET:HE1	2:G:1691:TRP:CD2	2.51	0.45
1:A:474:GLU:O	1:A:477:ILE:HG12	2.17	0.45
1:A:1205:ILE:HG22	1:A:1213:LEU:HD11	1.98	0.45
1:A:1722:VAL:HG23	1:A:1732:THR:C	2.41	0.45
2:G:278:VAL:HG23	2:G:279:THR:H	1.80	0.45
2:G:323:ILE:O	2:G:324:LEU:C	2.60	0.45
2:G:441:LYS:HD2	2:G:441:LYS:N	2.32	0.45
2:G:443:LEU:O	2:G:446:ASN:N	2.48	0.45
2:G:502:LEU:N	2:G:502:LEU:HD23	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1090:TYR:O	2:G:1093:ASP:OD1	2.34	0.45
1:A:703:VAL:HG12	1:A:704:VAL:N	2.32	0.45
1:A:1118:LYS:HA	1:A:1178:ALA:HB1	1.98	0.45
1:A:1137:SER:OG	1:A:1140:THR:N	2.38	0.45
1:A:1463:VAL:O	1:A:1466:GLU:N	2.47	0.45
1:A:1722:VAL:HG22	1:A:1723:SER:N	2.31	0.45
2:G:820:CYS:SG	2:G:821:ILE:N	2.89	0.45
1:A:50:SER:HB3	2:G:1671:SER:OG	2.17	0.45
1:A:57:ALA:C	1:A:59:ARG:N	2.73	0.45
1:A:395:SER:OG	1:A:398:LYS:N	2.43	0.45
1:A:985:ARG:HA	1:A:1086:ASP:OD2	2.16	0.45
1:A:1219:VAL:HA	1:A:1384:ILE:CD1	2.46	0.45
1:A:1555:ALA:O	1:A:1559:GLU:OE1	2.34	0.45
1:A:1655:VAL:CG1	1:A:1656:VAL:N	2.79	0.45
2:G:37:PHE:CE1	2:G:64:PHE:HA	2.52	0.45
2:G:854:ILE:HG21	2:G:856:LYS:HE2	1.98	0.45
2:G:934:SER:OG	2:G:935:THR:N	2.50	0.45
2:G:1353:LEU:HD11	2:G:1411:PHE:HB2	1.98	0.45
1:A:488:PRO:O	1:A:672:THR:OG1	2.32	0.45
1:A:768:ILE:C	1:A:769:ILE:HG13	2.41	0.45
1:A:1149:GLY:O	1:A:1151:LYS:HG2	2.17	0.45
1:A:1211:ILE:O	1:A:1215:VAL:HG23	2.17	0.45
1:A:1393:ALA:HB1	1:A:1398:VAL:HG23	1.97	0.45
2:G:249:TYR:CE1	2:G:283:ILE:HD12	2.51	0.45
2:G:270:ALA:C	2:G:271:THR:HG1	2.20	0.45
2:G:598:THR:OG1	2:G:599:PRO:HD3	2.17	0.45
2:G:1466:PHE:N	2:G:1466:PHE:CD2	2.84	0.45
2:G:1539:ILE:HD13	2:G:1626:ILE:HG22	1.99	0.45
1:A:493:VAL:HG12	1:A:493:VAL:O	2.15	0.45
1:A:936:LEU:HA	1:A:939:PHE:HB3	1.98	0.45
1:A:1051:VAL:HG13	1:A:1052:GLU:N	2.32	0.45
1:A:1685:TYR:CZ	2:G:993:GLN:NE2	2.84	0.45
2:G:494:THR:HG22	2:G:494:THR:O	2.16	0.45
2:G:1389:ILE:HG22	2:G:1390:VAL:N	2.31	0.45
1:A:483:VAL:O	1:A:484:LEU:C	2.56	0.45
1:A:980:VAL:HG12	2:G:968:GLN:CD	2.42	0.45
1:A:1442:ASN:O	1:A:1448:ARG:NE	2.49	0.45
2:G:1511:SER:C	2:G:1512:HIS:HD1	2.25	0.45
2:G:1604:ARG:CB	2:G:1657:ILE:HD11	2.47	0.45
1:A:486:VAL:HG22	1:A:487:ASP:N	2.31	0.45
1:A:519:VAL:HG11	1:A:528:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:LEU:HD23	1:A:749:ILE:N	2.32	0.45
1:A:822:VAL:O	1:A:865:CYS:N	2.43	0.45
2:G:1447:LYS:HD2	2:G:1449:TRP:NE1	2.31	0.45
2:G:1640:PHE:C	2:G:1640:PHE:CD1	2.95	0.45
1:A:79:LEU:HD21	1:A:87:GLU:HB3	1.99	0.45
1:A:768:ILE:CG2	1:A:770:PRO:HD3	2.47	0.45
1:A:1233:GLU:O	1:A:1234:MET:C	2.58	0.45
1:A:1636:VAL:CG1	1:A:1637:ARG:N	2.80	0.45
1:A:1714:VAL:HG13	1:A:1720:ALA:HB3	1.99	0.45
1:A:1743:SER:O	1:A:1746:ASN:N	2.49	0.45
2:G:199:ILE:HD11	2:G:213:LEU:HD23	1.99	0.45
2:G:569:LEU:HD21	2:G:1085:LEU:CD1	2.46	0.45
2:G:1225:GLU:OE2	2:G:1227:ARG:HB2	2.17	0.45
2:G:1270:TRP:HB2	2:G:1271:ILE:HD12	1.98	0.45
2:G:1739:GLU:O	2:G:1987:PRO:HG3	2.17	0.45
2:G:1797:LEU:HD12	2:G:1797:LEU:N	2.31	0.45
1:A:295:ALA:O	1:A:299:GLY:N	2.42	0.45
1:A:338:LEU:O	1:A:342:GLN:N	2.34	0.45
1:A:678:VAL:HG22	1:A:767:ALA:HB3	1.98	0.45
1:A:1238:VAL:HG22	1:A:1242:GLU:HB2	1.98	0.45
1:A:1704:ALA:HB1	1:A:1705:PRO:CD	2.47	0.45
2:G:59:GLU:HB3	2:G:122:LEU:HD21	1.99	0.45
2:G:461:ASP:O	2:G:465:GLY:N	2.43	0.45
2:G:570:ILE:HG22	2:G:571:LYS:N	2.32	0.45
2:G:573:LYS:CG	2:G:1101:GLU:HA	2.47	0.45
2:G:1151:HIS:O	2:G:1155:LEU:HD12	2.16	0.45
2:G:1201:VAL:N	2:G:1204:GLU:O	2.44	0.45
2:G:1862:VAL:HA	2:G:1918:LYS:HD2	1.99	0.45
2:G:1875:VAL:HG13	2:G:1876:GLU:N	2.32	0.45
2:G:2026:PHE:O	2:G:2029:VAL:HG22	2.16	0.45
1:A:14:LEU:HD23	1:A:14:LEU:O	2.16	0.44
1:A:78:ILE:O	1:A:79:LEU:HD12	2.16	0.44
1:A:329:GLU:HB2	1:A:333:LYS:NZ	2.33	0.44
1:A:358:GLU:O	1:A:361:PHE:N	2.50	0.44
1:A:767:ALA:HA	1:A:821:GLN:O	2.18	0.44
1:A:1583:HIS:C	1:A:1585:LYS:H	2.25	0.44
2:G:526:ARG:CG	2:G:558:ASN:H	2.30	0.44
2:G:1079:ASP:OD2	2:G:1080:GLY:N	2.50	0.44
2:G:1327:ILE:HG23	2:G:1328:VAL:N	2.32	0.44
2:G:1728:ARG:O	2:G:1731:GLU:HG3	2.17	0.44
2:G:1738:PHE:HB2	2:G:1751:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1815:LEU:HB3	2:G:1821:VAL:HG21	1.99	0.44
1:A:12:ILE:HG22	1:A:16:GLU:OE1	2.18	0.44
1:A:625:THR:HG22	1:A:627:SER:N	2.32	0.44
1:A:680:ILE:HG22	1:A:704:VAL:O	2.18	0.44
1:A:1009:LEU:HD13	1:A:1445:MET:HE1	1.99	0.44
2:G:125:ASN:OD1	2:G:126:TYR:N	2.50	0.44
2:G:203:LEU:HG	2:G:204:ASP:N	2.32	0.44
2:G:596:GLY:N	2:G:618:GLU:OE1	2.45	0.44
2:G:610:THR:CG2	2:G:617:ILE:HD11	2.48	0.44
2:G:869:ASP:HA	2:G:873:PHE:HD2	1.82	0.44
2:G:907:VAL:N	2:G:910:GLN:O	2.45	0.44
2:G:1051:THR:HG22	2:G:1052:CYS:N	2.32	0.44
2:G:1321:ALA:HB3	2:G:1366:LEU:HG	1.99	0.44
2:G:1792:LEU:HB2	2:G:1798:ILE:HD11	1.99	0.44
1:A:399:ALA:C	1:A:400:ARG:HG2	2.42	0.44
1:A:1445:MET:O	1:A:1446:LYS:C	2.60	0.44
2:G:321:PRO:HA	2:G:324:LEU:HB3	1.99	0.44
2:G:1382:VAL:HG22	2:G:1383:ASN:N	2.32	0.44
2:G:1511:SER:OG	2:G:1512:HIS:N	2.51	0.44
2:G:1695:ASP:OD2	2:G:1706:ILE:N	2.49	0.44
1:A:13:LEU:HD22	2:G:2026:PHE:HE1	1.81	0.44
1:A:91:THR:N	1:A:92:PRO:CD	2.80	0.44
1:A:1316:VAL:O	1:A:1320:LEU:HD23	2.17	0.44
1:A:1604:ILE:HG22	1:A:1605:ILE:N	2.31	0.44
2:G:88:LEU:HD23	2:G:135:ARG:HD2	1.99	0.44
2:G:159:ILE:HD12	2:G:271:THR:C	2.42	0.44
2:G:240:LEU:N	2:G:240:LEU:HD12	2.33	0.44
2:G:263:LEU:HD23	2:G:263:LEU:C	2.42	0.44
2:G:391:LEU:CD2	2:G:394:ARG:HE	2.31	0.44
2:G:1198:SER:OG	2:G:1206:LYS:N	2.50	0.44
2:G:1240:TYR:HD1	2:G:1253:GLU:HA	1.82	0.44
2:G:1264:GLU:OE1	2:G:1264:GLU:HA	2.18	0.44
2:G:1435:ILE:N	2:G:1435:ILE:HD12	2.32	0.44
1:A:365:LYS:O	1:A:368:VAL:N	2.46	0.44
1:A:496:PRO:HG2	1:A:521:LYS:O	2.17	0.44
1:A:959:ILE:HG13	1:A:960:GLU:N	2.32	0.44
1:A:1008:GLU:OE2	1:A:1446:LYS:NZ	2.50	0.44
1:A:1542:HIS:N	1:A:1553:GLU:OE2	2.43	0.44
2:G:610:THR:O	2:G:613:ALA:N	2.49	0.44
2:G:652:ILE:HG22	2:G:654:VAL:H	1.82	0.44
2:G:1040:LEU:O	2:G:1043:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1044:VAL:HG23	2:G:1045:ASP:OD1	2.18	0.44
2:G:1452:LEU:HD23	2:G:1502:GLY:CA	2.46	0.44
2:G:1563:ILE:O	2:G:1563:ILE:HG22	2.16	0.44
2:G:1811:GLU:O	2:G:1815:LEU:HG	2.18	0.44
1:A:337:VAL:HG23	1:A:338:LEU:N	2.33	0.44
1:A:931:GLN:H	1:A:931:GLN:CD	2.24	0.44
1:A:1055:TRP:CE2	1:A:1692:MET:O	2.71	0.44
1:A:1630:THR:HG22	1:A:1631:LEU:H	1.82	0.44
2:G:37:PHE:CE1	2:G:67:TYR:HB3	2.52	0.44
2:G:343:ASN:HB2	2:G:416:PHE:HB3	2.00	0.44
2:G:877:LYS:HG3	2:G:878:ASN:H	1.83	0.44
1:A:537:LYS:CE	1:A:634:THR:HG23	2.48	0.44
1:A:671:VAL:HG22	1:A:672:THR:O	2.18	0.44
1:A:873:ARG:N	1:A:898:GLN:OE1	2.51	0.44
1:A:1076:VAL:HG12	1:A:1077:ASP:N	2.32	0.44
2:G:336:SER:OG	2:G:337:PRO:CD	2.65	0.44
2:G:344:LEU:HD23	2:G:349:VAL:HG13	1.98	0.44
2:G:625:PHE:HA	2:G:661:TRP:CH2	2.51	0.44
2:G:1623:LYS:HB2	2:G:1643:ARG:HB2	2.00	0.44
2:G:1877:ARG:NE	2:G:1944:ILE:HD13	2.33	0.44
1:A:535:ILE:HD11	1:A:932:PHE:HB3	1.99	0.44
1:A:822:VAL:O	1:A:823:ILE:HD13	2.17	0.44
1:A:1263:ASP:O	1:A:1266:LYS:N	2.35	0.44
2:G:237:SER:O	2:G:238:CYS:C	2.61	0.44
2:G:1135:GLU:HA	2:G:1176:PRO:HG2	1.98	0.44
2:G:1489:ILE:HD11	2:G:1504:VAL:HG23	1.98	0.44
2:G:1490:LYS:HA	2:G:1499:VAL:O	2.17	0.44
2:G:1988:PHE:CE2	2:G:1992:LEU:HD21	2.53	0.44
2:G:1999:GLU:OE1	2:G:2000:ASN:N	2.50	0.44
1:A:395:SER:HG	1:A:398:LYS:H	1.64	0.44
1:A:727:ALA:O	1:A:728:LYS:C	2.61	0.44
1:A:964:GLU:OE1	1:A:965:HIS:N	2.51	0.44
1:A:1256:ALA:HB3	1:A:1278:SER:OG	2.17	0.44
