



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 11:56 AM UTC

PDB ID : 6HV9 / pdb_00006hv9
EMDB ID : EMD-0288
Title : S. cerevisiae CMG-Pol epsilon-DNA
Authors : Abid Ali, F.; Purkiss, A.G.; Cheung, A.; Costa, A.
Deposited on : 2018-10-10
Resolution : 4.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

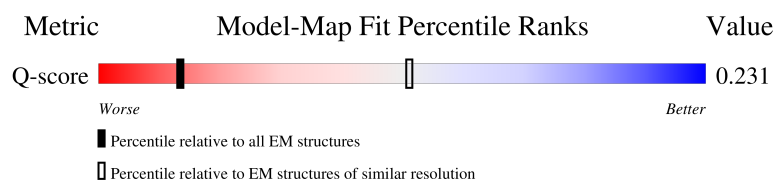
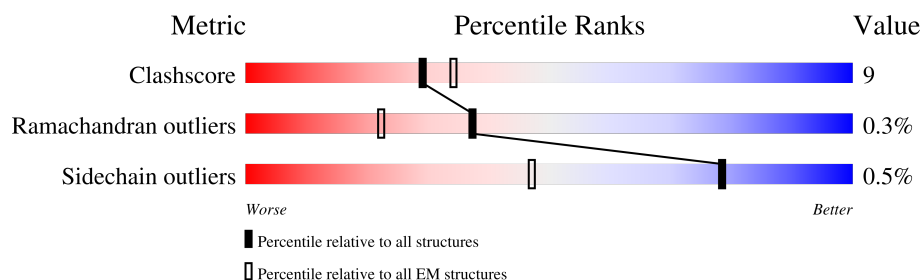
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.98 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1031 (4.48 - 5.48)

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	3	971	
2	4	933	
3	5	775	
4	6	1017	

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Mol	Chain	Length	Quality of chain
5	2	868	
6	7	845	
7	C	208	
8	D	213	
9	E	194	
10	F	294	
11	G	650	
12	X	21	
13	Y	21	
14	J	7	
15	B	689	
16	A	914	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 47617 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 DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	558	Total	C	N	O	S	0	0
			4270	2689	753	818	10		

- Molecule 2 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	589	Total	C	N	O	S	0	0
			4543	2848	796	873	26		

- Molecule 3 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	628	Total	C	N	O	S	0	0
			4690	2942	820	907	21		

- Molecule 4 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	571	Total	C	N	O	S	0	0
			4307	2704	766	821	16		

- Molecule 5 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	549	Total	C	N	O	S	0	0
			4184	2639	745	785	15		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	616	Total	C	N	O	S	0	0
			4785	3024	820	916	25		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	194	Total	C	N	O	S	0	0
			1492	934	265	287	6		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	181	Total	C	N	O	S	0	0
			1461	935	257	265	4		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	159	Total	C	N	O	S	0	0
			1262	824	207	226	5		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	218	Total	C	N	O	S	0	0
			1743	1099	292	339	13		

- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	541	Total	C	N	O	S	0	0
			4239	2684	737	808	10		

- Molecule 12 is a DNA chain called DNA (5'-D(*GP*CP*AP*GP*CP*CP*AP*CP*GP*CP*TP*GP*GP*CP*CP*GP*TP*TP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	21	Total	C	N	O	P	0	0
			425	203	76	126	20		

- Molecule 13 is a DNA chain called DNA (5'-D(P*TP*AP*AP*AP*AP*CP*GP*GP*CP*C*P*AP*GP*CP*GP*TP*GP*GP*CP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	21	Total	C	N	O	P	0	0
			433	204	84	124	21		

- Molecule 14 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	7	Total	C	N	O	P	0	0
			140	70	14	49	7		

- Molecule 15 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B	465	Total	C	N	O	S	0	0
			3661	2346	620	681	14		

