



Full wwPDB EM Validation Report ⓘ

Mar 22, 2025 – 05:08 PM EDT

PDB ID : 6U5T
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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

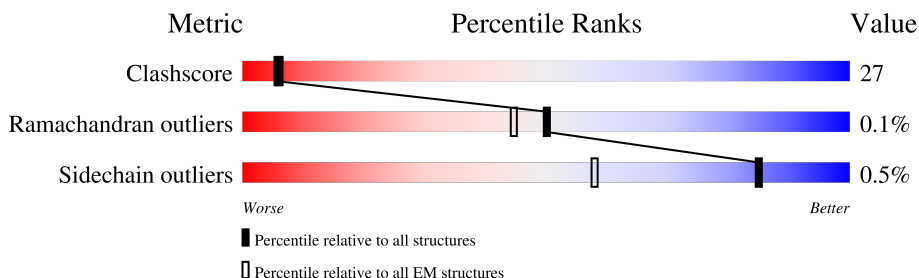
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1887	<div> <div>26%</div> <div>47%</div> <div>38%</div> <div>14%</div> </div>
2	G	2073	<div> <div>46%</div> <div>50%</div> <div>48%</div> <div>.</div> </div>

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:

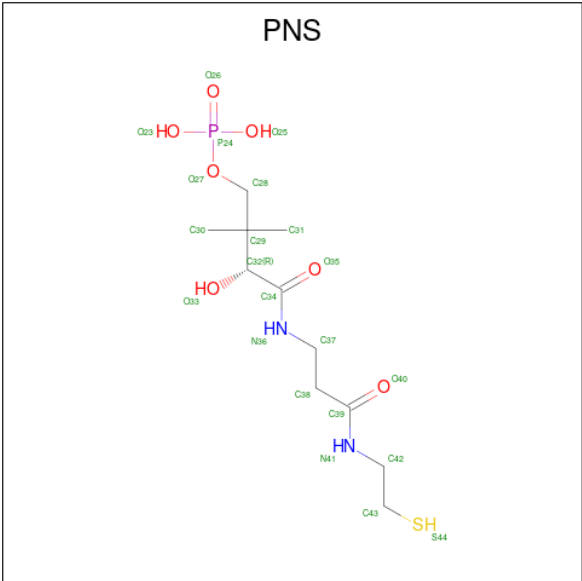
Chain	Residue	Modelled	Actual	Comment	Reference
G	2052	ASP	-	expression tag	UNP P07149
G	2053	TYR	-	expression tag	UNP P07149
G	2054	LYS	-	expression tag	UNP P07149
G	2055	ASP	-	expression tag	UNP P07149
G	2056	HIS	-	expression tag	UNP P07149
G	2057	ASP	-	expression tag	UNP P07149
G	2058	GLY	-	expression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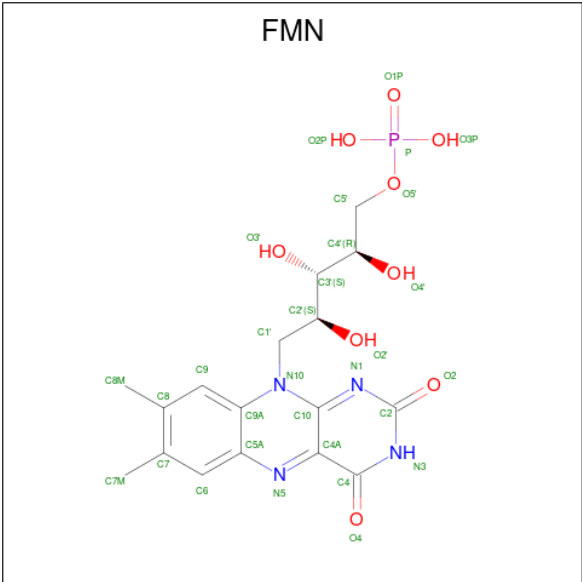
Chain	Residue	Modelled	Actual	Comment	Reference
G	2073	LYS	-	expression tag	UNP P07149

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C₁₁H₂₃N₂O₇PS).



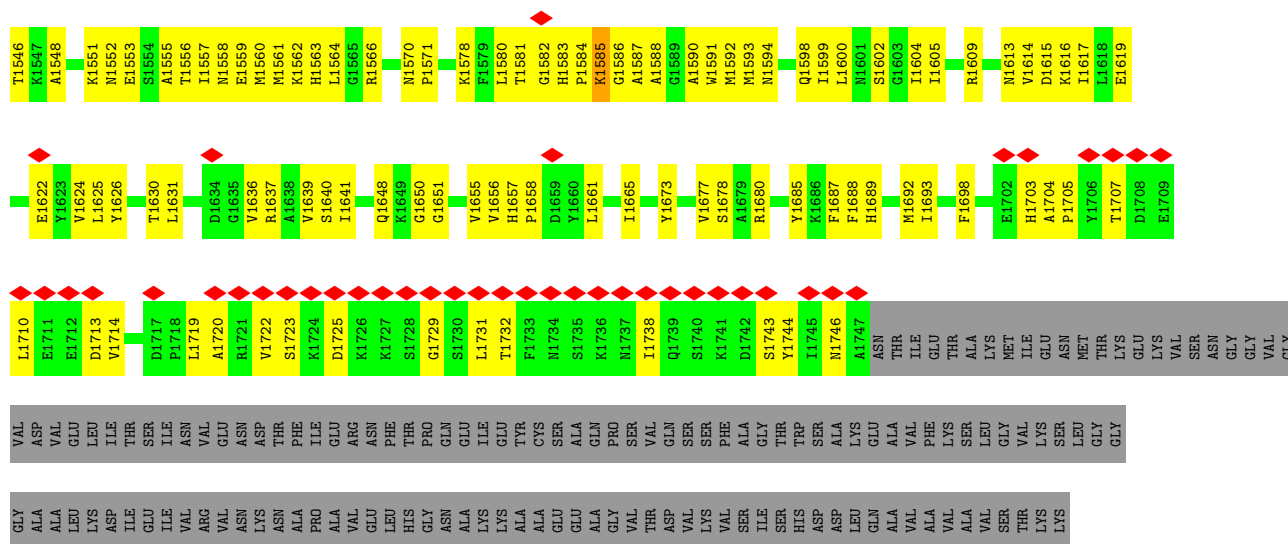
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			5	1	3	1	