1:A:1287:VAL:O	1:A:1291:LEU:N	2.42	0.44
1:A:1307:THR:HG23	1:A:1586:GLY:O	2.18	0.44
1:A:1673:TYR:O	1:A:1677:VAL:HG23	2.18	0.44
2:G:818:LYS:HA	2:G:821:ILE:HG22	2.00	0.44
2:G:1452:LEU:HD22	2:G:1501:ILE:CG2	2.46	0.44
2:G:1830:VAL:HG12	2:G:1991:PHE:CD2	2.52	0.44
1:A:446:ALA:O	1:A:449:LYS:N	2.51	0.43
1:A:527:GLN:HG3	1:A:626:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:GLY:O	1:A:696:LEU:C	2.61	0.43
1:A:915:GLU:O	1:A:918:GLN:N	2.51	0.43
1:A:1106:ILE:HG13	1:A:1185:VAL:HA	2.00	0.43
1:A:1138:LYS:HA	1:A:1163:TYR:CD2	2.52	0.43
1:A:1360:ARG:NH2	1:A:1372:THR:HG23	2.33	0.43
1:A:1680:ARG:O	1:A:1681:GLU:C	2.61	0.43
2:G:72:VAL:CG1	2:G:73:GLU:N	2.81	0.43
2:G:180:TYR:O	2:G:181:HIS:C	2.61	0.43
2:G:695:ILE:HD11	2:G:723:HIS:ND1	2.33	0.43
2:G:894:ARG:O	2:G:895:LEU:C	2.59	0.43
2:G:899:PHE:O	2:G:1050:ARG:HD3	2.17	0.43
2:G:904:PHE:CE2	2:G:1003:PHE:CZ	3.06	0.43
2:G:1267:TRP:HB3	2:G:1275:PHE:CE1	2.53	0.43
2:G:1918:LYS:O	2:G:1921:LYS:HG2	2.18	0.43
1:A:430:ARG:NE	1:A:605:LEU:HB3	2.33	0.43
1:A:938:GLU:HA	1:A:941:ALA:HB3	2.00	0.43
1:A:1039:MET:HE3	1:A:1039:MET:HB3	1.87	0.43
1:A:1154:ILE:O	1:A:1164:SER:O	2.37	0.43
1:A:1252:GLY:O	1:A:1254:VAL:N	2.51	0.43
1:A:1327:CYS:SG	1:A:1328:ILE:N	2.91	0.43
1:A:1335:PHE:C	1:A:1336:GLN:HG2	2.43	0.43
1:A:1344:GLY:O	1:A:1347:LYS:N	2.35	0.43
1:A:1354:GLU:O	1:A:1358:HIS:ND1	2.51	0.43
2:G:395:LYS:CE	2:G:396:ALA:HB2	2.48	0.43
2:G:1041:GLU:HA	2:G:1046:GLN:OE1	2.18	0.43
2:G:1363:ALA:O	2:G:1606:ARG:NH2	2.51	0.43
2:G:1628:HIS:HA	2:G:1638:ILE:HD13	1.99	0.43
2:G:1741:ILE:HD11	2:G:1986:LYS:HG2	1.99	0.43
1:A:748:LEU:O	1:A:751:PHE:HB3	2.17	0.43
1:A:948:VAL:HG23	1:A:949:GLU:N	2.32	0.43
1:A:953:VAL:HG12	2:G:1439:LYS:CB	2.44	0.43
1:A:1200:ILE:HG13	1:A:1698:PHE:CD1	2.54	0.43
1:A:1326:ILE:HG22	1:A:1327:CYS:N	2.33	0.43
1:A:1367:ARG:HD3	1:A:1370:THR:HG21	1.99	0.43
2:G:698:LEU:O	2:G:700:LEU:N	2.50	0.43
2:G:751:LEU:C	2:G:751:LEU:HD23	2.43	0.43
2:G:1612:PHE:HD1	2:G:1651:LEU:HD21	1.83	0.43
2:G:1861:ARG:O	2:G:1921:LYS:NZ	2.51	0.43
2:G:1917:ILE:HD11	2:G:1922:ILE:O	2.18	0.43
2:G:1917:ILE:HD13	2:G:1924:ILE:HD11	2.00	0.43
1:A:334:ASP:O	1:A:338:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ALA:HA	1:A:342:GLN:CG	2.48	0.43
1:A:365:LYS:O	1:A:368:VAL:HB	2.18	0.43
1:A:678:VAL:HG12	1:A:679:LEU:N	2.33	0.43
1:A:1012:LEU:O	1:A:1012:LEU:HD12	2.17	0.43
1:A:1103:ILE:HG22	1:A:1104:ARG:N	2.34	0.43
1:A:1656:VAL:HG12	1:A:1657:HIS:H	1.84	0.43
1:A:1685:TYR:CE1	1:A:1689:HIS:CE1	3.06	0.43
2:G:273:HIS:CG	2:G:274:SER:H	2.37	0.43
2:G:1697:HIS:O	2:G:1701:THR:OG1	2.36	0.43
2:G:1878:VAL:CG2	2:G:1944:ILE:HD11	2.48	0.43
1:A:1102:GLY:O	1:A:1104:ARG:HG3	2.18	0.43
1:A:1393:ALA:HB1	1:A:1398:VAL:CG2	2.49	0.43
1:A:1535:ASP:OD2	1:A:1637:ARG:NH1	2.49	0.43
2:G:272:GLY:N	2:G:277:LEU:HD12	2.34	0.43
2:G:397:LYS:HE3	2:G:416:PHE:O	2.18	0.43
2:G:649:ILE:HG13	2:G:679:LEU:HD12	1.99	0.43
2:G:943:TRP:O	2:G:946:PHE:HB3	2.19	0.43
2:G:1166:VAL:HG22	2:G:1167:SER:N	2.34	0.43
2:G:1255:MET:N	2:G:1256:GLU:OE2	2.51	0.43
2:G:1455:GLU:OE1	2:G:1455:GLU:N	2.47	0.43
2:G:1783:LEU:O	2:G:1784:MET:C	2.61	0.43
1:A:1384:ILE:HG13	1:A:1385:GLN:N	2.31	0.43
1:A:1544:THR:HG23	1:A:1546:THR:HG23	2.00	0.43
2:G:138:ASP:OD1	2:G:138:ASP:N	2.47	0.43
2:G:241:ILE:HG21	2:G:275:GLN:HE21	1.83	0.43
2:G:846:VAL:O	2:G:853:PRO:HA	2.19	0.43
2:G:881:VAL:N	2:G:882:PRO:HD3	2.33	0.43
2:G:1476:ASN:OD1	2:G:1479:ILE:HD12	2.18	0.43
2:G:1833:TYR:O	2:G:1837:THR:HG23	2.18	0.43
2:G:1911:THR:CG2	2:G:1966:CYS:SG	3.07	0.43
1:A:640:LEU:CD1	1:A:659:PHE:CD2	3.01	0.43
1:A:703:VAL:CG1	1:A:704:VAL:N	2.81	0.43
1:A:893:VAL:CG1	1:A:894:ARG:N	2.82	0.43
1:A:1138:LYS:CG	1:A:1138:LYS:O	2.66	0.43
1:A:1260:MET:HE3	1:A:1275:LEU:HD12	2.01	0.43
2:G:10:THR:O	2:G:10:THR:HG23	2.18	0.43
2:G:214:ASN:O	2:G:218:TRP:CE2	2.72	0.43
2:G:217:GLU:O	2:G:221:ASN:OD1	2.37	0.43
1:A:337:VAL:HA	1:A:340:ARG:HB3	1.99	0.43
1:A:791:ALA:O	1:A:792:HIS:C	2.60	0.43
1:A:795:MET:O	1:A:799:ILE:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1414:ILE:HG22	1:A:1415:GLY:N	2.33	0.43
2:G:118:LYS:O	2:G:122:LEU:HD23	2.18	0.43
2:G:238:CYS:HB2	2:G:239:PRO:HD3	2.01	0.43
2:G:590:PRO:HB3	2:G:1078:HIS:CD2	2.54	0.43
2:G:765:LEU:HD23	2:G:796:PHE:HD1	1.80	0.43
2:G:1360:ILE:O	2:G:1606:ARG:NH2	2.51	0.43
1:A:350:LEU:N	1:A:350:LEU:HD12	2.34	0.43
1:A:430:ARG:CZ	1:A:495:LYS:HG2	2.49	0.43
1:A:677:TYR:CB	1:A:764:ASP:O	2.67	0.43
1:A:795:MET:O	1:A:799:ILE:HD12	2.18	0.43
1:A:959:ILE:O	1:A:963:LEU:N	2.46	0.43
1:A:1219:VAL:O	1:A:1220:VAL:C	2.62	0.43
1:A:1233:GLU:HA	1:A:1731:LEU:CD1	2.48	0.43
2:G:284:ALA:CB	2:G:455:ILE:HG22	2.47	0.43
2:G:471:LEU:HD23	2:G:473:GLY:N	2.34	0.43
2:G:692:SER:O	2:G:696:GLU:OE1	2.37	0.43
2:G:768:GLY:O	2:G:769:SER:OG	2.34	0.43
2:G:821:ILE:HD11	2:G:1055:HIS:CE1	2.53	0.43
2:G:1100:VAL:CG1	2:G:1147:ILE:HG21	2.46	0.43
2:G:1260:GLN:O	2:G:1264:GLU:HG2	2.19	0.43
2:G:1343:VAL:O	2:G:1343:VAL:HG13	2.18	0.43
2:G:1543:ASP:HA	2:G:1622:LEU:O	2.18	0.43
2:G:1680:LEU:C	2:G:1680:LEU:HD23	2.44	0.43
2:G:1773:ALA:C	2:G:1777:THR:HG23	2.43	0.43
2:G:1816:ALA:O	2:G:1820:ASP:N	2.48	0.43
2:G:1821:VAL:HG23	2:G:1822:MET:HG2	2.00	0.43
2:G:1867:SER:O	2:G:1871:LEU:HD12	2.19	0.43
1:A:34:VAL:HG13	1:A:35:PHE:H	1.83	0.43
1:A:58:GLN:HB3	1:A:78:ILE:HD13	2.00	0.43
1:A:1151:LYS:O	1:A:1152:VAL:C	2.61	0.43
1:A:1207:GLN:HG2	1:A:1208:VAL:HG23	2.01	0.43
2:G:621:GLY:CA	2:G:658:MET:HE1	2.49	0.43
2:G:750:MET:HE2	2:G:750:MET:HA	2.00	0.43
2:G:873:PHE:CD1	2:G:1026:GLU:HB3	2.54	0.43
2:G:1392:VAL:HG12	2:G:1393:VAL:N	2.33	0.43
2:G:1435:ILE:O	2:G:1436:LYS:HE2	2.19	0.43
2:G:1480:PHE:N	2:G:1480:PHE:CD1	2.87	0.43
2:G:1605:VAL:CG2	2:G:1657:ILE:HD13	2.49	0.43
2:G:1616:VAL:CG1	2:G:1650:VAL:HG11	2.49	0.43
2:G:1719:ILE:O	2:G:1761:SER:HA	2.19	0.43
2:G:1905:ARG:HD2	2:G:1958:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:O	1:A:34:VAL:HG12	2.19	0.42
1:A:49:PRO:HG2	2:G:1671:SER:OG	2.19	0.42
1:A:509:ILE:O	1:A:509:ILE:CG2	2.67	0.42
1:A:994:GLU:OE1	1:A:994:GLU:N	2.52	0.42
1:A:1223:PHE:CD1	1:A:1228:ILE:HG21	2.54	0.42
1:A:1230:ASP:O	1:A:1231:PRO:C	2.61	0.42
1:A:1370:THR:H	1:A:1373:ARG:HE	1.66	0.42
2:G:11:LEU:HD12	2:G:11:LEU:N	2.34	0.42
2:G:198:LEU:O	2:G:202:THR:HG22	2.18	0.42
2:G:864:LEU:HD11	2:G:868:PHE:CE2	2.54	0.42
2:G:1020:VAL:HG22	2:G:1021:LEU:N	2.34	0.42
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.81	0.42
2:G:1789:PHE:CD2	2:G:1817:SER:HB2	2.54	0.42
2:G:2037:PRO:HA	2:G:2040:GLU:HG2	2.01	0.42
1:A:475:GLN:OE1	1:A:614:ALA:HB2	2.19	0.42
1:A:527:GLN:CG	1:A:626:VAL:HG21	2.49	0.42
1:A:1238:VAL:HG22	1:A:1239:HIS:H	1.84	0.42
1:A:1316:VAL:HG22	1:A:1320:LEU:HD22	2.01	0.42
1:A:1333:ASP:OD2	1:A:1584:PRO:C	2.61	0.42
2:G:108:LEU:HD12	2:G:112:ASN:HB3	2.00	0.42
2:G:112:ASN:OD1	2:G:113:ASP:N	2.47	0.42
2:G:334:VAL:O	2:G:334:VAL:HG23	2.18	0.42
2:G:587:ILE:HG13	2:G:589:ARG:H	1.84	0.42
2:G:637:VAL:HG23	2:G:638:VAL:N	2.34	0.42
2:G:1386:THR:HG23	2:G:1411:PHE:CZ	2.52	0.42
2:G:1770:LEU:HD23	2:G:1776:PHE:HE1	1.84	0.42
2:G:1889:VAL:HG23	2:G:1899:VAL:HG23	2.01	0.42
2:G:1981:LEU:N	2:G:1981:LEU:HD12	2.34	0.42
1:A:12:ILE:O	1:A:13:LEU:C	2.61	0.42
1:A:57:ALA:C	1:A:59:ARG:H	2.28	0.42
1:A:1316:VAL:O	1:A:1317:GLU:C	2.63	0.42
2:G:6:THR:HG22	2:G:23:PRO:HA	2.00	0.42
2:G:195:LEU:HD23	2:G:213:LEU:HD21	2.00	0.42