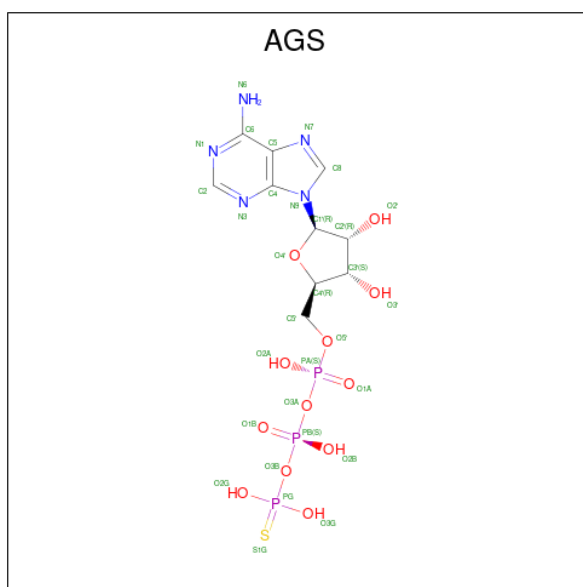
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	266	ASN	MET	conflict	UNP P24482

- Molecule 16 is a protein called DNA polymerase epsilon catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	771	Total	C	N	O	S	0	0
			5918	3797	988	1101	32		

- Molecule 17 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
17	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

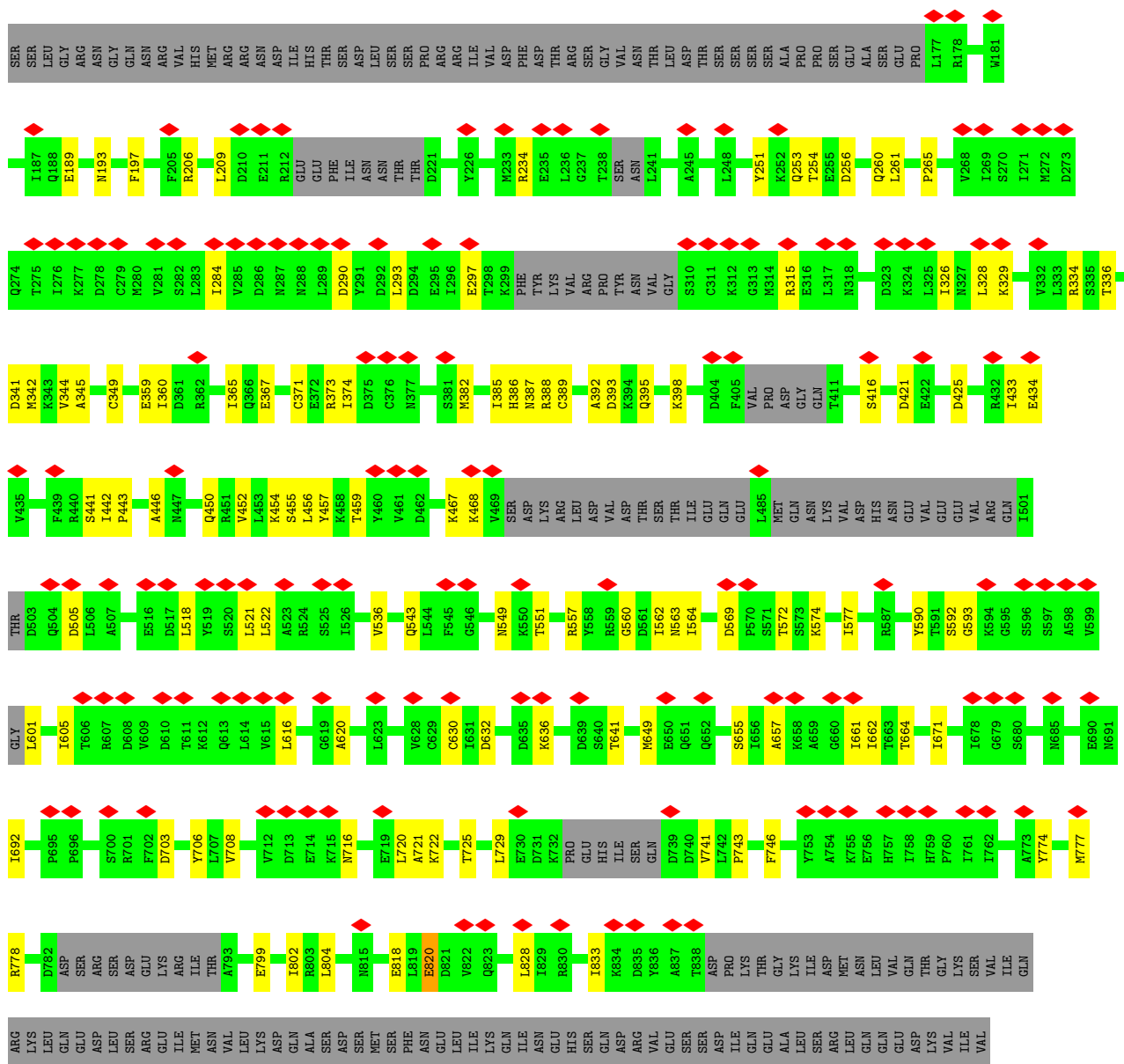
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	