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

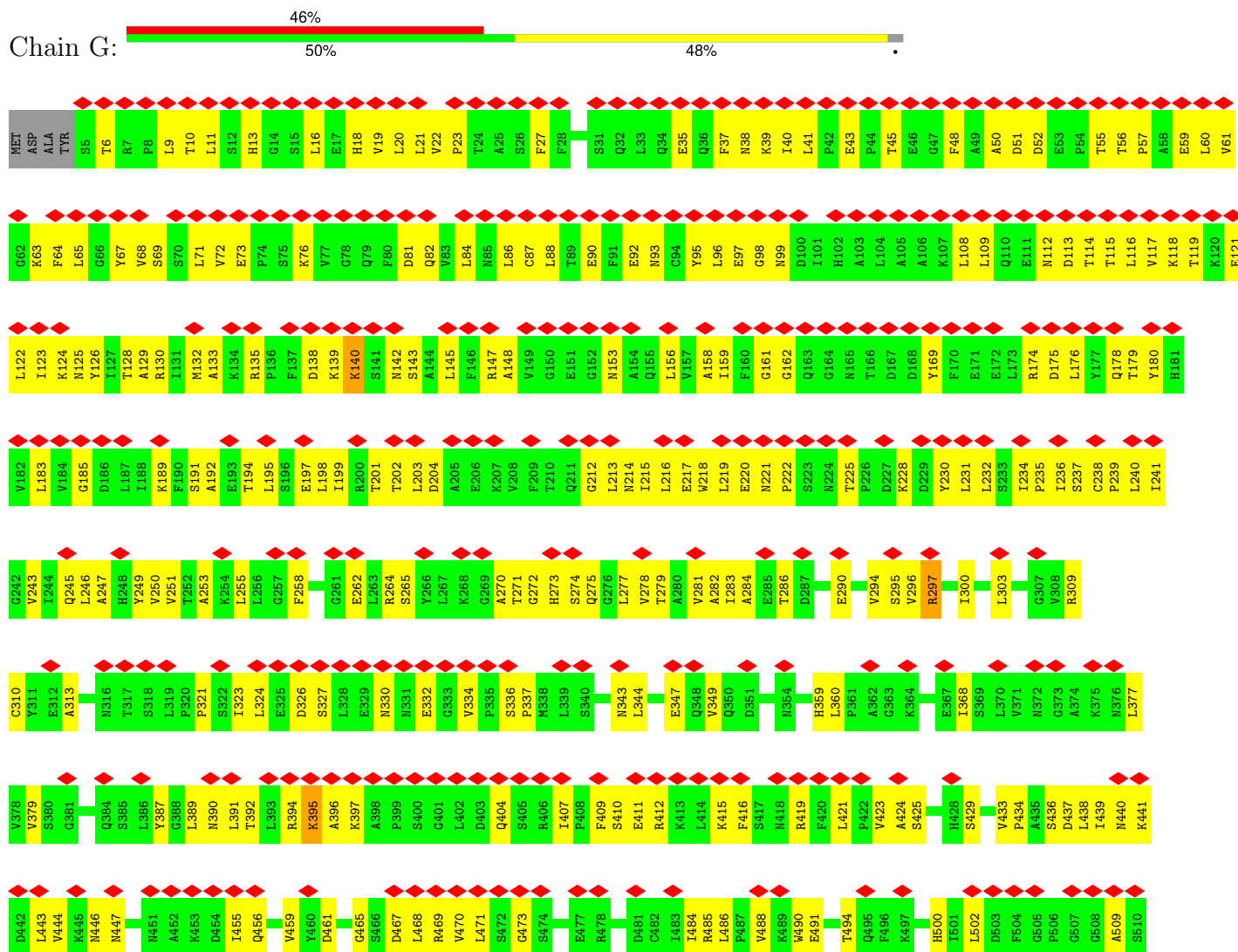


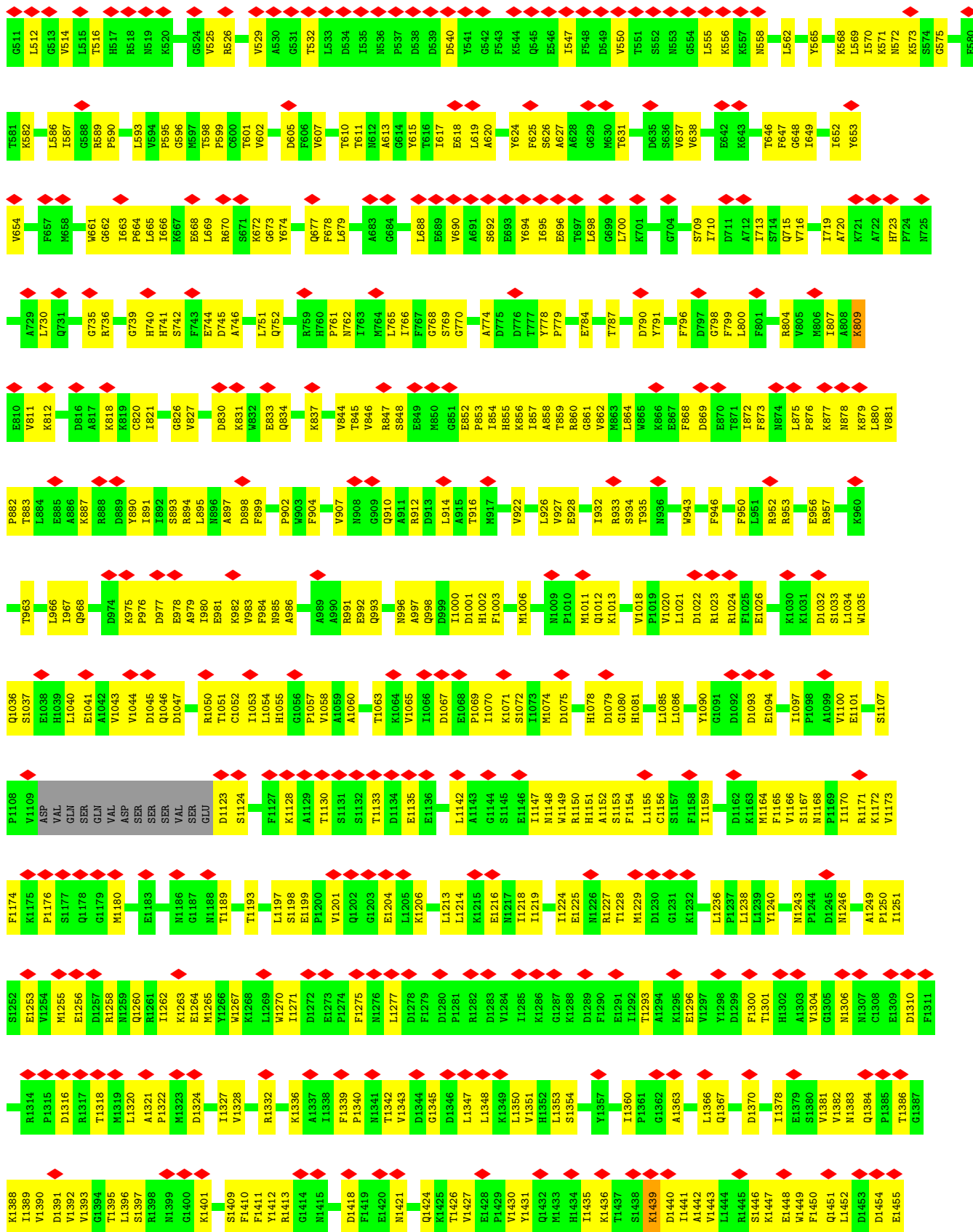
Mol	Chain	Residues	Atoms					AltConf
4	G	1	Total	C	N	O	P	0
			31	17	4	9	1	

GLU	GLU	D600	◆
SER	SER	V601	◆
SER	SER	E602	◆
LVS	LVS	D603	◆
GLU	GLU	A604	◆
ILE	ILE	L605	◆
ASP	ASP	D606	◆
PRO	PRO	K607	◆
SER	SER	D608	◆
GLN	GLN	S609	◆
THR	THR	T610	◆
THR	THR	K611	◆
GLN	GLN	E612	◆
LEU	LEU	V613	◆
ALA	ALA	A614	◆
GLY	GLY	S615	◆
MET	MET	L616	◆
D600	K650	◆	◆
V601	T651	◆	◆
E602	D652	◆	◆
D603	R653	◆	◆
A604	Q654	◆	◆
L605	L655	◆	◆
D606	S656	◆	◆
K607	S657	◆	◆
D608	L658	◆	◆
S609	F659	◆	◆
T610	L660	◆	◆
K611	D661	◆	◆
E612	G662	◆	◆
V613	L663	◆	◆
A614	E664	◆	◆
S615	K665	◆	◆
L616	A666	◆	◆
K619	V671	◆	◆
S620	T672	◆	◆
T621	T673	◆	◆
I622	Y677	◆	◆
S623	V678	◆	◆
K624	L679	◆	◆
T625	I680	◆	◆
V626	G684	◆	◆
S627	G685	◆	◆
S628	T686	◆	◆
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R632	T688	◆	◆
E633	T689	◆	◆
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V649	T696	◆	◆
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T651	T698	◆	◆
D652	T699	◆	◆
R653	T700	◆	◆
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L658	T705	◆	◆
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L660	T707	◆	◆
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T987	T1024	◆	◆
T988	T1025</		



• Molecule 2: Fatty acid synthase subunit beta





E2046	DI456	V1531	G1668	DI743	A1805	S1865	I1925	V1985	E2046
K2047	DI457	N1532	Q1669	G1744	G1806	F1866	E1926	K1986	K2047
Y2048	DI458	L1533	G1670	K1745	H1807	S1867	L1927	F1987	Y2048
E2049	L1459	E1534	S1671	L1746	S1808	Q1868	Q1928	K1989	E2049
Q2050	L1460	N1535	Q1672	K1747	L1809	L1810	S1930	S1990	Q2050
SER	N1461	P1536	E1673	T1748	G1811	E1811	L1871	F1991	SER
ASP	F1466	I1537	Q1674	E1749	Y1812	Y1812	L1931	L1992	ASP
TYR	E1467	P1538	G1675	K1750	A1813	Q1872	S1932	K1993	TYR
LYS	T1468	I1539	M1676	I1751	L1814	Y1873	L1933	K1994	LYS
ASP	E1469	A1540	M1678	K1753	L1815	V1874	L1934	N1995	ASP
ASP	V1472	V1541	D1679	E1754	A1816	V1875	E1935	I1996	ASP
GLY	K1475	L1542	L1680	I1755	S1817	E1876	V1936	I1997	GLY
TYR	N1476	D1543	Y1681	E1757	L1818	R1877	E1937	K1998	TYR
LYS	A1477	S1544	Y1682	K1758	A1819	V1878	G1938	E1999	LYS
ASP	N1478	T1546	T1682	H1759	D1820	G1879	H1939	N2000	ASP
HIS	I1479	Y1546	T1683	S1760	V1821	K1880	L1940	V2001	HIS
ASP	F1480	P1547	S1684	T1760	M1822	R1881	F1941	K2002	ASP
ASP	K1484	S1548	K1685	S1761	S1823	T1882	E1942	A2004	ASP
ASP	C1485	T1549	A1686	Y1762	I1824	G1883	I1943	R2005	ASP
ASP	I1489	N1550	A1687	T1763	E1825	W1884	I1944	G2008	ASP
ASP	K1490	E1551	Q1688	F1764	S1826	L1885	D1945	K2009	ASP
LYS	V1491	P1552	W1690	S1765	L1827	V1886	E1946	Y2010	LYS
K1496	D1559	R1555	V1691	E1767	V1828	E1887	A1947	T2011	K1496
E1497	L1560	D1569	K1692	K1768	E1829	I1888	S1948	P2012	E1497
T1498	I1563	I1563	A1693	L1770	V1830	M1889	K1949	N2013	T1498
V1499	H1564	I1563	A1694	L1771	F1832	N1890	L2014	L2014	V1499
E1500	S1565	E1500	D1695	S1772	Y1833	Y1891	S1951	A2016	E1500
I1501	S1566	I1501	F1698	A1773	G1834	M1892	A1952	K2017	I1501
G1502	S1567	G1502	S1705	I1774	E1835	V1893	E1894	P2018	G1502
V1504	R1567	V1504	L1707	K1775	M1836	M1895	T1837	F2019	V1504
D1505	H1568	D1505	DI708	Q1776	N1838	Q1896	Q1955	Q2020	D1505
Y1506	F1569	Y1506	I1709	F1776	Q1839	Q1897	R1956	Q2020	Y1506
E1507	Y1572	E1507	V1710	T1777	V1840	Y1898	P1957	V2021	E1507
A1510	N1573	A1510	I1711	Q1778	A1841	V1899	L1958	T2022	A1510
S1511	L1575	S1511	M1712	T1778	V1842	A1900	K1959	E2024	S1511
H1512	P1576	H1512	N1713	P1783	P1843	A1901	L1960	Y2025	H1512
G1513	G1577	G1513	P1714	L1783	D1845	G1902	E1961	F2026	G1513
N1514	T1578	N1514	V1715	M1784	E1846	D1903	R1962	Q2027	N1514
D1518	I1579	D1518	T1718	A1787	L1847	R1905	G1963	D2028	D1518
F1519	T1580	F1519	I1719	A1788	G1848	A1906	F1964	V2029	F1519
L1520	H1581	L1520	R1728	F1789	L1849	L1907	A1965	Y2030	L1520
K1521	G1582	K1521	R1729	E1790	S1850	D1908	C1966	D2031	K1521
R1522	M1583	R1522	R1730	L1792	N1851	T1909	I1967	L2032	R1522
N1523	F1584	N1523	E1731	E1793	Y1852	V1910	L1969	T2033	N1523
G1524	R1590	G1524	S1734	K1793	G1853	T1911	V1970	G2034	G1524
S1525	A1591	S1525	A1735	S1794	M1854	N1912	G1971	S2035	S1525
T1526	S1592	T1526	M1736	K1795	I1855	V1913	I1972	E2036	T1526
L1527	I1593	L1527	I1737	G1796	T1856	L1914	L1973	T2037	L1527
E1528	E1594	E1528	F1738	L1797	A1856	N1915	V1974	I2038	E1528
Q1529	N1595	Q1529	E1739	I1798	I1857	F1916	N1975	K2039	Q1529
K1530	W1596	K1530	T1740	P1799	M1858	I1917	P1976	E2040	K1530
	A1597		I1741	A1800	G1860	K1918	F1977	I2041	
	A1598		VI742	D1801	R1861	L1919	H1977	I2042	
	D1599			A1802	Y1862	Q1920	S1978	D2043	
				T1803	V1863	K1921	T1979	N2044	
				F1804	A1864	I1922	Y1980	W2045	
						D1923	L1981		
						I1924	M1982		
							N1983		
							G1984		