2:G:326:ASP:OD1	2:G:326:ASP:C	2.61	0.42
2:G:741:HIS:O	2:G:853:PRO:HG2	2.18	0.42
2:G:872:ILE:HG22	2:G:880:LEU:HD11	2.00	0.42
2:G:1685:LYS:NZ	2:G:1689:ASP:OD2	2.35	0.42
1:A:36:LEU:HD23	1:A:65:TYR:HD2	1.84	0.42
1:A:430:ARG:HE	1:A:606:ASP:CG	2.26	0.42
1:A:715:THR:O	1:A:718:TYR:N	2.52	0.42
1:A:725:TYR:O	1:A:726:GLY:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:LYS:HZ2	1:A:861:GLN:CD	2.20	0.42
1:A:1361:THR:O	1:A:1362:PRO:C	2.62	0.42
1:A:1423:LYS:O	1:A:1424:GLY:C	2.62	0.42
1:A:1533:ILE:HD11	1:A:1561:MET:CE	2.49	0.42
2:G:809:LYS:HB3	2:G:1067:ASP:HB2	2.01	0.42
2:G:860:ARG:HB3	2:G:898:ASP:HB3	2.00	0.42
2:G:1642:THR:OG1	2:G:1651:LEU:HB2	2.19	0.42
2:G:1739:GLU:HG2	2:G:1746:LEU:HG	2.01	0.42
2:G:1866:PHE:HA	2:G:1925:ILE:HD11	2.01	0.42
2:G:1991:PHE:HA	2:G:1994:LYS:HE2	2.01	0.42
1:A:367:THR:O	1:A:371:LEU:HB2	2.19	0.42
1:A:734:VAL:C	1:A:735:VAL:HG23	2.45	0.42
1:A:1179:LEU:O	1:A:1180:ARG:C	2.61	0.42
1:A:1246:CYS:HB3	1:A:1314:ILE:HG13	2.02	0.42
2:G:57:PRO:HA	2:G:60:LEU:HB3	2.01	0.42
2:G:68:VAL:O	2:G:72:VAL:HG23	2.18	0.42
2:G:169:TYR:OH	2:G:231:LEU:O	2.25	0.42
2:G:176:LEU:HD13	2:G:247:ALA:CB	2.50	0.42
2:G:715:GLN:O	2:G:719:ILE:HG12	2.20	0.42
2:G:1660:PRO:O	2:G:1662:THR:OG1	2.37	0.42
2:G:1931:LEU:HD13	2:G:1935:GLU:OE1	2.19	0.42
1:A:911:PRO:O	1:A:915:GLU:OE1	2.38	0.42
1:A:917:CYS:HA	1:A:920:SER:O	2.19	0.42
1:A:1320:LEU:HD23	1:A:1320:LEU:N	2.35	0.42
1:A:1378:GLU:HA	1:A:1583:HIS:O	2.20	0.42
2:G:672:LYS:HD2	2:G:674:TYR:CE2	2.54	0.42
2:G:826:GLY:CA	2:G:1060:ALA:HB3	2.50	0.42
2:G:916:THR:O	2:G:916:THR:CG2	2.67	0.42
2:G:2030:TYR:HA	2:G:2033:THR:HG22	2.01	0.42
1:A:21:GLN:O	2:G:1977:HIS:CD2	2.73	0.42
1:A:522:LEU:HA	1:A:525:TYR:HB3	2.01	0.42
1:A:1688:PHE:O	1:A:1692:MET:HB2	2.20	0.42
1:A:1740:SER:C	1:A:1742:ASP:N	2.78	0.42
2:G:92:GLU:OE2	2:G:93:ASN:ND2	2.52	0.42
2:G:122:LEU:O	2:G:125:ASN:OD1	2.36	0.42
2:G:345:THR:OG1	2:G:348:GLN:OE1	2.27	0.42
2:G:565:TYR:N	2:G:565:TYR:CD2	2.88	0.42
2:G:827:VAL:HG12	2:G:1057:PRO:HB2	2.02	0.42
2:G:846:VAL:HG12	2:G:847:ARG:O	2.20	0.42
2:G:1612:PHE:CD1	2:G:1651:LEU:HD21	2.55	0.42
1:A:12:ILE:O	1:A:15:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:HB3	2:G:1989:LYS:HZ3	1.84	0.42
1:A:442:ARG:HA	1:A:728:LYS:HG3	2.01	0.42
1:A:601:VAL:O	1:A:601:VAL:HG12	2.20	0.42
1:A:683:ALA:O	1:A:684:GLY:C	2.62	0.42
1:A:872:THR:HA	1:A:896:PHE:O	2.19	0.42
1:A:1017:ARG:NH1	1:A:1320:LEU:O	2.48	0.42
1:A:1280:ILE:O	1:A:1280:ILE:HG22	2.19	0.42
1:A:1638:ALA:C	1:A:1639:VAL:HG23	2.45	0.42
2:G:669:LEU:HD22	2:G:674:TYR:CE2	2.54	0.42
2:G:846:VAL:O	2:G:854:ILE:N	2.52	0.42
2:G:857:ILE:HG22	2:G:858:ALA:N	2.34	0.42
2:G:872:ILE:O	2:G:875:LEU:HB3	2.20	0.42
1:A:47:ILE:HG21	2:G:1666:PHE:HE2	1.84	0.42
1:A:368:VAL:O	1:A:369:ALA:C	2.63	0.42
1:A:798:ASN:O	1:A:802:MET:N	2.51	0.42
1:A:809:GLN:N	1:A:809:GLN:OE1	2.52	0.42
1:A:916:LEU:HD12	1:A:916:LEU:HA	1.92	0.42
1:A:977:TYR:N	1:A:977:TYR:CD1	2.86	0.42
1:A:1259:GLY:O	1:A:1270:VAL:HG21	2.20	0.42
2:G:68:VAL:HG13	2:G:69:SER:N	2.33	0.42
2:G:228:LYS:O	2:G:230:TYR:N	2.52	0.42
2:G:398:ALA:O	2:G:399:PRO:C	2.62	0.42
2:G:404:GLN:O	2:G:407:ILE:HG22	2.20	0.42
2:G:1960:LEU:HD23	2:G:1968:PRO:HB3	2.02	0.42
2:G:1985:VAL:CG2	2:G:1986:LYS:N	2.82	0.42
1:A:1:MET:HE2	1:A:2:LYS:HB3	2.02	0.42
1:A:28:TRP:HB3	2:G:1891:TYR:O	2.19	0.42
1:A:156:ALA:O	1:A:160:LYS:N	2.52	0.42
1:A:663:LEU:HA	1:A:666:ALA:HB3	2.01	0.42
1:A:1154:ILE:O	1:A:1155:PHE:C	2.63	0.42
1:A:1333:ASP:OD1	1:A:1584:PRO:O	2.37	0.42
1:A:1602:SER:OG	1:A:1604:ILE:HD12	2.19	0.42
2:G:145:LEU:HD23	2:G:145:LEU:H	1.85	0.42
2:G:185:GLY:O	2:G:189:LYS:HD3	2.20	0.42
2:G:441:LYS:HA	2:G:444:VAL:HG22	2.02	0.42
2:G:932:ILE:HD12	2:G:932:ILE:N	2.35	0.42
2:G:1037:SER:O	2:G:1040:LEU:HD13	2.20	0.42
2:G:1214:LEU:HD21	2:G:1220:GLN:CD	2.45	0.42
1:A:533:GLY:O	1:A:536:THR:N	2.47	0.41
1:A:625:THR:O	1:A:628:SER:OG	2.25	0.41
1:A:640:LEU:N	1:A:656:SER:OG	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:VAL:O	2:G:968:GLN:NE2	2.53	0.41
1:A:1025:ALA:HB3	1:A:1218:SER:O	2.19	0.41
1:A:1089:VAL:CG1	1:A:1090:LYS:N	2.82	0.41
1:A:1117:GLU:OE2	1:A:1184:LEU:HD22	2.20	0.41
1:A:1440:SER:OG	1:A:1443:LEU:HD12	2.20	0.41
2:G:677:GLN:NE2	2:G:1165:PHE:CD2	2.88	0.41
2:G:1313:SER:O	2:G:1314:ARG:C	2.62	0.41
2:G:1330:GLY:C	2:G:1334:ILE:HD12	2.45	0.41
2:G:1378:ILE:CD1	2:G:1392:VAL:HG22	2.47	0.41
2:G:1775:GLN:HE22	2:G:1836:MET:HB2	1.85	0.41
2:G:1985:VAL:O	2:G:1988:PHE:N	2.53	0.41
2:G:1997:ILE:HD12	2:G:2000:ASN:ND2	2.34	0.41
1:A:69:ASP:OD1	1:A:69:ASP:C	2.62	0.41
1:A:332:THR:O	1:A:333:LYS:C	2.63	0.41
1:A:424:VAL:O	1:A:425:LEU:HD23	2.20	0.41
1:A:1149:GLY:O	1:A:1150:ASP:HB3	2.21	0.41
1:A:1283:MET:O	1:A:1287:VAL:HG23	2.20	0.41
1:A:1316:VAL:HG13	1:A:1317:GLU:H	1.85	0.41
1:A:1340:SER:O	1:A:1344:GLY:N	2.53	0.41
1:A:1569:GLY:C	1:A:1571:PRO:HD3	2.45	0.41
2:G:778:TYR:HB3	2:G:779:PRO:HD3	2.02	0.41
2:G:804:ARG:HD2	2:G:1063:THR:HG22	2.00	0.41
2:G:914:LEU:CD2	2:G:1000:ILE:HG23	2.46	0.41
2:G:1148:ASN:O	2:G:1151:HIS:N	2.53	0.41
2:G:1381:VAL:O	2:G:1381:VAL:CG2	2.67	0.41
2:G:1812:TYR:OH	2:G:1834:ARG:NE	2.52	0.41
2:G:1923:ASP:C	2:G:1925:ILE:N	2.77	0.41
2:G:1929:LYS:HD2	2:G:1929:LYS:N	2.35	0.41
1:A:442:ARG:CG	1:A:727:ALA:HA	2.49	0.41
1:A:467:GLN:O	1:A:471:THR:HG22	2.20	0.41
1:A:649:TRP:O	1:A:650:LYS:HE2	2.20	0.41
1:A:678:VAL:CG1	1:A:679:LEU:N	2.83	0.41
1:A:942:LYS:O	1:A:943:LEU:C	2.63	0.41
1:A:1029:PRO:HA	1:A:1190:PRO:HD3	2.01	0.41
1:A:1164:SER:O	1:A:1165:VAL:HG13	2.20	0.41
1:A:1317:GLU:HA	1:A:1320:LEU:HD21	2.02	0.41
1:A:1399:PRO:HG2	1:A:1401:TYR:HE2	1.85	0.41
2:G:786:SER:OG	2:G:794:MET:HE3	2.19	0.41
2:G:1428:GLU:CD	2:G:1470:THR:HG23	2.45	0.41
2:G:1501:ILE:N	2:G:1501:ILE:HD12	2.36	0.41
1:A:490:TYR:CE2	1:A:906:LEU:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:PHE:CE1	1:A:663:LEU:HD21	2.55	0.41
1:A:913:VAL:O	1:A:914:VAL:C	2.63	0.41
1:A:1154:ILE:HD13	1:A:1154:ILE:N	2.35	0.41
2:G:827:VAL:N	2:G:1057:PRO:O	2.44	0.41
2:G:1766:SER:OG	2:G:1770:LEU:N	2.54	0.41
1:A:472:LEU:O	1:A:473:GLY:C	2.64	0.41
1:A:1030:TRP:CZ2	1:A:1102:GLY:HA3	2.55	0.41
1:A:1235:TYR:OH	1:A:1292:ILE:HG22	2.21	0.41
1:A:1256:ALA:HB1	1:A:1274:ILE:HG13	2.02	0.41
1:A:1286:TRP:O	1:A:1290:LEU:HD12	2.19	0.41
1:A:1584:PRO:HG2	1:A:1588:ALA:N	2.36	0.41
1:A:1590:ALA:O	1:A:1591:TRP:C	2.64	0.41
2:G:67:TYR:CE1	2:G:71:LEU:HD21	2.55	0.41
2:G:99:ASN:OD1	2:G:550:VAL:HG22	2.20	0.41
2:G:162:GLY:N	2:G:273:HIS:HB3	2.35	0.41
2:G:250:VAL:HG23	2:G:251:VAL:N	2.34	0.41
2:G:1489:ILE:HD12	2:G:1502:GLY:C	2.46	0.41
2:G:1638:ILE:HG22	2:G:1639:LYS:N	2.34	0.41
2:G:1804:PHE:CG	2:G:1818:LEU:HG	2.56	0.41
2:G:2032:LEU:HD12	2:G:2032:LEU:C	2.45	0.41
1:A:373:ALA:O	1:A:376:ASP:OD1	2.39	0.41
1:A:652:ASP:OD1	1:A:654:GLN:N	2.53	0.41
1:A:1219:VAL:O	1:A:1222:ALA:HB3	2.20	0.41
1:A:1234:MET:HG2	1:A:1396:MET:HE1	2.03	0.41
1:A:1378:GLU:CB	1:A:1585:LYS:HE2	2.39	0.41
1:A:1463:VAL:O	1:A:1467:LEU:N	2.39	0.41
2:G:652:ILE:CG2	2:G:654:VAL:HG22	2.49	0.41
2:G:1604:ARG:HB3	2:G:1657:ILE:HD11	2.03	0.41
2:G:1711:ILE:HG13	2:G:1712:ASN:N	2.36	0.41
2:G:1718:THR:HG22	2:G:1763:THR:HG22	2.03	0.41
2:G:1917:ILE:CD1	2:G:1924:ILE:HD11	2.50	0.41
1:A:2:LYS:CG	1:A:5:VAL:HG12	2.51	0.41
1:A:459:ASP:CG	1:A:461:THR:HG22	2.46	0.41
1:A:1226:SER:O	1:A:1226:SER:OG	2.26	0.41