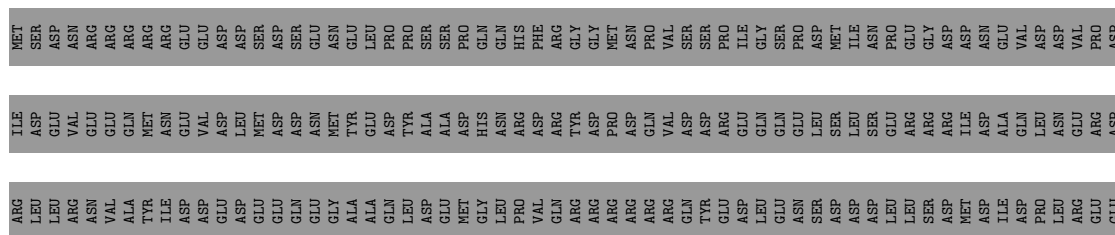
- Molecule 2: DNA replication licensing factor MCM4

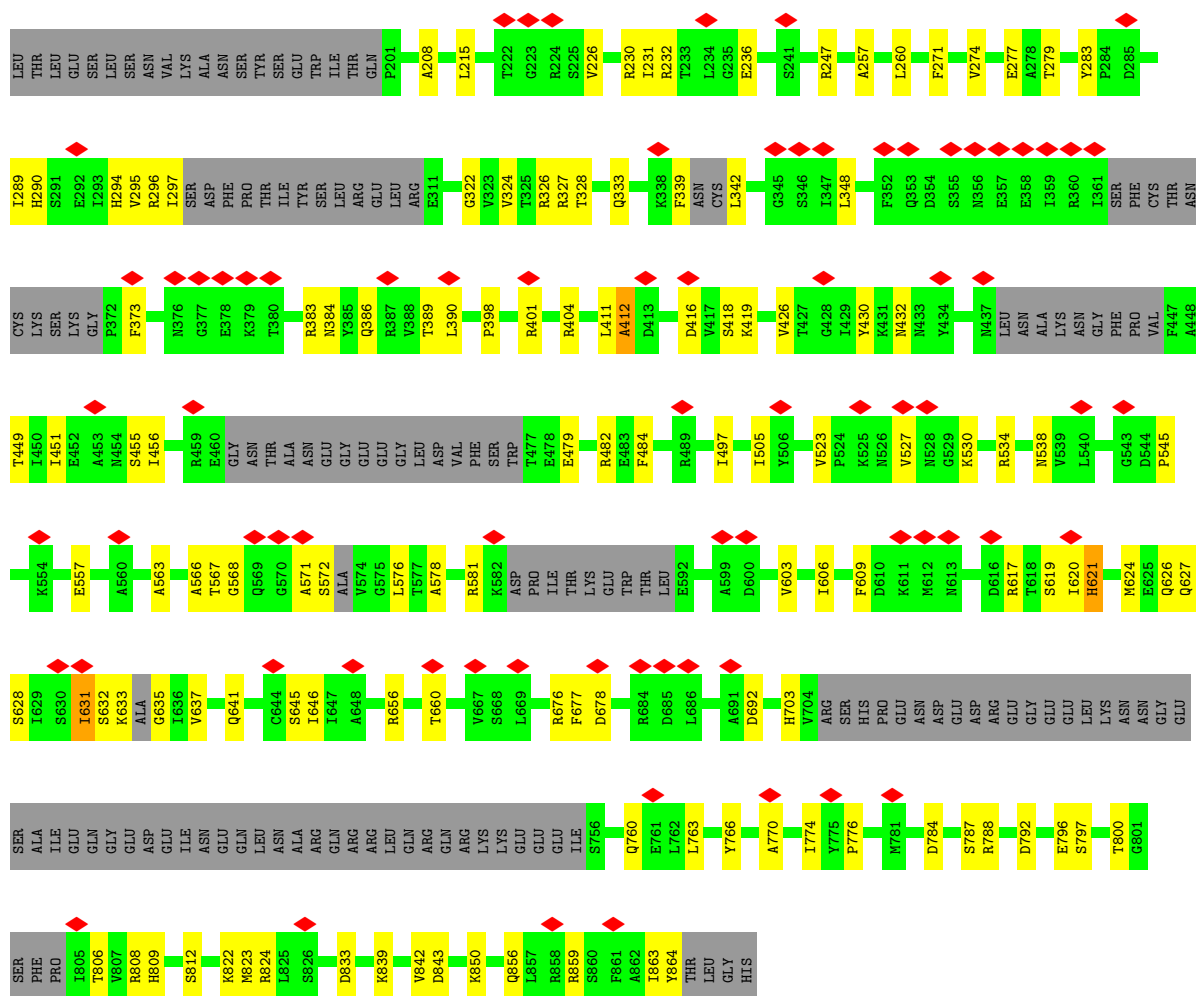


ASN	ILE	ARG	ALA	ALA	ILE	GLY	SER	SER	PRO	LEU	ASN	PHE	PRO	SER	SER	SER	SER	GLN	ARG	