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 (\AA)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PNS, FMN

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	0.64	0/12424	0.54	0/16819
2	G	0.47	0/16360	0.49	0/22198
All	All	0.55	0/28784	0.51	0/39017

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

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12202	0	11715	648	0
2	G	15995	0	15978	878	0
3	A	5	0	0	0	0
4	G	31	0	19	1	0
All	All	28233	0	27712	1488	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 27.

All (1488) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1054:LEU:HD12	4:G:3051:FMN:HM72	1.72	0.71
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
2:G:1236:LEU:HD22	2:G:1265:MET:CE	2.21	0.70
1:A:1584:PRO:CB	1:A:1587:ALA:HB3	2.19	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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:582:LYS:NZ	2:G:761:PRO:O	2.26	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
1:A:1107:GLU:OE1	1:A:1191:THR:OG1	2.11	0.66
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
1:A:695:GLY:O	1:A:698:GLN:N	2.27	0.66
2:G:270:ALA:O	2:G:271:THR:OG1	2.08	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:1318:THR:O	2:G:1318:THR:HG23	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:27:ARG:NH1	2:G:2014:LEU:O	2.30	0.64
1:A:519:VAL:HG11	1:A:894:ARG:HH12	1.63	0.64
1:A:78:ILE:C	1:A:79:LEU:HD12	2.18	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
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
2:G:115:THR:HG21	2:G:118:LYS:HZ3	1.63	0.64
1:A:430:ARG:NE	1:A:606:ASP:OD1	2.31	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:1501:LEU:HD23	1:A:1502:ARG:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:655:LEU:C	1:A:655:LEU:HD23	2.19	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:748:LEU:HD23	1:A:748:LEU:C	2.20	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
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
2:G:1013:LYS:NZ	2:G:1032:ASP:OD2	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1213:LEU:C	2:G:1214:LEU:HD22	2.21	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:1236:LEU:HD22	2:G:1265:MET:HE1	1.82	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
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:626:SER:OG	2:G:627:ALA:N	2.34	0.60
2:G:1710:VAL:HA	2:G:1771:LEU:HD21	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:142:ASN:C	2:G:550:VAL:HG12	2.23	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:893:VAL:HG12	1:A:894:ARG:N	2.18	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
1:A:1333:ASP:CG	1:A:1584:PRO:O	2.42	0.58
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:THR:HG21	2:G:108:LEU:HD11	1.86	0.58
1:A:1335:PHE:CE1	1:A:1378:GLU:CD	2.77	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: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
1:A:1501:LEU:O	1:A:1504:ALA:N	2.35	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:1236:LEU:HD22	2:G:1265:MET:HE3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:G:1850:SER:OG	2:G:1851:ASN:N	2.37	0.57
1:A:1333:ASP:OD2	1:A:1586:GLY:N	2.32	0.56
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
1:A:1544:THR:O	1:A:1545:SER:HB3	2.06	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
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
2:G:975:LYS:NZ	2:G:978:GLU:OE1	2.27	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	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:470:VAL:HG23	2:G:470:VAL:O	2.07	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1033:SER:C	2:G:1034:LEU:HD12	2.28	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:9:LEU:HD23	2:G:9:LEU:C	2.29	0.53
2:G:568:LYS:C	2:G:569:LEU:HD22	2.29	0.53
2:G:1351:VAL:HG21	2:G:1413:ARG:NH2	2.23	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: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:1185:VAL:HB	1:A:1377:MET:HE1	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:20:LEU:HD12	2:G:90:GLU:CD	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:800:LEU:C	2:G:800:LEU:HD12	2.28	0.53
2:G:1032:ASP:O	2:G:1036:GLN:NE2	2.39	0.53
2:G:1926:GLU:O	2:G:1930:SER:OG	2.11	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: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
2:G:1685:LYS:NZ	2:G:1689:ASP:OD2	2.35	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
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:988:ILE:HG22	1:A:989:GLN:N	2.25	0.52
1:A:1115:ASN:O	1:A:1118:LYS:N	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
1:A:1636:VAL:HG12	1:A:1637:ARG:N	2.24	0.51
1:A:420:ILE:HG21	1:A:469:VAL:HG13	1.92	0.51
1:A:1106:ILE:HD12	1:A:1184:LEU:C	2.30	0.51
1:A:1648:GLN:O	1:A:1650:GLY:N	2.43	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: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: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:1424:GLY:O	1:A:1427:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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: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
1:A:14:LEU:C	1:A:14:LEU:HD23	2.32	0.50
1:A:608:ASP:OD2	1:A:611:LYS:NZ	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1581:THR:OG1	1:A:1582:GLY:N	2.45	0.50
2:G:174:ARG:NH2	2:G:219:LEU:HA	2.27	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:71:ALA:C	1:A:72:LEU:HD23	2.32	0.49
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
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: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:1403:ILE:CG2	1:A:1404:VAL:N	2.75	0.49
1:A:1463:VAL:HG23	1:A:1464:GLU:N	2.27	0.49
1:A:1555:ALA:O	1:A:1558:ASN:N	2.44	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
2:G:1173:VAL:HG13	2:G:1174:PHE:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:927:VAL:HG13	2:G:928:GLU:N	2.28	0.49
2:G:1458:ASP:C	2:G:1459:LEU:HD12	2.34	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:270:ALA:C	2:G:271:THR:HG1	2.11	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:732:LEU:C	1:A:733:ILE:HD12	2.34	0.48
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:1321:ALA:HB1	2:G:1322:PRO:HD2	1.95	0.48
2:G:1737:ILE:O	2:G:1833:TYR:OH	2.25	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
1:A:1110:LEU:HD12	1:A:1110:LEU:N	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1854:MET:HG3	2:G:1969:LEU:HD12	1.94	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: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:1625:LEU:C	1:A:1626:TYR:CD2	2.87	0.48
1:A:658:LEU:C	1:A:658:LEU:HD12	2.33	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:1877:ARG:CZ	2:G:1944:ILE:HD13	2.44	0.48
1:A:1185:VAL:CG2	1:A:1377:MET:CE	2.92	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:753:TYR:O	1:A:813:ARG:NH2	2.47	0.47
1:A:953:VAL:HG23	1:A:954:ARG:N	2.29	0.47
2:G:21:LEU:C	2:G:21:LEU:HD23	2.35	0.47
2:G:807:ILE:HD13	2:G:1065:VAL:O	2.14	0.47
2:G:1484:LYS:HZ3	2:G:1507:GLU:HB3	1.80	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: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
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:1454:ASP:OD1	2:G:1454:ASP:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:359:HIS:C	2:G:360:LEU:HD12	2.34	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:1186:ALA:HB2	1:A:1378:GLU:OE1	2.14	0.47
2:G:387:TYR:CE2	2:G:391:LEU:HD11	2.49	0.47
2:G:766:ILE:HG23	2:G:798:GLY:C	2.35	0.47
2:G:1316:ASP:OD1	2:G:1316:ASP:C	2.53	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
1:A:1335:PHE:HE1	1:A:1378:GLU:CD	2.19	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:1796:GLY:C	2:G:1797:LEU:HD12	2.35	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
1:A:427:ASN:ND2	1:A:608:ASP:OD1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:806:VAL:HG23	1:A:807:LYS:N	2.30	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
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: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:1918:LYS:HD3	2:G:1964:PHE:HB3	1.97	0.46
1:A:1040:GLU:HA	1:A:1580:LEU:HD11	1.97	0.46
1:A:1075:TRP:C	1:A:1076:VAL:HG23	2.36	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
2:G:1737:ILE:C	2:G:1751:ILE:HD11	2.35	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:493:VAL:HG12	1:A:493:VAL:O	2.15	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
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:1:MET:HE1	2:G:2048:TYR:HA	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1501:LEU:HD23	1:A:1501:LEU:C	2.36	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
1:A:420:ILE:HD13	1:A:469:VAL:CG1	2.45	0.46
1:A:1384:ILE:HG13	1:A:1385:GLN:N	2.31	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:861:GLY:HA2	2:G:898:ASP:O	2.16	0.45
2:G:996:ASN:OD1	2:G:996:ASN:C	2.54	0.45