1:A:1713:ASP:HB3	1:A:1738:ILE:HG21	2.02	0.41
2:G:191:SER:O	2:G:194:THR:HG22	2.21	0.41
2:G:720:ALA:HB1	2:G:762:ASN:HD21	1.85	0.41
2:G:831:LYS:HE2	2:G:834:GLN:HG3	2.01	0.41
2:G:1151:HIS:HD2	2:G:1155:LEU:HD12	1.84	0.41
2:G:1345:GLY:HA3	2:G:1412:TYR:CD1	2.56	0.41
2:G:1478:ASN:N	2:G:1478:ASN:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1713:ASN:CB	2:G:1771:LEU:HD13	2.51	0.41
2:G:1776:PHE:C	2:G:1779:PRO:HD2	2.46	0.41
2:G:1871:LEU:O	2:G:1875:VAL:HG12	2.20	0.41
2:G:1953:VAL:HG12	2:G:1953:VAL:O	2.20	0.41
1:A:8:GLU:HG2	2:G:1998:LYS:HD3	2.02	0.41
1:A:80:CYS:SG	1:A:83:LYS:HB3	2.61	0.41
1:A:632:ARG:C	1:A:634:THR:N	2.77	0.41
1:A:1157:ILE:HG12	1:A:1162:GLU:O	2.21	0.41
1:A:1412:ASP:O	1:A:1413:LYS:HG2	2.21	0.41
1:A:1558:ASN:O	1:A:1562:LYS:HB2	2.21	0.41
2:G:40:ILE:CD1	2:G:67:TYR:CE2	3.04	0.41
2:G:488:VAL:O	2:G:488:VAL:HG23	2.20	0.41
2:G:1002:HIS:CE1	2:G:1006:MET:SD	3.13	0.41
2:G:1489:ILE:HD12	2:G:1502:GLY:O	2.20	0.41
2:G:1742:VAL:O	2:G:1745:LYS:HB3	2.20	0.41
2:G:1779:PRO:O	2:G:1782:THR:OG1	2.35	0.41
2:G:1940:LEU:HD12	2:G:1941:PHE:HD1	1.86	0.41
1:A:1:MET:HE2	1:A:5:VAL:CG1	2.51	0.41
1:A:35:PHE:CD2	1:A:35:PHE:C	2.98	0.41
1:A:90:TYR:HB2	2:G:1533:LEU:HD11	2.02	0.41
1:A:420:ILE:HG21	1:A:469:VAL:CG1	2.51	0.41
1:A:475:GLN:OE1	1:A:614:ALA:N	2.53	0.41
1:A:706:THR:C	1:A:707:THR:HG23	2.46	0.41
1:A:735:VAL:HG12	1:A:736:PRO:N	2.36	0.41
1:A:1083:PRO:O	1:A:1084:VAL:HG23	2.21	0.41
1:A:1185:VAL:O	1:A:1186:ALA:HB2	2.21	0.41
1:A:1234:MET:SD	1:A:1326:ILE:HD13	2.60	0.41
1:A:1369:ALA:O	1:A:1614:VAL:HA	2.20	0.41
1:A:1384:ILE:O	1:A:1385:GLN:OE1	2.39	0.41
1:A:1513:TYR:CD1	1:A:1524:GLY:HA3	2.56	0.41
1:A:1548:ALA:O	1:A:1549:ASN:C	2.64	0.41
2:G:38:ASN:HA	2:G:41:LEU:CD2	2.51	0.41
2:G:421:LEU:HB2	2:G:423:VAL:HG23	2.02	0.41
2:G:500:HIS:HA	2:G:526:ARG:O	2.21	0.41
2:G:589:ARG:HG2	2:G:590:PRO:HD2	2.03	0.41
2:G:1033:SER:O	2:G:1052:CYS:HB2	2.21	0.41
2:G:1228:THR:CG2	2:G:1229:MET:N	2.84	0.41
2:G:1491:VAL:CB	2:G:1501:ILE:HD11	2.51	0.41
2:G:1745:LYS:HD2	2:G:1747:LYS:HB2	2.02	0.41
2:G:1792:LEU:O	2:G:1795:LYS:N	2.54	0.41
2:G:1822:MET:SD	2:G:1996:ILE:HG22	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1911:THR:HG23	2:G:1966:CYS:SG	2.61	0.41
1:A:450:PHE:CE1	1:A:454:HIS:CD2	3.08	0.41
1:A:529:MET:O	1:A:636:PRO:HB2	2.20	0.41
1:A:533:GLY:O	1:A:534:PRO:C	2.64	0.41
1:A:771:PHE:CD1	1:A:825:PRO:HG3	2.56	0.41
1:A:799:ILE:O	1:A:802:MET:HB3	2.21	0.41
1:A:985:ARG:NH1	1:A:1085:ASP:OD1	2.54	0.41
1:A:1051:VAL:CG1	1:A:1052:GLU:N	2.83	0.41
1:A:1334:ASP:CG	1:A:1335:PHE:H	2.28	0.41
1:A:1592:MET:SD	1:A:1641:ILE:HG23	2.61	0.41
2:G:174:ARG:HH21	2:G:219:LEU:HA	1.85	0.41
2:G:309:ARG:CG	2:G:439:ILE:HG12	2.51	0.41
2:G:332:GLU:HG3	2:G:390:ASN:HD21	1.86	0.41
2:G:1397:SER:HA	2:G:1401:LYS:O	2.21	0.41
2:G:1584:PHE:CD2	2:G:1584:PHE:C	2.99	0.41
2:G:1595:ASN:OD1	2:G:1595:ASN:N	2.53	0.41
2:G:1707:LEU:N	2:G:1707:LEU:HD23	2.35	0.41
2:G:1808:SER:H	2:G:2013:ASN:ND2	2.17	0.41
2:G:1924:ILE:HG22	2:G:1928:GLN:OE1	2.21	0.41
2:G:2015:THR:HG21	2:G:2025:TYR:CE1	2.56	0.41
1:A:788:SER:O	1:A:791:ALA:N	2.53	0.40
1:A:1288:ASN:OD1	1:A:1293:SER:CA	2.69	0.40
1:A:1308:SER:O	1:A:1312:VAL:HG23	2.22	0.40
1:A:1624:VAL:HG22	1:A:1626:TYR:CE2	2.55	0.40
2:G:716:VAL:O	2:G:719:ILE:HB	2.20	0.40
2:G:1262:ILE:HD13	2:G:1348:LEU:HD23	2.04	0.40
2:G:1310:ASP:OD2	2:G:1320:LEU:HD21	2.21	0.40
2:G:1447:LYS:HG3	2:G:1448:GLU:N	2.36	0.40
2:G:1764:PHE:C	2:G:1765:ARG:HD2	2.47	0.40
2:G:1797:LEU:N	2:G:1797:LEU:CD1	2.84	0.40
2:G:1988:PHE:C	2:G:1992:LEU:HD23	2.46	0.40
1:A:46:GLU:HA	2:G:1665:VAL:HG23	2.04	0.40
1:A:47:ILE:HB	2:G:1666:PHE:CD2	2.56	0.40
1:A:677:TYR:HB3	1:A:764:ASP:O	2.21	0.40
1:A:788:SER:C	1:A:790:PHE:N	2.78	0.40
1:A:1167:LEU:O	1:A:1168:LEU:HD13	2.21	0.40
1:A:1185:VAL:CG2	1:A:1377:MET:CE	2.92	0.40
1:A:1247:SER:OG	1:A:1248:GLY:N	2.53	0.40
1:A:1251:MET:HE2	1:A:1254:VAL:HG22	2.02	0.40
1:A:1375:GLY:O	1:A:1545:SER:OG	2.35	0.40
1:A:1603:GLY:O	1:A:1633:THR:OG1	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:18:HIS:CD2	2:G:19:VAL:O	2.74	0.40
2:G:159:ILE:HD12	2:G:271:THR:O	2.22	0.40
2:G:180:TYR:O	2:G:183:LEU:N	2.43	0.40
2:G:253:ALA:HB1	2:G:258:PHE:O	2.21	0.40
2:G:690:VAL:O	2:G:693:GLU:CD	2.64	0.40
2:G:713:ILE:HA	2:G:716:VAL:HG12	2.03	0.40
2:G:845:THR:HA	2:G:854:ILE:O	2.20	0.40
2:G:875:LEU:HD23	2:G:876:PRO:N	2.36	0.40
1:A:80:CYS:SG	1:A:83:LYS:N	2.89	0.40
1:A:346:LEU:O	1:A:347:ALA:C	2.64	0.40
1:A:519:VAL:HG23	1:A:524:GLN:HB2	2.03	0.40
1:A:701:ALA:O	1:A:730:SER:HA	2.21	0.40
1:A:1049:GLY:O	1:A:1053:MET:HB2	2.21	0.40
1:A:1189:ILE:HD12	1:A:1193:TRP:HB3	2.02	0.40
1:A:1538:VAL:CG1	1:A:1539:ALA:N	2.83	0.40
2:G:741:HIS:CE1	2:G:855:HIS:NE2	2.89	0.40
2:G:1218:ILE:HG22	2:G:1219:ILE:N	2.36	0.40
2:G:1323:MET:HE3	2:G:1357:TYR:CG	2.56	0.40
2:G:1339:PHE:O	2:G:1340:PRO:C	2.63	0.40
2:G:1592:LEU:HD23	2:G:1592:LEU:C	2.47	0.40
1:A:20:TYR:C	1:A:22:PHE:H	2.30	0.40
1:A:355:ASP:O	1:A:358:GLU:N	2.42	0.40
1:A:394:PHE:HB2	1:A:744:ASP:OD1	2.20	0.40
1:A:440:MET:O	1:A:443:SER:OG	2.36	0.40
1:A:626:VAL:HA	1:A:629:THR:HG23	2.02	0.40
1:A:768:ILE:C	1:A:769:ILE:CG1	2.94	0.40
1:A:1059:PHE:HA	1:A:1079:LYS:NZ	2.36	0.40
1:A:1244:GLY:O	1:A:1327:CYS:HA	2.21	0.40
1:A:1673:TYR:CE1	1:A:1677:VAL:CG2	3.05	0.40
2:G:118:LYS:O	2:G:121:GLU:N	2.55	0.40
2:G:409:PHE:HA	2:G:412:ARG:HD2	2.02	0.40
2:G:573:LYS:HG2	2:G:1101:GLU:HA	2.03	0.40
2:G:616:THR:C	2:G:617:ILE:HG13	2.46	0.40
2:G:875:LEU:HD23	2:G:876:PRO:O	2.22	0.40
2:G:1267:TRP:CE3	2:G:1271:ILE:HG21	2.56	0.40
2:G:1448:GLU:O	2:G:1451:GLN:OE1	2.38	0.40
2:G:1916:PHE:O	2:G:1919:LEU:HG	2.21	0.40
2:G:1988:PHE:O	2:G:1989:LYS:C	2.63	0.40
2:G:2036:GLU:N	2:G:2037:PRO:HD3	2.36	0.40
1:A:688:ILE:C	1:A:690:ALA:H	2.28	0.40
1:A:765:LEU:HA	1:A:765:LEU:HD23	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ARG:HH11	1:A:818:ARG:CB	2.35	0.40
1:A:833:PHE:HZ	1:A:871:TRP:CZ3	2.39	0.40
1:A:862:LEU:C	1:A:863:THR:HG23	2.46	0.40
1:A:1539:ALA:HB3	1:A:1541:PHE:HE1	1.87	0.40
2:G:143:SER:OG	2:G:547:ILE:O	2.38	0.40
2:G:158:ALA:O	2:G:270:ALA:HB1	2.22	0.40
2:G:214:ASN:O	2:G:218:TRP:NE1	2.55	0.40
2:G:247:ALA:O	2:G:251:VAL:HG13	2.21	0.40
2:G:1129:ALA:C	2:G:1130:THR:HG23	2.46	0.40
2:G:1152:ALA:O	2:G:1153:SER:C	2.65	0.40
2:G:1175:LYS:O	2:G:1180:MET:HE1	2.22	0.40
2:G:1216:GLU:O	2:G:1216:GLU:CG	2.70	0.40
2:G:1236:LEU:HD23	2:G:1238:LEU:HD11	2.03	0.40
2:G:1381:VAL:HG12	2:G:1390:VAL:HG12	2.04	0.40
2:G:1472:VAL:HG21	2:G:1480:PHE:CD2	2.56	0.40
2:G:1539:ILE:HB	2:G:1626:ILE:HG22	2.04	0.40
2:G:1567:ARG:O	2:G:1567:ARG:HD2	2.22	0.40
2:G:1687:ALA:HB1	2:G:1787:ALA:HB1	2.03	0.40
2:G:1791:ASP:O	2:G:1794:SER:HB3	2.21	0.40
2:G:1925:ILE:H	2:G:1925:ILE:HD12	1.86	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	1608/1887 (85%)	1329 (83%)	275 (17%)	4 (0%)	43	72
2	G	2029/2073 (98%)	1771 (87%)	258 (13%)	0	100	100
All	All	3637/3960 (92%)	3100 (85%)	533 (15%)	4 (0%)	49	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1585	LYS
1	A	179	LYS
1	A	1168	LEU
1	A	58	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1233/1566 (79%)	1231 (100%)	2 (0%)	87	96
2	G	1772/1810 (98%)	1772 (100%)	0	100	100
All	All	3005/3376 (89%)	3003 (100%)	2 (0%)	87	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1200	ILE
1	A	1378	GLU