GLN	ASN	SER	SER	ASP	VAL	PHE	GLN	SER	SER	GLY	ARG	GLN	GLY	ARG	ILE	ILE	SER	SER	ALA	ALA	ALA	HIS	TYR	ARG	SER	ARG	LEU	LEU	THR	SER
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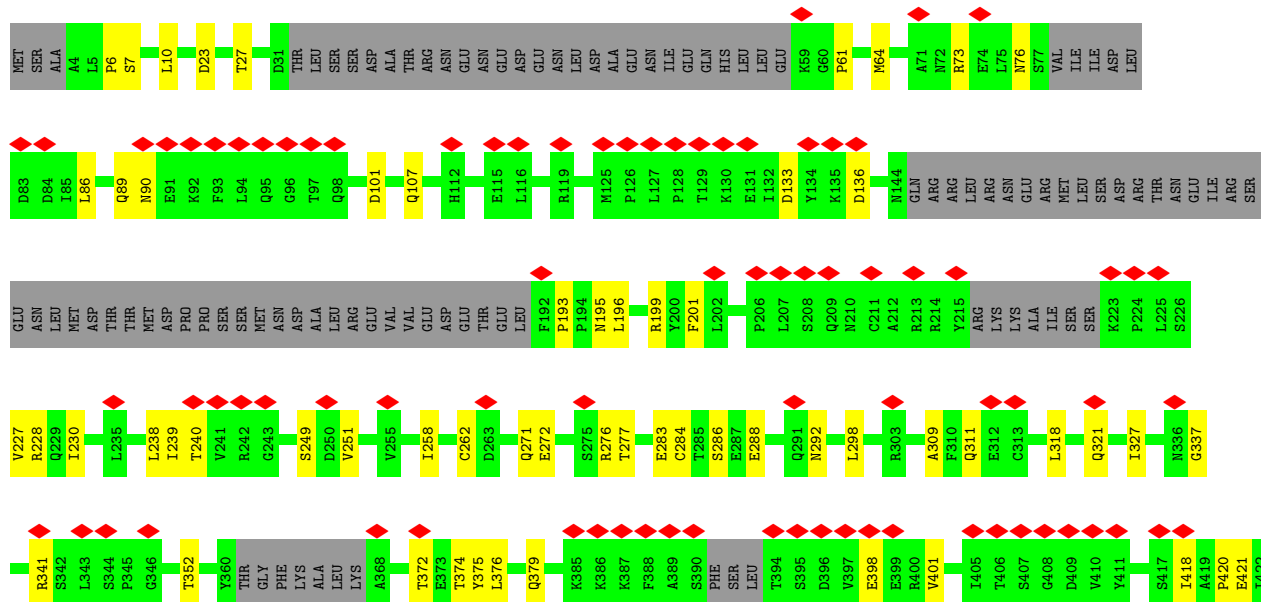