2:G:1170:ILE:HA	2:G:1173:VAL:HG12	1.99	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
2:G:278:VAL:HG23	2:G:279:THR:H	1.80	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
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:395:SER:OG	1:A:398:LYS:N	2.43	0.45
1:A:948:VAL:HG23	1:A:949:GLU:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1149:GLY:O	1:A:1151:LYS:HG2	2.17	0.45
1:A:1184:LEU:HD12	1:A:1184:LEU:C	2.36	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:525:VAL:C	2:G:526:ARG:HD3	2.37	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: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:1604:ILE:HG22	1:A:1605:ILE:N	2.31	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:1442:ASN:O	1:A:1448:ARG:NE	2.49	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
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
1:A:79:LEU:HD21	1:A:87:GLU:HB3	1.99	0.45
1:A:745:VAL:C	1:A:747:ALA:H	2.20	0.45
1:A:768:ILE:CG2	1:A:770:PRO:HD3	2.47	0.45
1:A:1076:VAL:HG12	1:A:1077:ASP:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1245:ASN:OD1	1:A:1245:ASN:C	2.56	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
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:1624:VAL:C	1:A:1625:LEU:HD23	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:88:LEU:HD23	2:G:135:ARG:HD2	1.99	0.44
2:G:240:LEU:N	2:G:240:LEU:HD12	2.33	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
2:G:1678:MET:HE1	2:G:1691:TRP:CD2	2.53	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
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: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
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:1012:LEU:C	1:A:1013:LEU:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1263:ASP:O	1:A:1266:LYS:N	2.35	0.44
2:G:126:TYR:C	2:G:126:TYR:CD2	2.91	0.44
2:G:1135:GLU:HA	2:G:1176:PRO:HG2	1.98	0.44
2:G:1395:THR:C	2:G:1396:LEU:HD12	2.38	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: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:86:LEU:HD23	2:G:86:LEU:C	2.38	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
1:A:915:GLU:O	1:A:918:GLN:N	2.51	0.43
1:A:1063:HIS:CE1	1:A:1081:LYS:HZ1	2.36	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
2:G:72:VAL:CG1	2:G:73:GLU:N	2.81	0.43
2:G:695:ILE:HD11	2:G:723:HIS:ND1	2.33	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:644:THR:OG1	1:A:648:ASP:OD2	2.32	0.43
1:A:748:LEU:O	1:A:751:PHE:HB3	2.17	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:10:THR:HG23	2:G:10:THR:O	2.18	0.43
2:G:698:LEU:O	2:G:700:LEU:N	2.50	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
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:1388:MET:HE3	1:A:1392:LEU:HD23	2.01	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:334:VAL:HG23	2:G:334:VAL:O	2.18	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
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:637:VAL:HG23	2:G:638:VAL:N	2.34	0.43
2:G:846:VAL:O	2:G:853:PRO:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:795:MET:O	1:A:799:ILE:HB	2.19	0.43
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: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: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:1207:GLN:HG2	1:A:1208:VAL:HG23	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:587:ILE:HG13	2:G:589:ARG:H	1.84	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:1185:VAL:HB	1:A:1377:MET:CE	2.49	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: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
1:A:36:LEU:HD23	1:A:65:TYR:HD2	1.84	0.42
1:A:715:THR:O	1:A:718:TYR:N	2.52	0.42
1:A:1303:GLY:O	1:A:1304:ALA:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1822:MET:HE3	2:G:1827:LEU:HD13	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:1229:THR:OG1	1:A:1687:PHE:CD1	2.63	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:1638:ILE:HG22	2:G:1639:LYS:N	2.34	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:803:MET:C	1:A:805:CYS:H	2.23	0.42
1:A:1688:PHE:O	1:A:1692:MET:HB2	2.20	0.42
2:G:68:VAL:HG13	2:G:69:SER:N	2.33	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:273:HIS:O	2:G:274:SER:C	2.58	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
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: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:1185:VAL:C	1:A:1377:MET:HE3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:ILE:O	1:A:1280:ILE:HG22	2.19	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
2:G:1236:LEU:HB2	2:G:1265:MET:HE3	2.02	0.42
1:A:47:ILE:HG21	2:G:1666:PHE:HE2	1.84	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:228:LYS:O	2:G:230:TYR:N	2.52	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: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:451:MET:O	1:A:452:GLU:C	2.57	0.42
1:A:663:LEU:HA	1:A:666:ALA:HB3	2.01	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
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
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
1:A:1677:VAL:O	1:A:1678:SER:C	2.57	0.41
2:G:677:GLN:NE2	2:G:1165:PHE:CD2	2.88	0.41
2:G:1378:ILE:CD1	2:G:1392:VAL:HG22	2.47	0.41
2:G:1593:ILE:O	2:G:1594:GLU:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1997:ILE:HD12	2:G:2000:ASN:ND2	2.34	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
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:1929:LYS:HD2	2:G:1929:LYS:N	2.35	0.41
2:G:2041:ILE:HG23	2:G:2047:LYS:HZ1	1.85	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: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: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
1:A:659:PHE:CE1	1:A:663:LEU:HD21	2.55	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: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
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:1595:ASN:N	2:G:1595:ASN:OD1	2.53	0.41
2:G:1804:PHE:CG	2:G:1818:LEU:HG	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:ILE:C	1:A:769:ILE:HG13	2.41	0.41
1:A:1219:VAL:O	1:A:1222:ALA:HB3	2.20	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:665:LEU:HD23	2:G:665:LEU:C	2.40	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:57:ALA:C	1:A:59:ARG:N	2.73	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
2:G:1713:ASN:CB	2:G:1771:LEU:HD13	2.51	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1722:VAL:HG23	1:A:1732:THR:C	2.41	0.41
2:G:38:ASN:HA	2:G:41:LEU:CD2	2.51	0.41
2:G:323:ILE:O	2:G:324:LEU:C	2.60	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
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: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:1592:MET:SD	1:A:1641:ILE:HG23	2.61	0.41
2:G:69:SER:O	2:G:132:MET:HE1	2.21	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: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:1225:ALA:O	1:A:1401:TYR:OH	2.26	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:652:ILE:HG22	2:G:653:TYR:N	2.36	0.40
2:G:716:VAL:O	2:G:719:ILE:HB	2.20	0.40
2:G:784:GLU:O	2:G:787:THR:OG1	2.16	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1797:LEU:N	2:G:1797:LEU:CD1	2.84	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:1167:LEU:O	1:A:1168:LEU:HD13	2.21	0.40
1:A:1247:SER:OG	1:A:1248:GLY:N	2.53	0.40
1:A:1375:GLY:O	1:A:1545:SER:OG	2.35	0.40
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: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: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:894:ARG:O	2:G:895:LEU:C	2.59	0.40
2:G:1218:ILE:HG22	2:G:1219:ILE:N	2.36	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:483:VAL:O	1:A:484:LEU:C	2.56	0.40
1:A:626:VAL:HA	1:A:629:THR:HG23	2.02	0.40
1:A:980:VAL:HG12	2:G:968:GLN:CD	2.42	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: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:1511:SER:C	2:G:1512:HIS:HD1	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1916:PHE:O	2:G:1919:LEU:HG	2.21	0.40
2:G:2036:GLU:N	2:G:2037:PRO:HD3	2.36	0.40
1:A:765:LEU:HA	1:A:765:LEU:HD23	1.84	0.40
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:1233:GLU:O	1:A:1234:MET:C	2.58	0.40
1:A:1539:ALA:HB3	1:A:1541:PHE:HE1	1.87	0.40
2:G:60:LEU:C	2:G:60:LEU:HD23	2.41	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:159:ILE:HD12	2:G:271:THR:C	2.42	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: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:1640:PHE:CD1	2:G:1640:PHE:C	2.95	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%)	44	73
2	G	2029/2073 (98%)	1771 (87%)	258 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3637/3960 (92%)	3100 (85%)	533 (15%)	4 (0%)	50	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%)	1230 (100%)	3 (0%)	92	98
2	G	1772/1810 (98%)	1761 (99%)	11 (1%)	84	95
All	All	3005/3376 (89%)	2991 (100%)	14 (0%)	85	96