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

Mol	Chain	Res	Type
1	A	344	GLN
1	A	407	ASN
1	A	441	ASN
1	A	465	ASN
1	A	479	ASN
1	A	654	GLN
1	A	669	ASN
1	A	698	GLN
1	A	965	HIS
1	A	969	ASN
1	A	1146	HIS
1	A	1148	HIS
1	A	1442	ASN

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Mol	Chain	Res	Type
1	A	1444	ASN
1	A	1483	ASN
1	A	1549	ASN
1	A	1598	GLN
1	A	1610	ASN
1	A	1689	HIS
1	A	1746	ASN
2	G	34	GLN
2	G	93	ASN
2	G	102	HIS
2	G	248	HIS
2	G	275	GLN
2	G	330	ASN
2	G	359	HIS
2	G	384	GLN
2	G	390	ASN
2	G	451	ASN
2	G	517	HIS
2	G	908	ASN
2	G	1002	HIS
2	G	1008	GLN
2	G	1039	HIS
2	G	1061	GLN
2	G	1087	HIS
2	G	1088	GLN
2	G	1186	ASN
2	G	1341	ASN
2	G	1383	ASN
2	G	1424	GLN
2	G	1611	GLN
2	G	1619	ASN
2	G	1778	GLN
2	G	1896	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	FMN	G	3051	-	33,33,33	1.15	2 (6%)	48,50,50	1.28	8 (16%)
3	PNS	A	1888	1	1,4,21	0.62	0	0,4,29	-	-