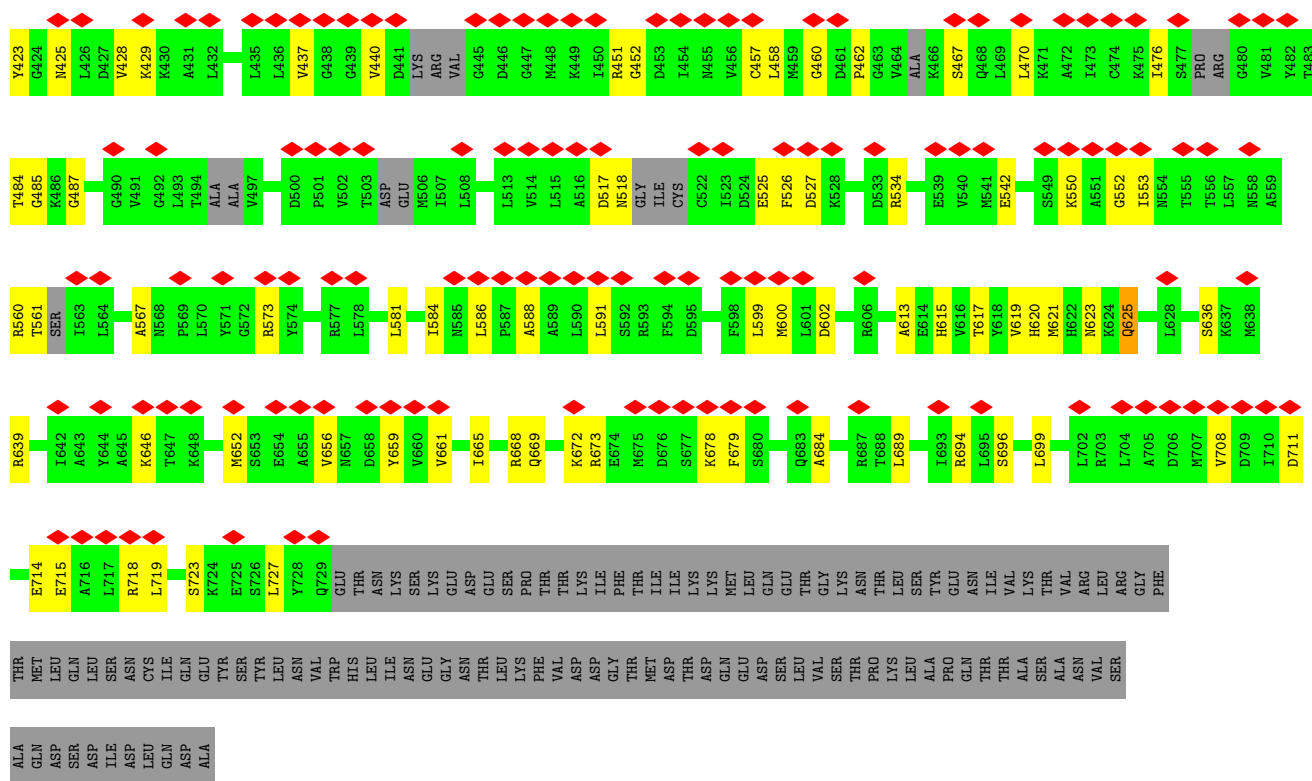
- Molecule 5: DNA replication licensing factor MCM2