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	83	LYS
1	A	1378	GLU
2	G	63	LYS
2	G	76	LYS
2	G	140	LYS
2	G	297	ARG
2	G	395	LYS
2	G	415	LYS
2	G	419	ARG
2	G	809	LYS
2	G	1023	ARG
2	G	1128	LYS
2	G	1439	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	344	GLN
1	A	407	ASN
1	A	465	ASN
1	A	479	ASN
1	A	618	ASN
1	A	654	GLN
1	A	882	ASN
1	A	904	ASN
1	A	965	HIS
1	A	969	ASN
1	A	1146	HIS
1	A	1345	ASN
1	A	1442	ASN
1	A	1483	ASN
1	A	1549	ASN
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	390	ASN
2	G	440	ASN
2	G	451	ASN
2	G	517	HIS
2	G	1002	HIS
2	G	1008	GLN
2	G	1061	GLN
2	G	1383	ASN
2	G	1399	ASN
2	G	1424	GLN
2	G	1688	GLN
2	G	1712	ASN
2	G	1775	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

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

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
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:

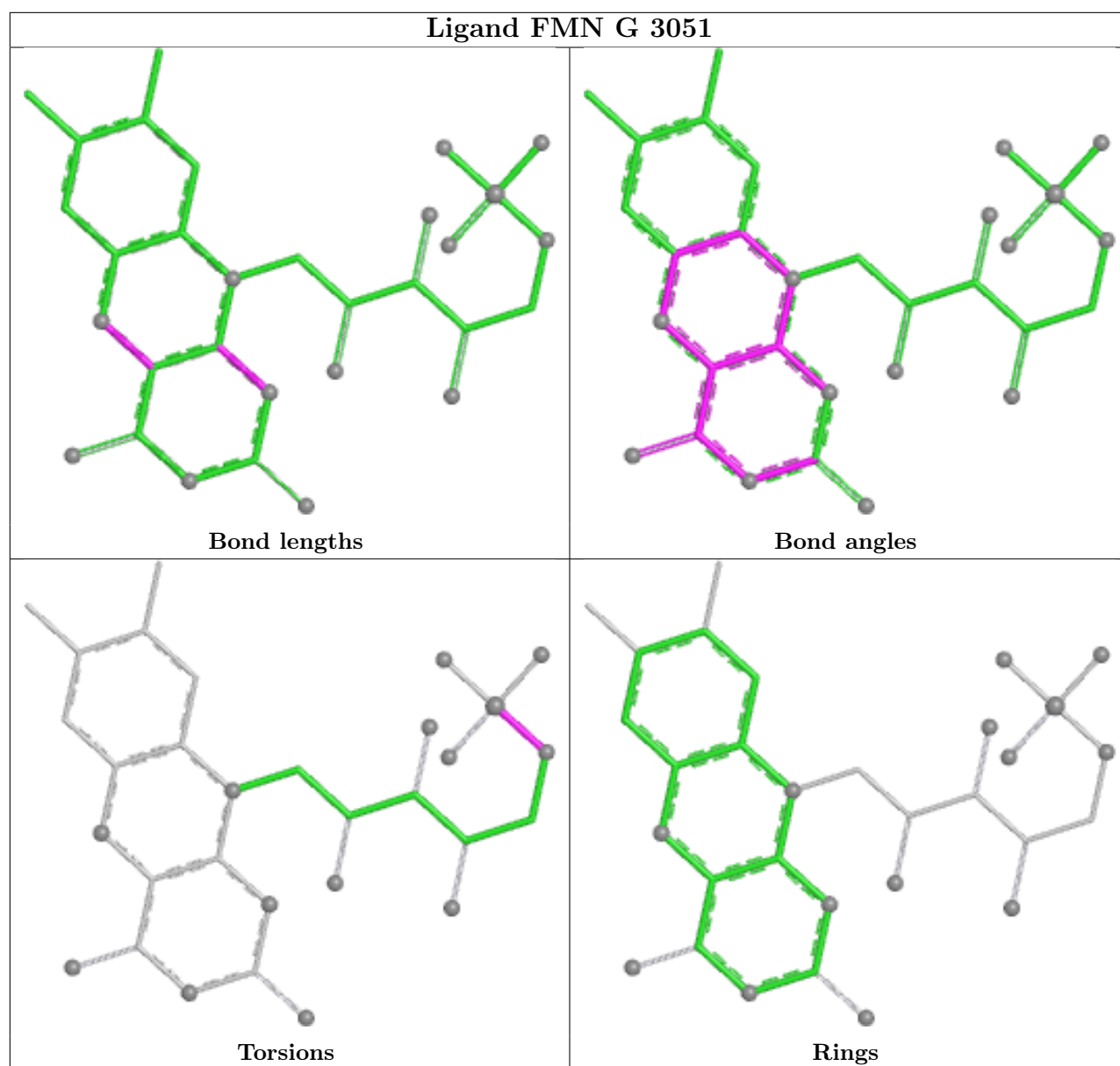
Mol	Chain	Res	Type	Atoms
4	G	3051	FMN	C5'-O5'-P-O1P
4	G	3051	FMN	C5'-O5'-P-O2P
4	G	3051	FMN	C5'-O5'-P-O3P

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.

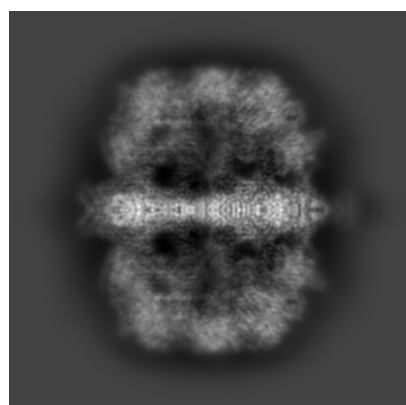
6 Map visualisation [i](#)

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.

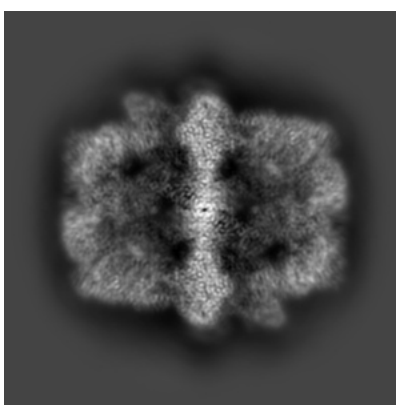
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

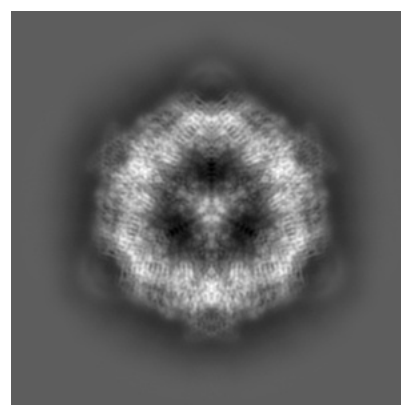
6.1.1 Primary map



X



Y

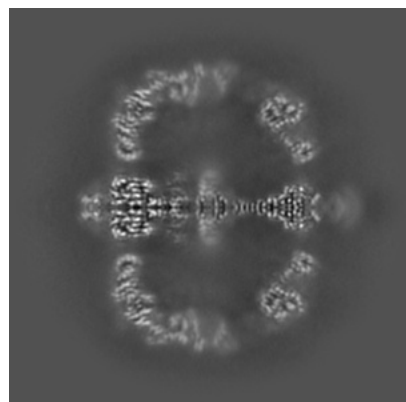


Z

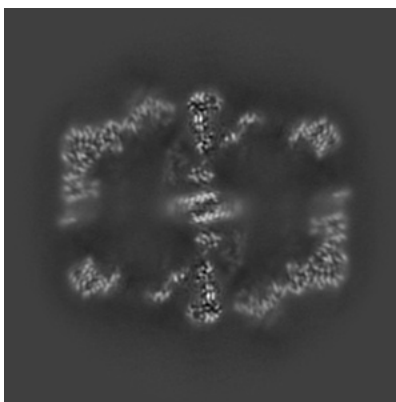
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