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	G	3051	-	-	3/18/18/18	0/3/3/3
3	PNS	A	1888	1	-	0/0/2/27	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C4A-N5	3.05	1.37	1.30
4	G	3051	FMN	C10-N1	2.21	1.37	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3051	FMN	C4-N3-C2	-3.52	119.38	125.64
4	G	3051	FMN	C4A-C4-N3	2.74	120.23	113.25
4	G	3051	FMN	C5A-C9A-N10	2.69	120.40	117.97
4	G	3051	FMN	C4A-C10-N10	2.65	120.28	116.48
4	G	3051	FMN	O4-C4-C4A	-2.61	119.65	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3051	FMN	C10-C4A-N5	-2.20	120.33	124.81
4	G	3051	FMN	C4A-C10-N1	-2.17	119.27	124.59
4	G	3051	FMN	C9A-C5A-N5	-2.01	120.33	122.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

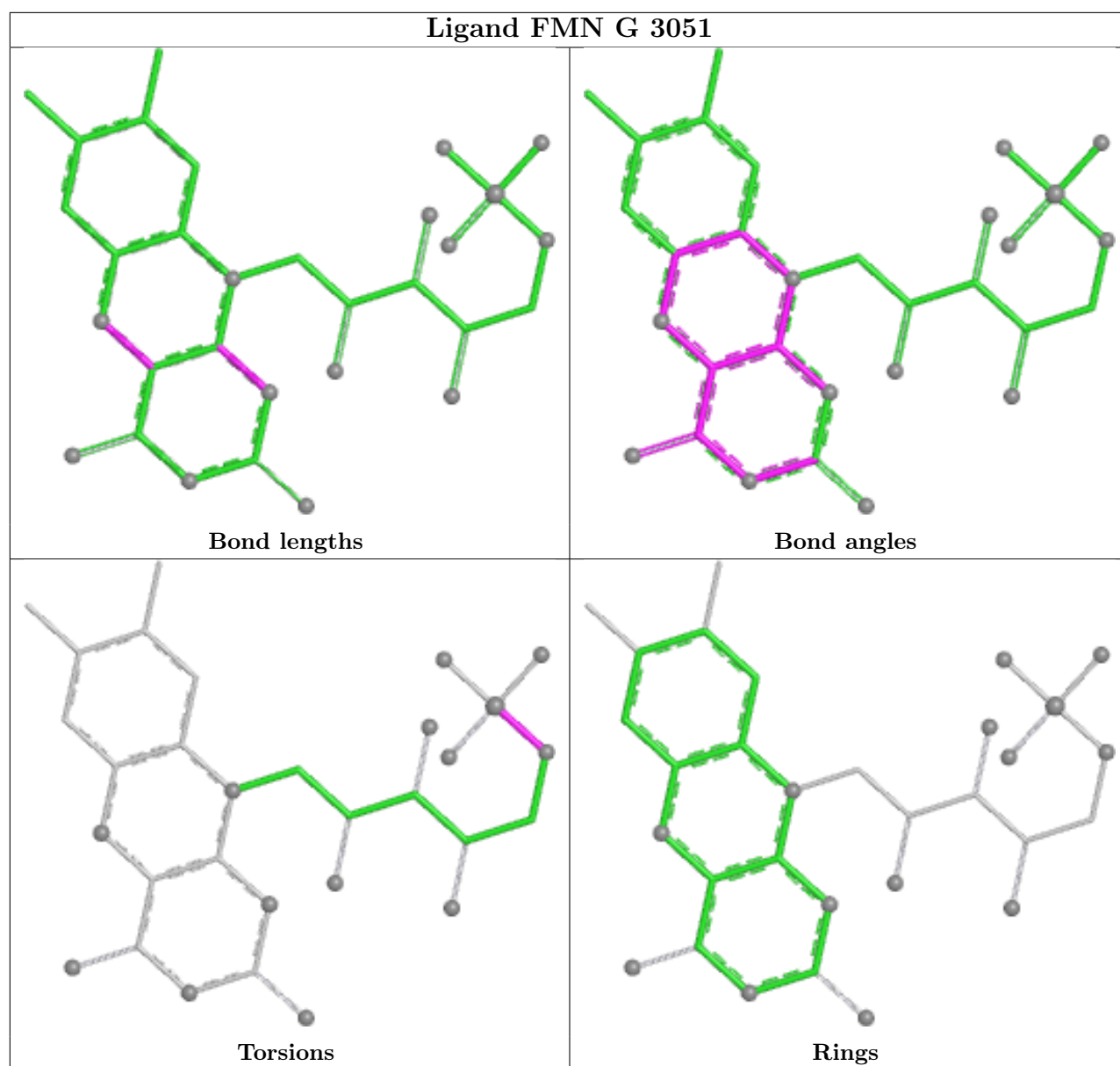
Mol	Chain	Res	Type	Atoms
4	G	3051	FMN	C5'-O5'-P-O1P
4	G	3051	FMN	C5'-O5'-P-O2P
4	G	3051	FMN	C5'-O5'-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3051	FMN	1	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.

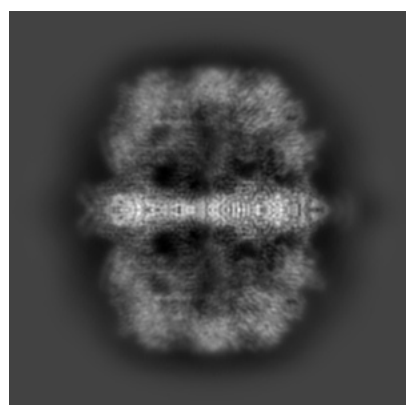
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20655. These allow visual inspection of the internal detail of the map and identification of artifacts.

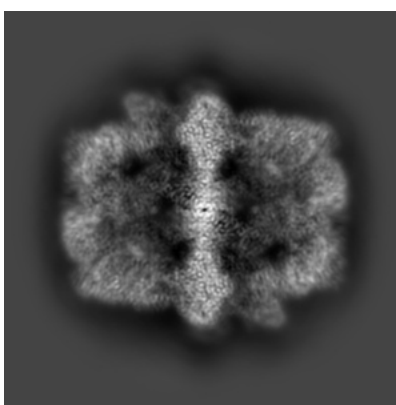
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

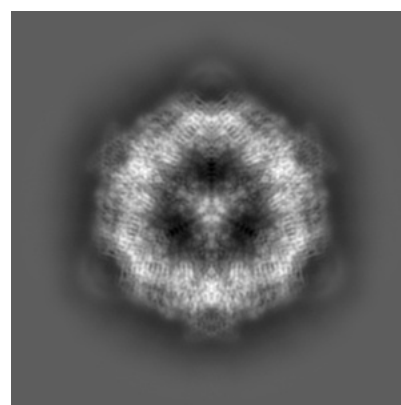
6.1.1 Primary map



X



Y

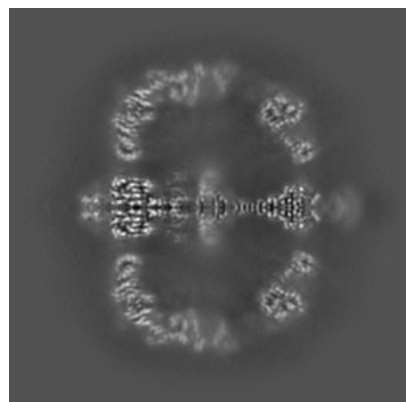


Z

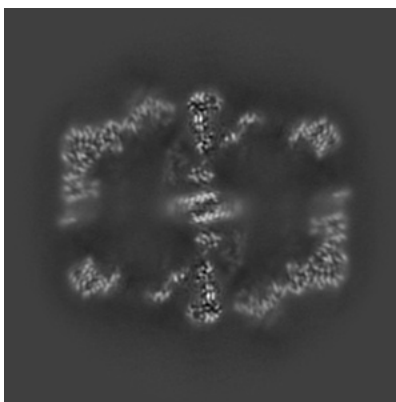
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

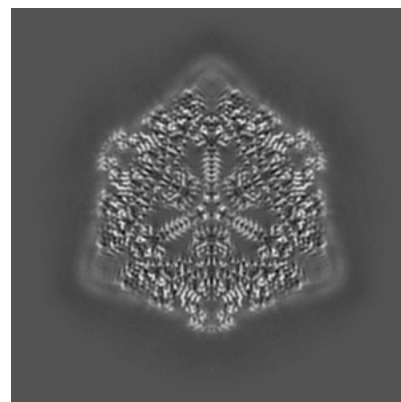
6.2.1 Primary map



X Index: 176



Y Index: 176

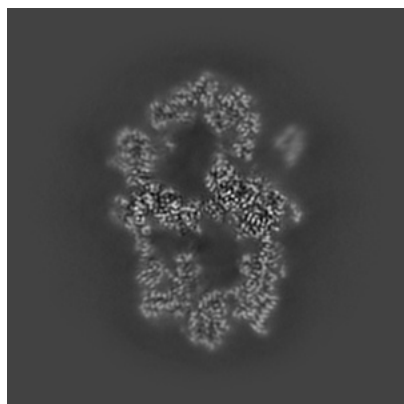


Z Index: 176

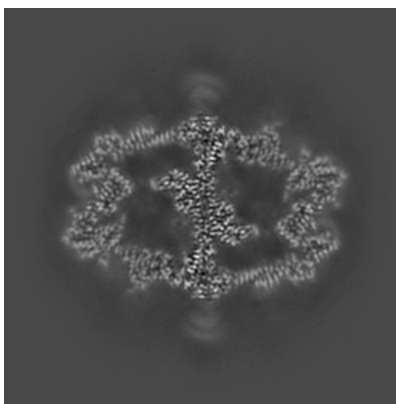
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

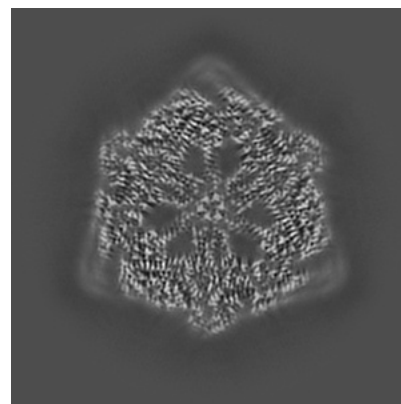
6.3.1 Primary map



X Index: 237



Y Index: 121

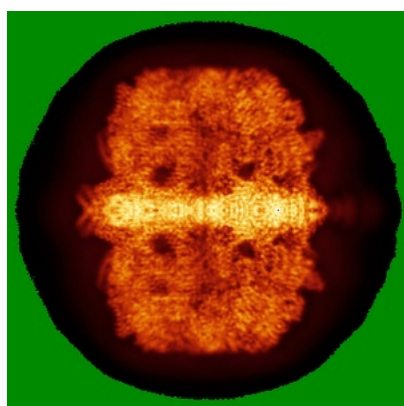


Z Index: 172

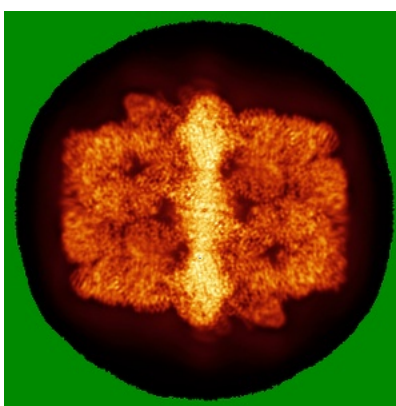
The images above show the largest variance slices of the map in three orthogonal directions.