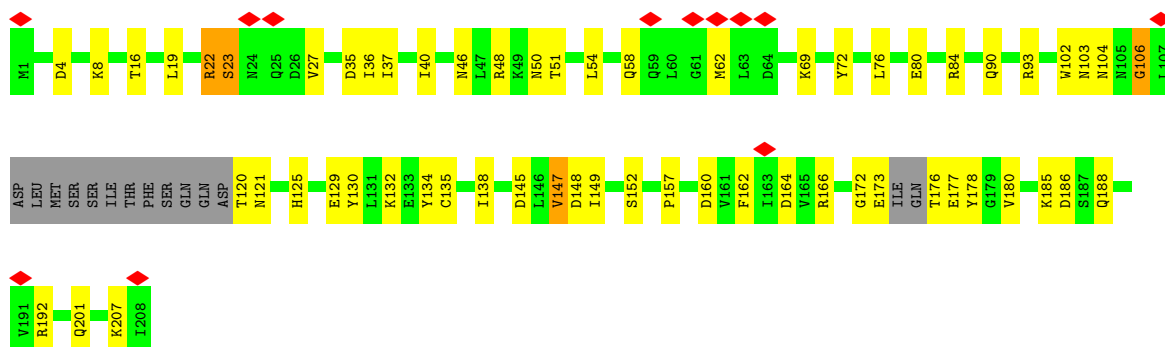


• Molecule 6: DNA replication licensing factor MCM7

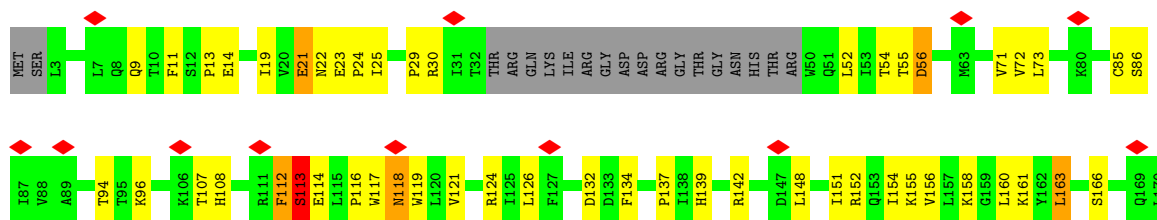


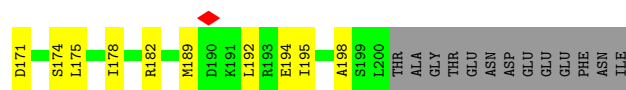


• Molecule 7: DNA replication complex GINS protein PSF1

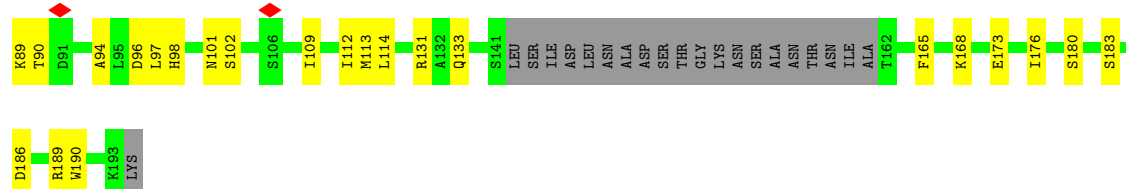


• Molecule 8: DNA replication complex GINS protein PSF2

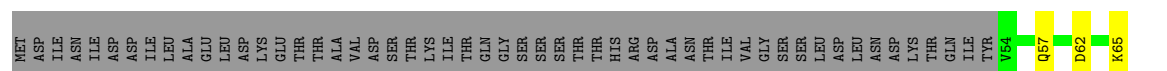


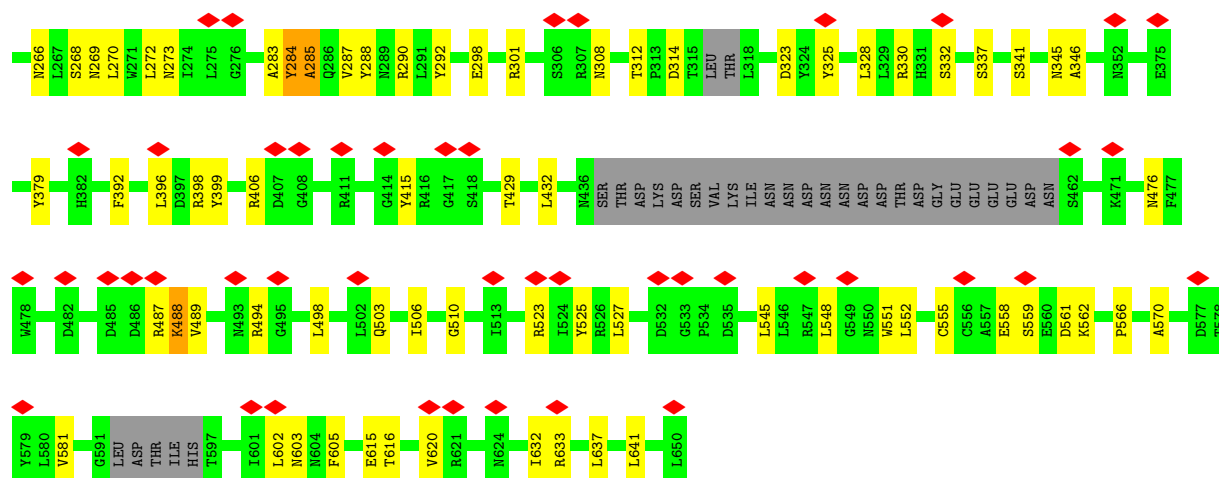