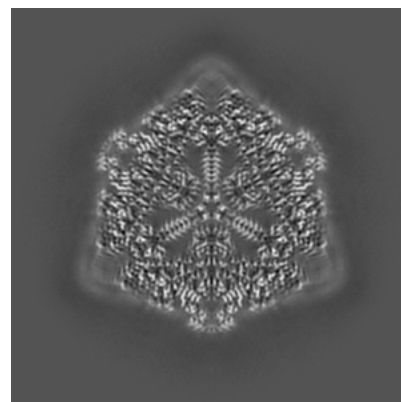
6.2.1 Primary map



X Index: 176



Y Index: 176

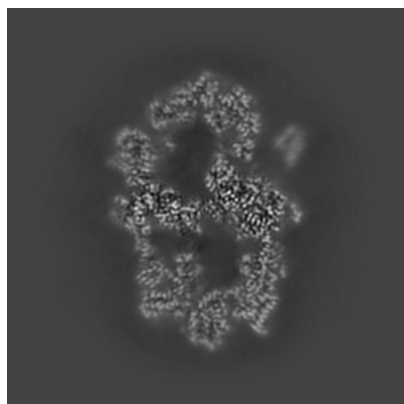


Z Index: 176

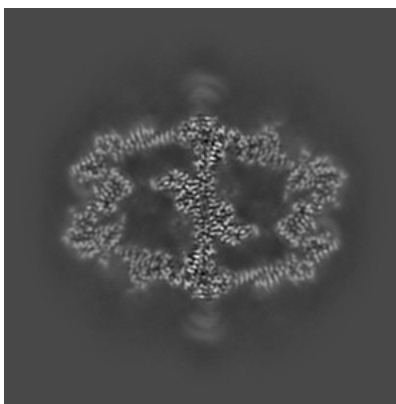
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

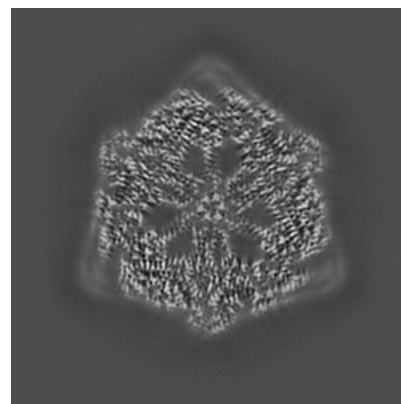
6.3.1 Primary map



X Index: 237



Y Index: 121

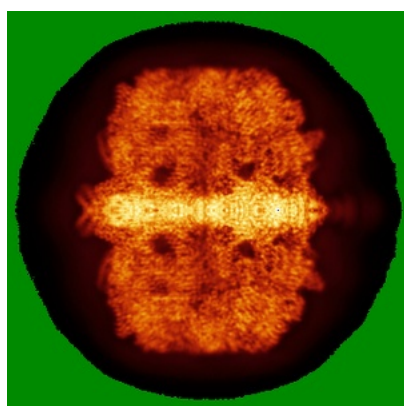


Z Index: 172

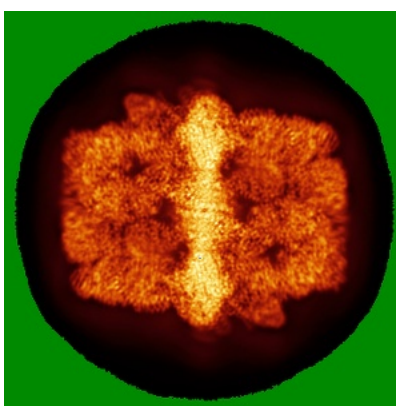
The images above show the largest variance slices of the map in three orthogonal directions.

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

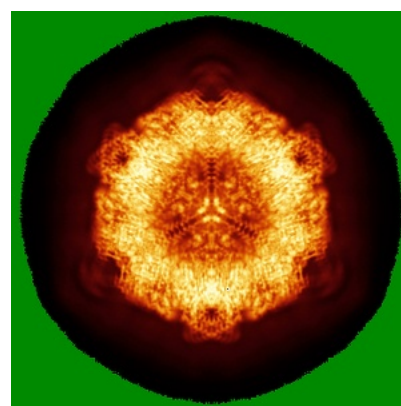
6.4.1 Primary map



X



Y

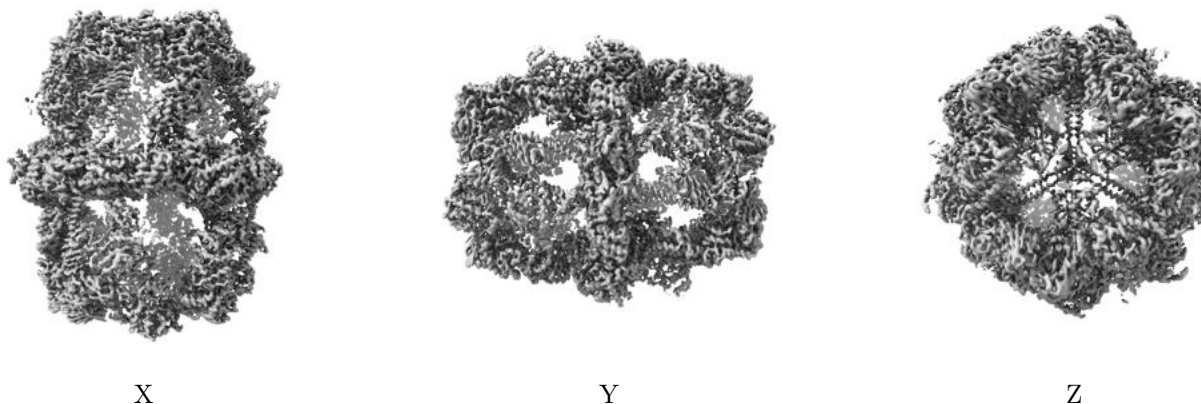


Z

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.

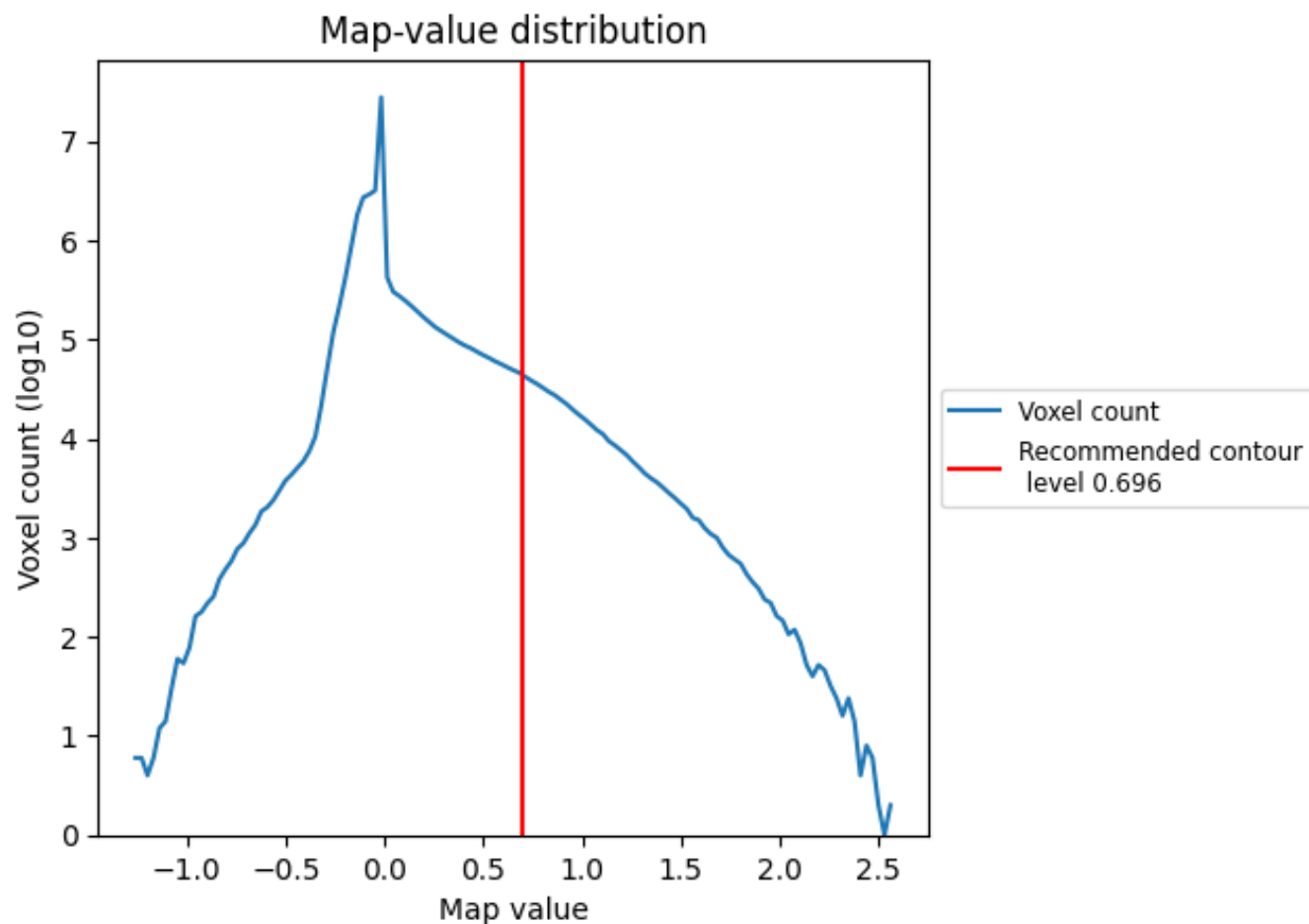
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