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

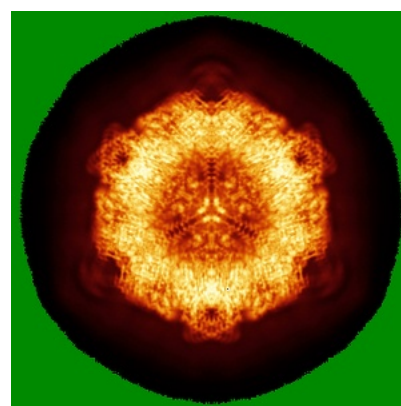
6.4.1 Primary map



X



Y

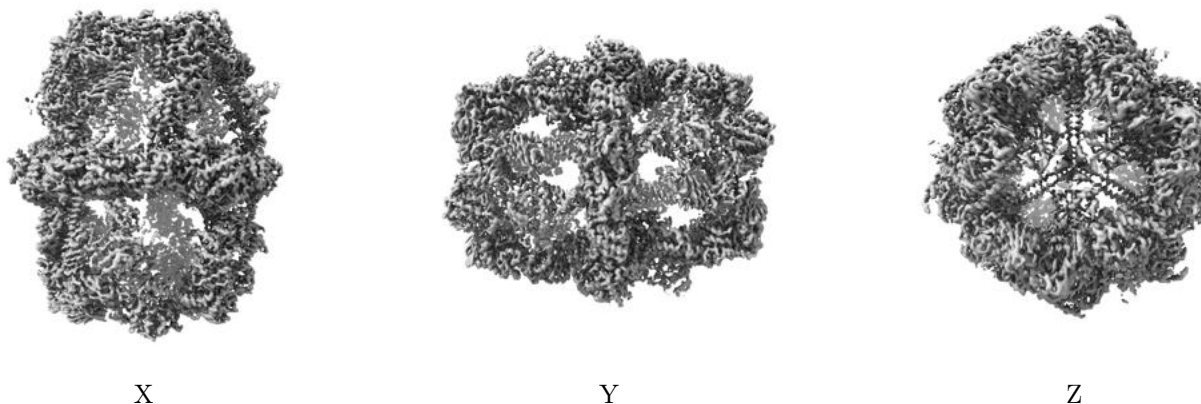


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.696. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

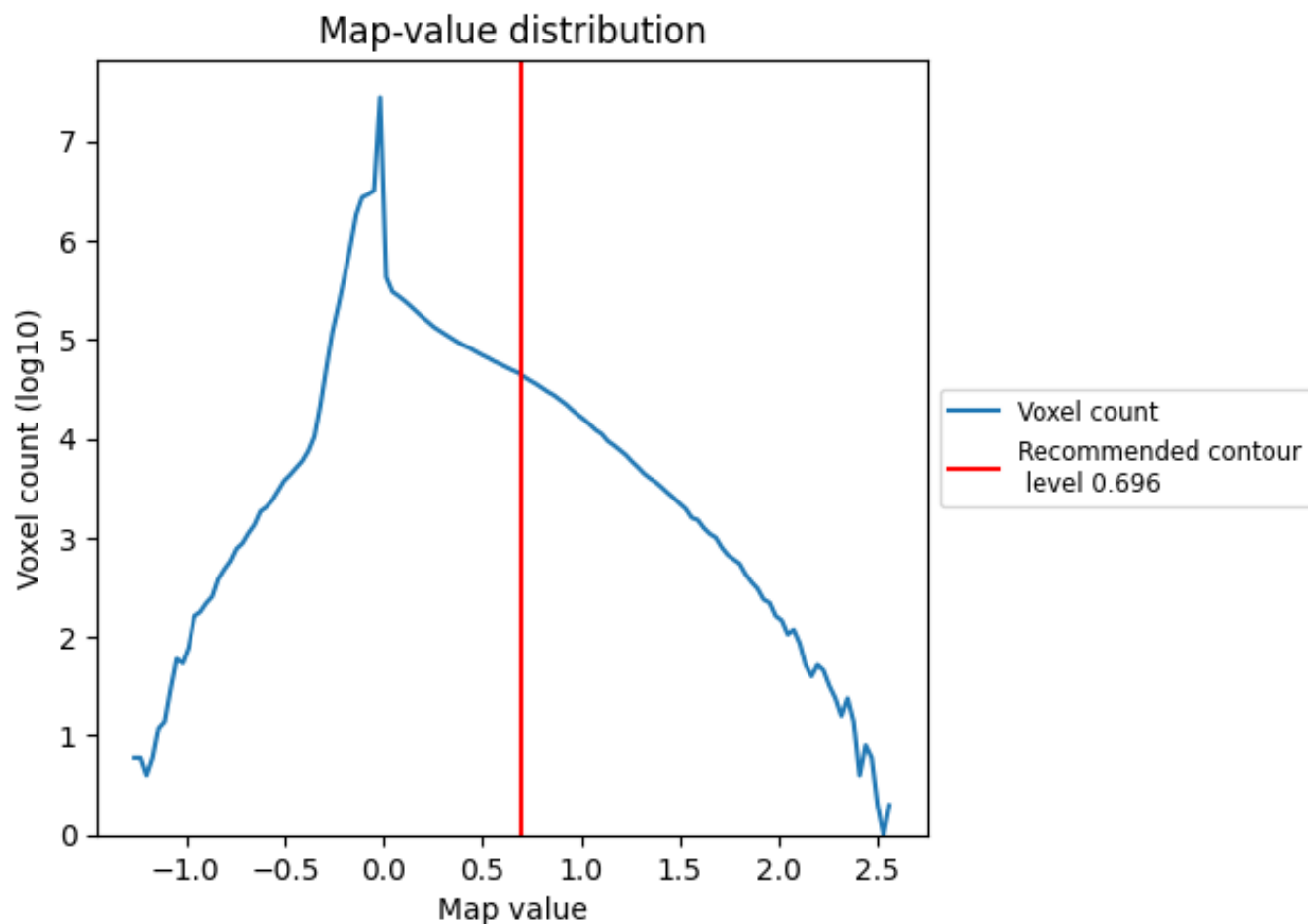
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

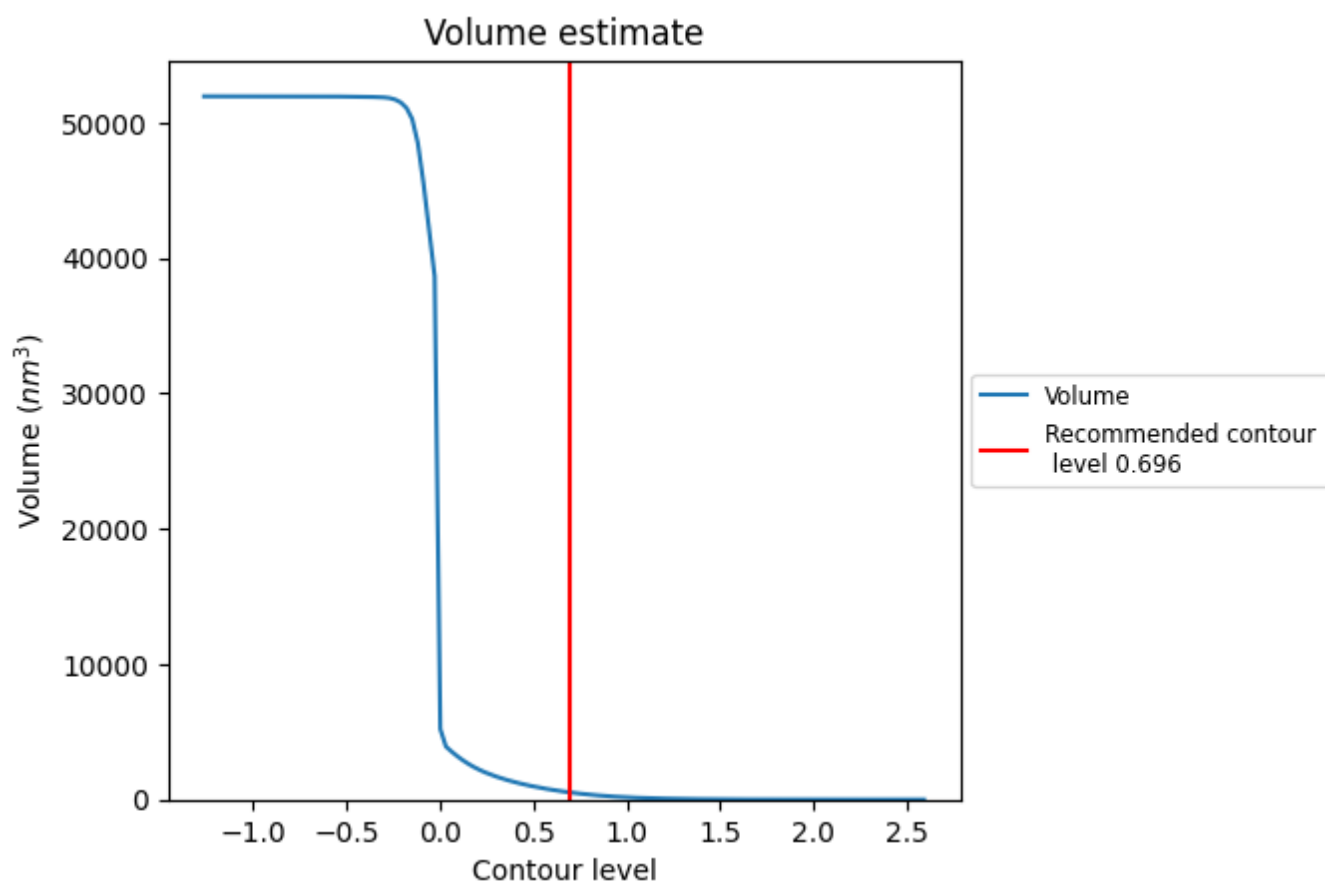
This section contains the results of statistical analysis of the map.

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.