- Molecule 9: DNA replication complex GINS protein PSF3

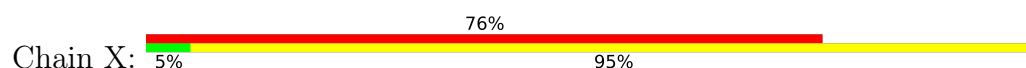


- Molecule 10: DNA replication complex GINS protein SLD5

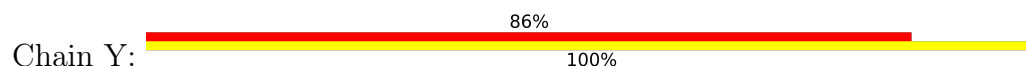




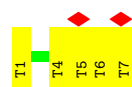
- Molecule 12: DNA (5'-D(*GP*CP*AP*GP*CP*CP*AP*CP*GP*CP*TP*GP*GP*CP*CP*GP*TP*TP*TP*TP*A)-3')



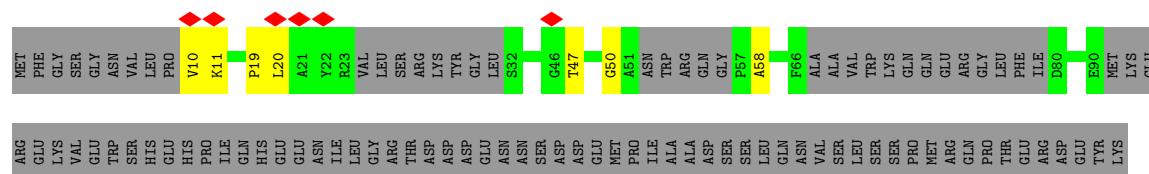
- Molecule 13: DNA (5'-D(P*TP*AP*AP*AP*AP*CP*GP*GP*CP*CP*AP*GP*CP*GP*TP*GP*GP*CP*TP*GP*C)-3')