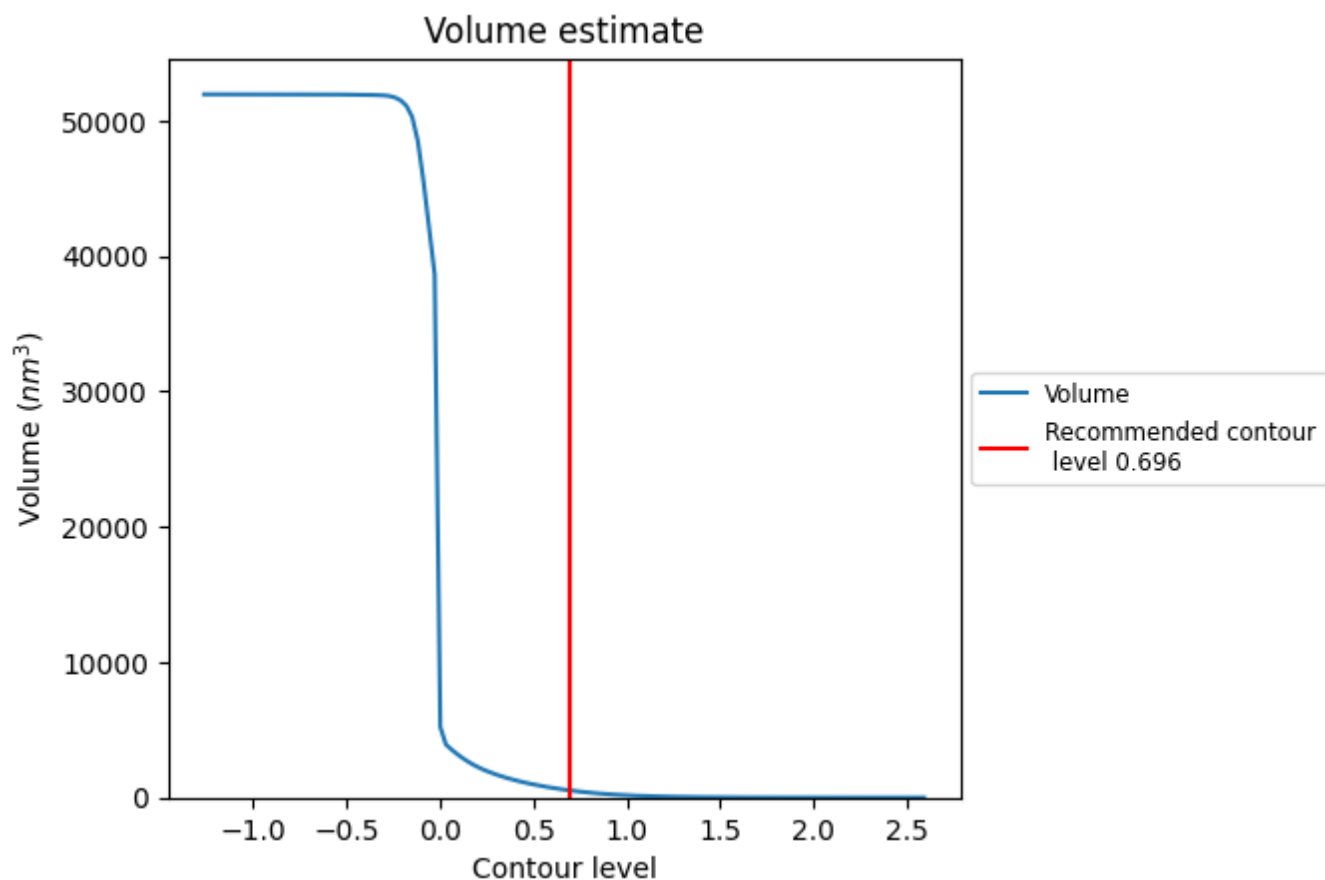
This section contains the results of statistical analysis of the map.

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.

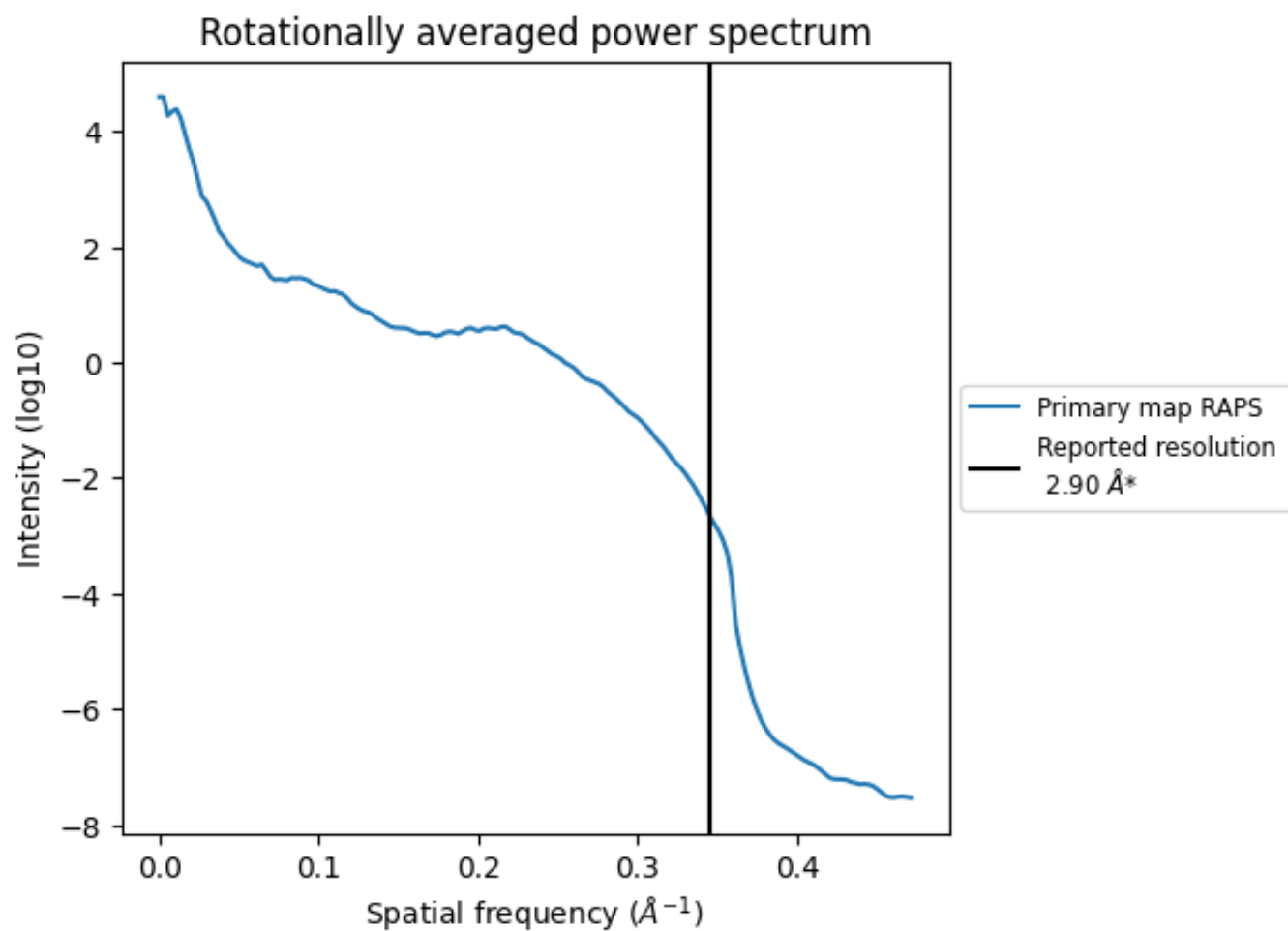
7.2 Volume estimate [i](#)



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 ⓘ

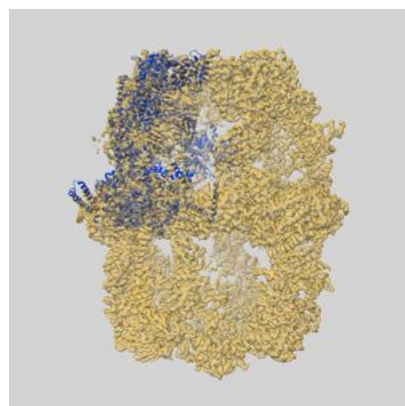
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

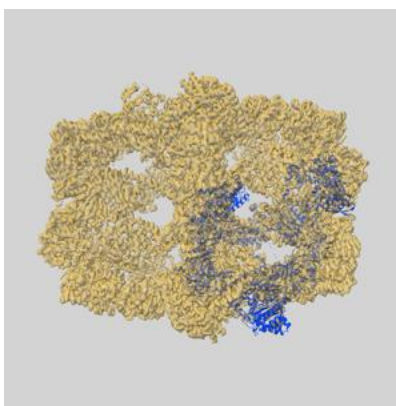
This section contains information regarding the fit between EMDB map EMD-20655 and PDB model 6U5T. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

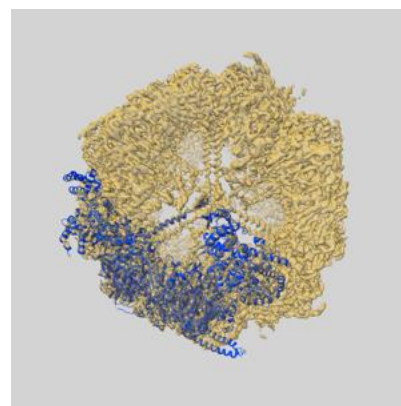
9.1.1 Map-model overlay [i](#)