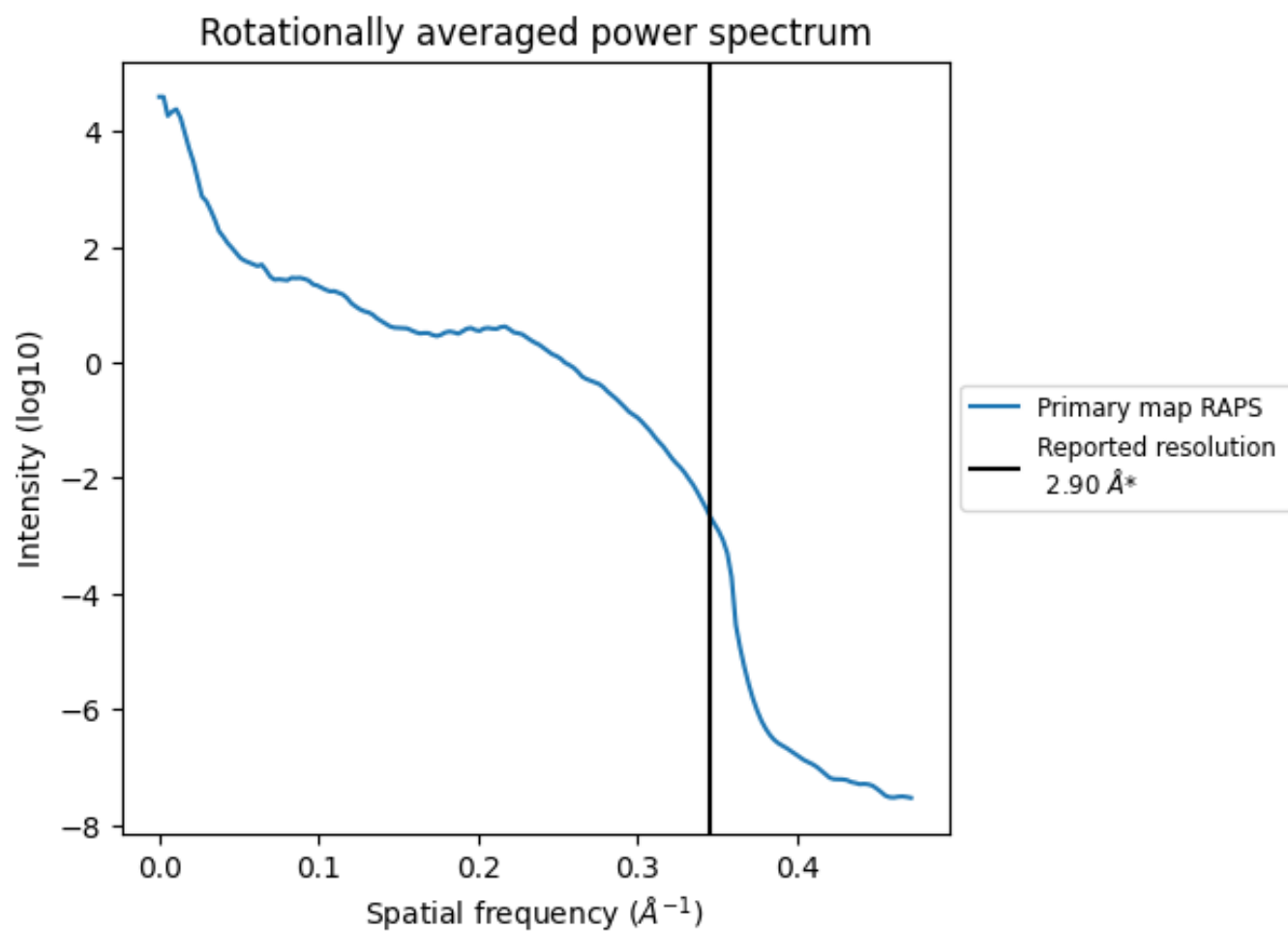
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 528 nm³; this corresponds to an approximate mass of 477 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

8 Fourier-Shell correlation ⓘ

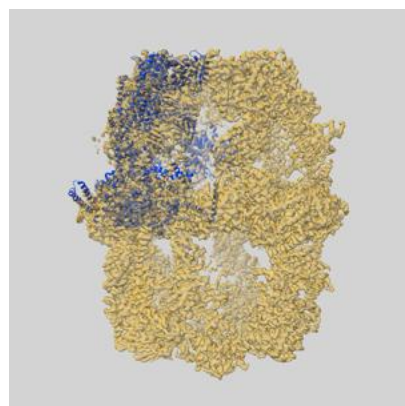
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

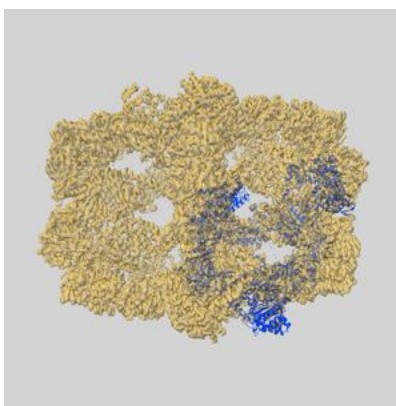
This section contains information regarding the fit between EMDB map EMD-20655 and PDB model 6U5T. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

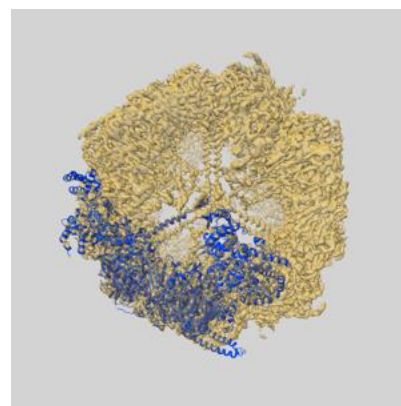
9.1.1 Map-model overlay [i](#)



X

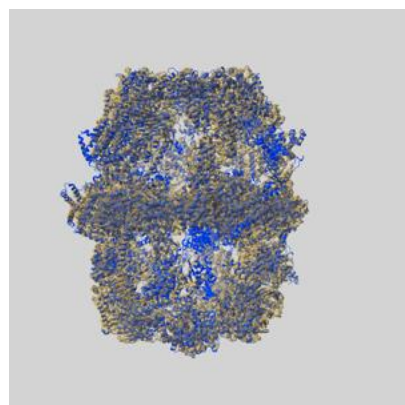


Y

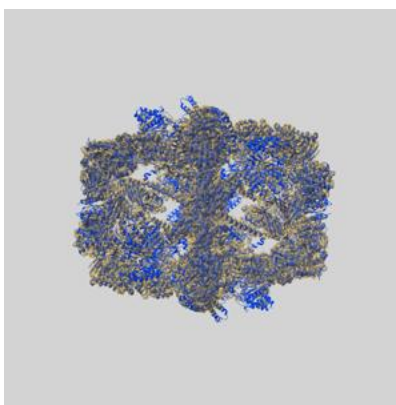


Z

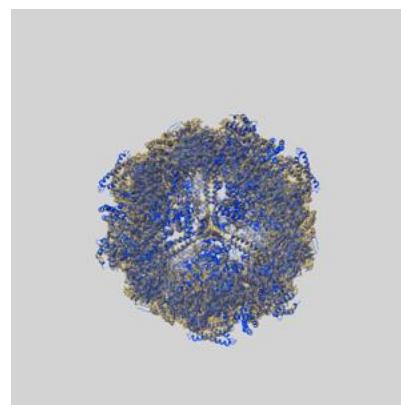
9.1.2 Map-model assembly overlay [i](#)



X



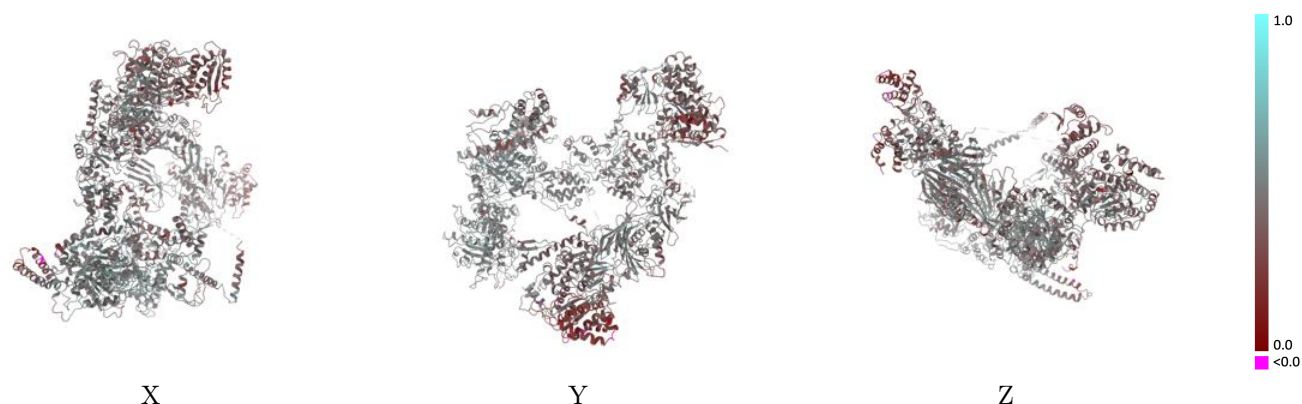
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.696 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](#)

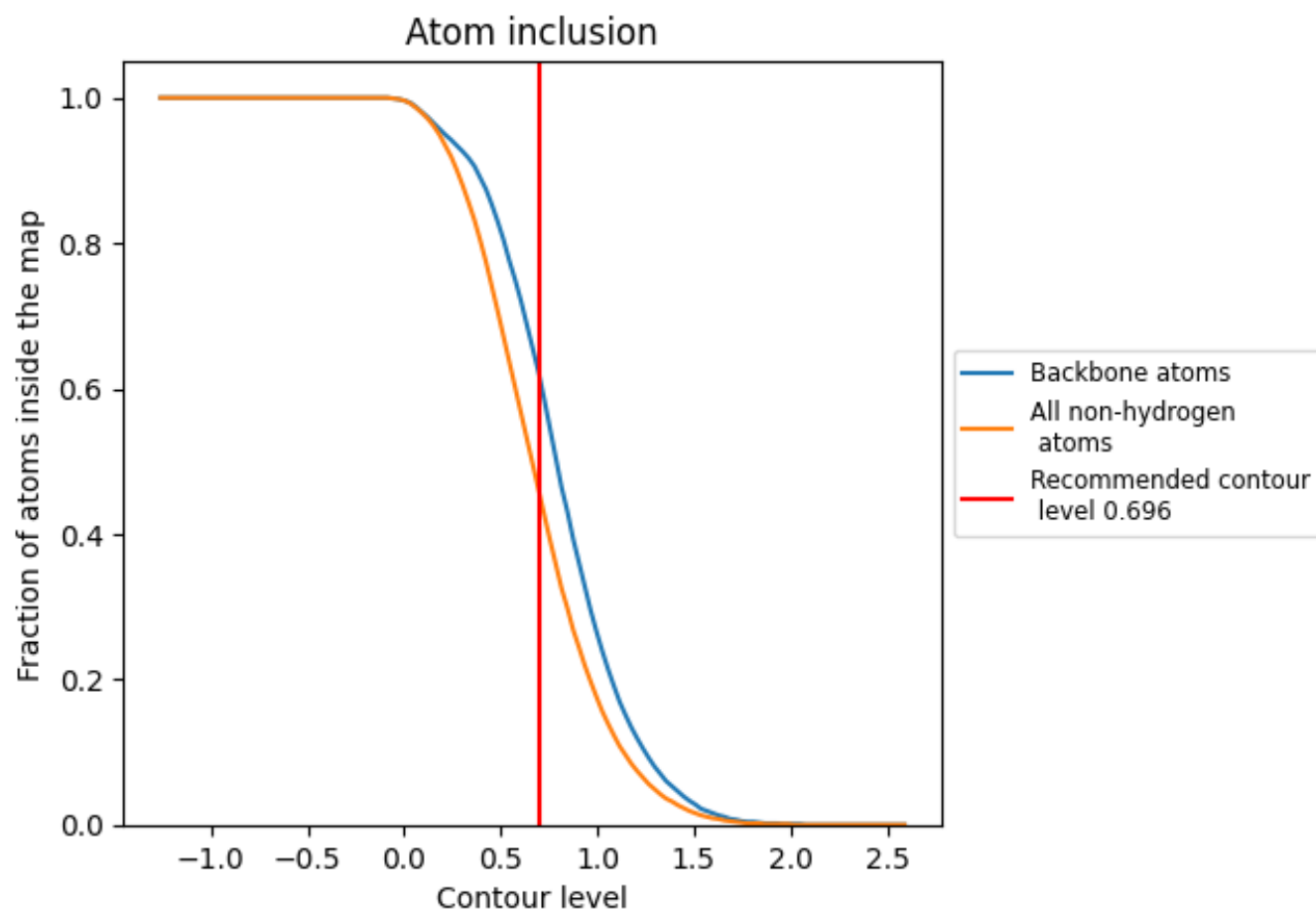


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.696) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4620	0.4420
A	0.5340	0.4690
G	0.4070	0.4210