X

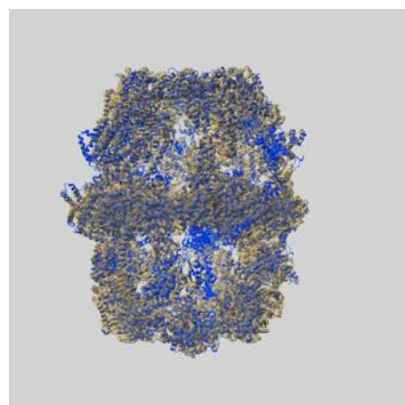


Y

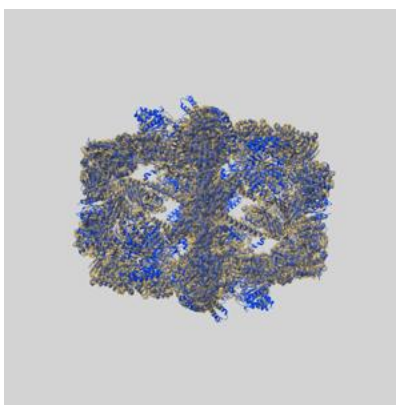


Z

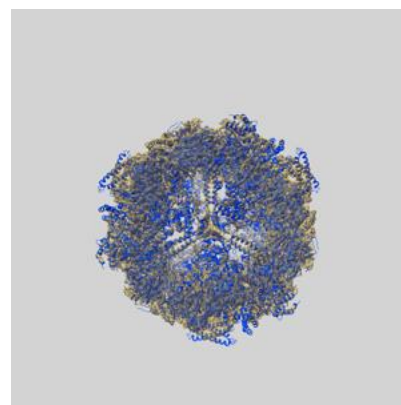
9.1.2 Map-model assembly overlay [i](#)



X



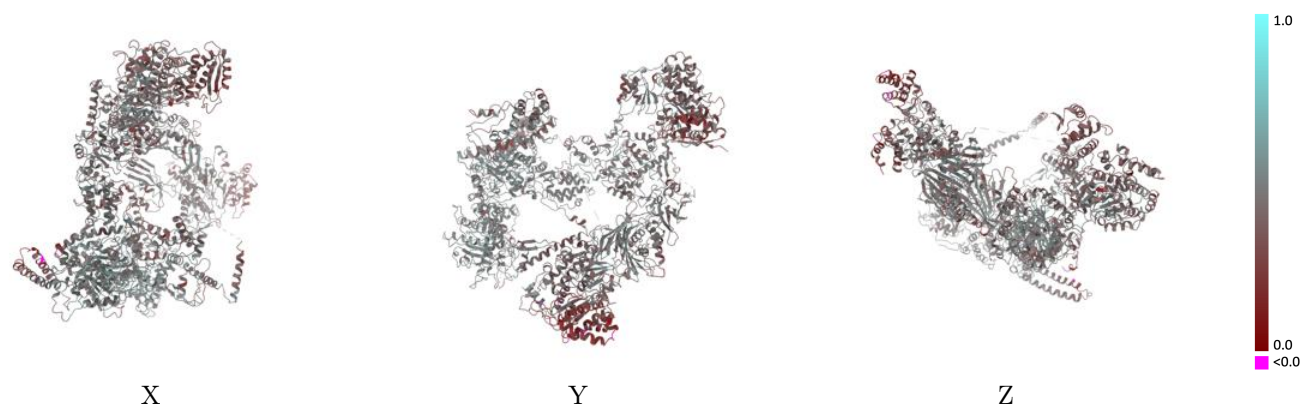
Y



Z

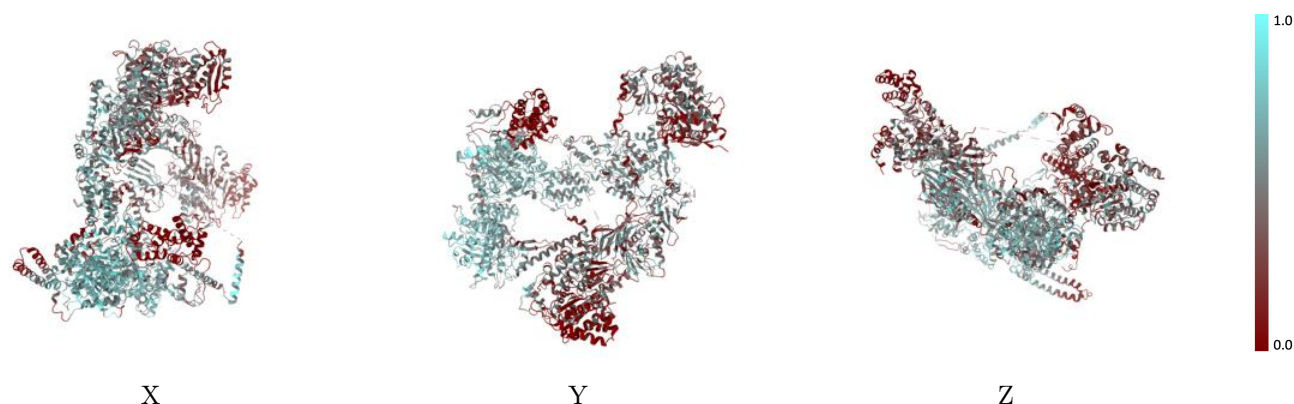
The images above show the 3D surface view of the map at the recommended contour level 0.696 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



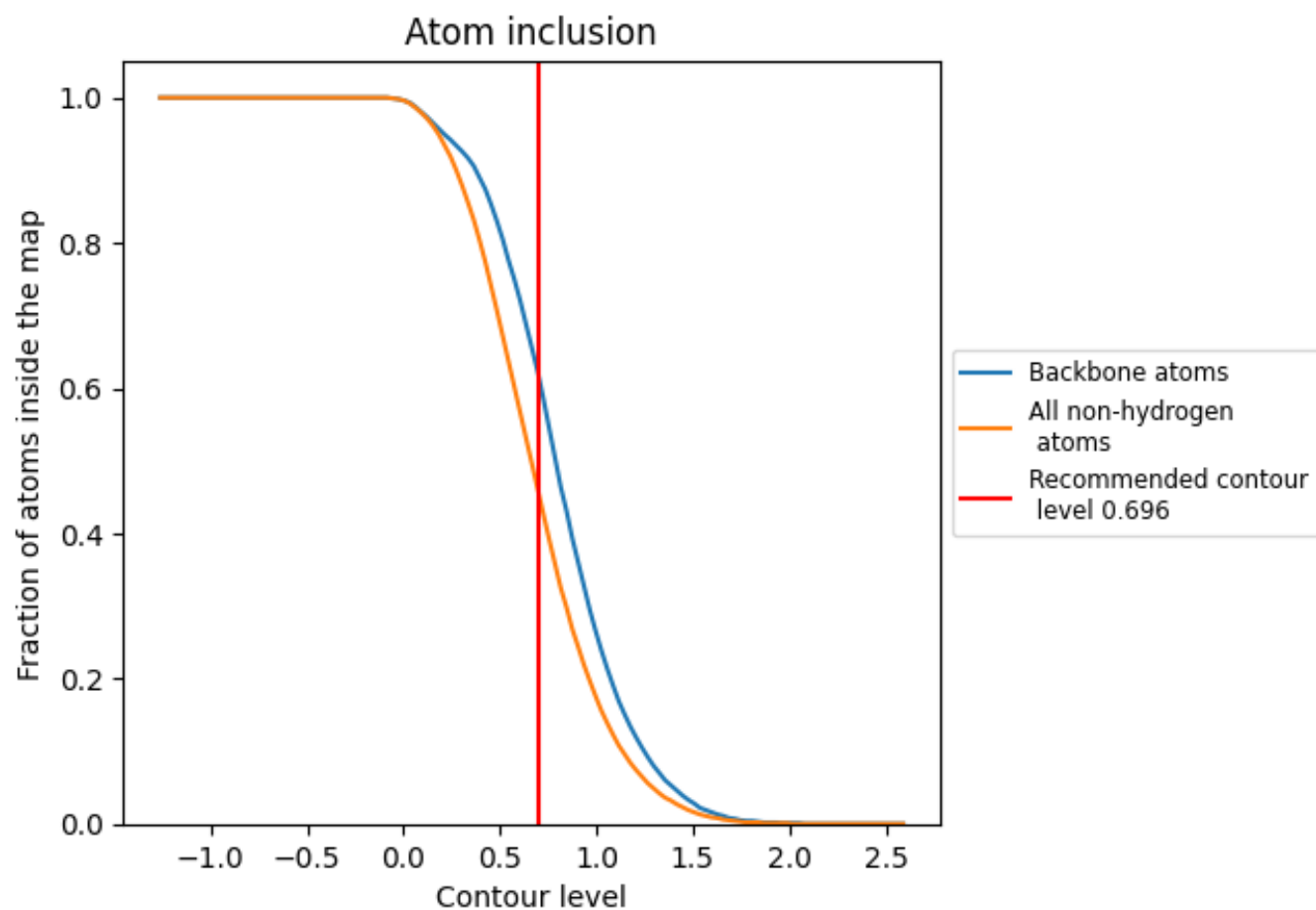
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.696).

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	<div></div> 0.4620	<div></div> 0.4420
A	<div></div> 0.5340	<div></div> 0.4690
G	<div></div> 0.4070	<div></div> 0.4210