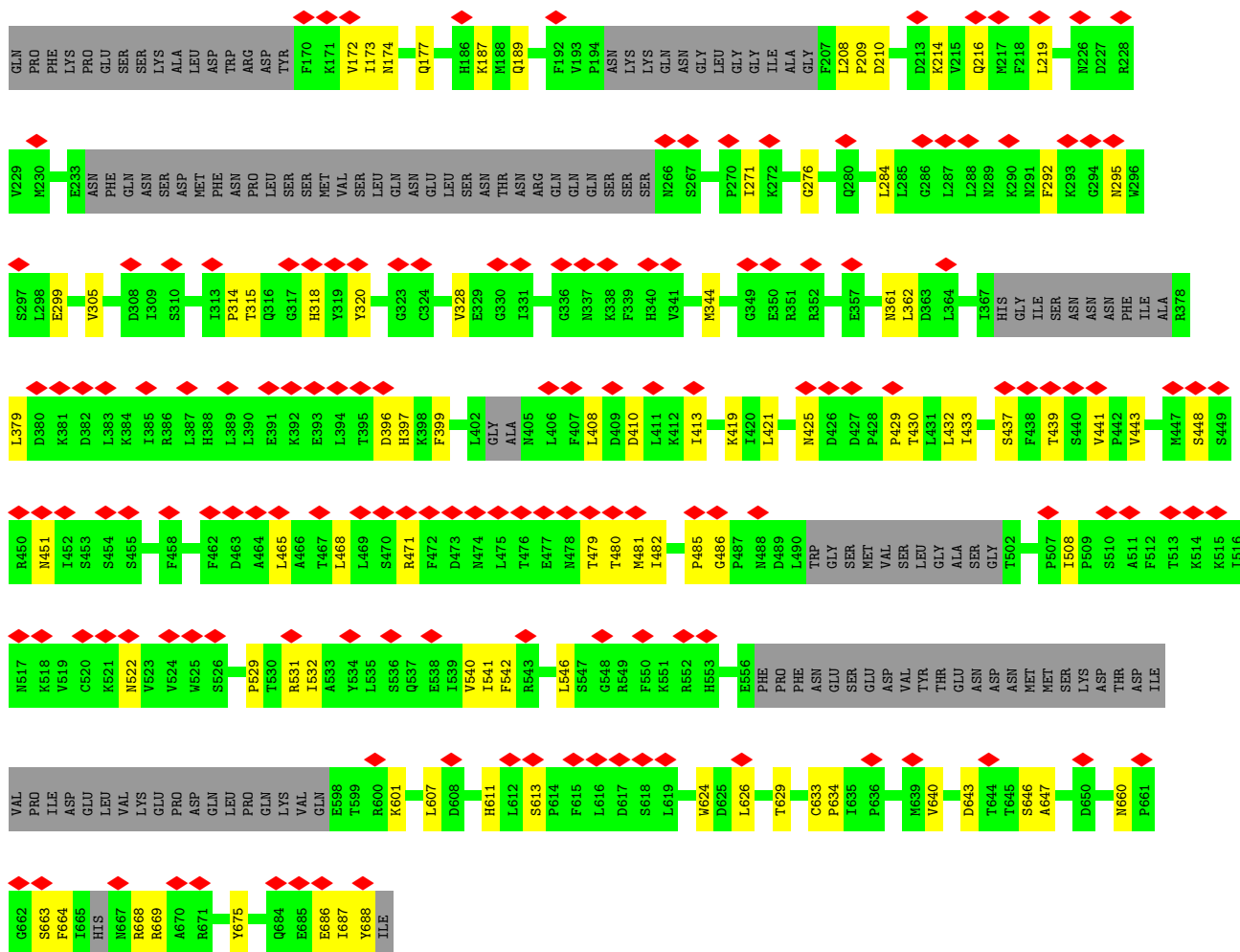


- Molecule 14: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*T)-3')

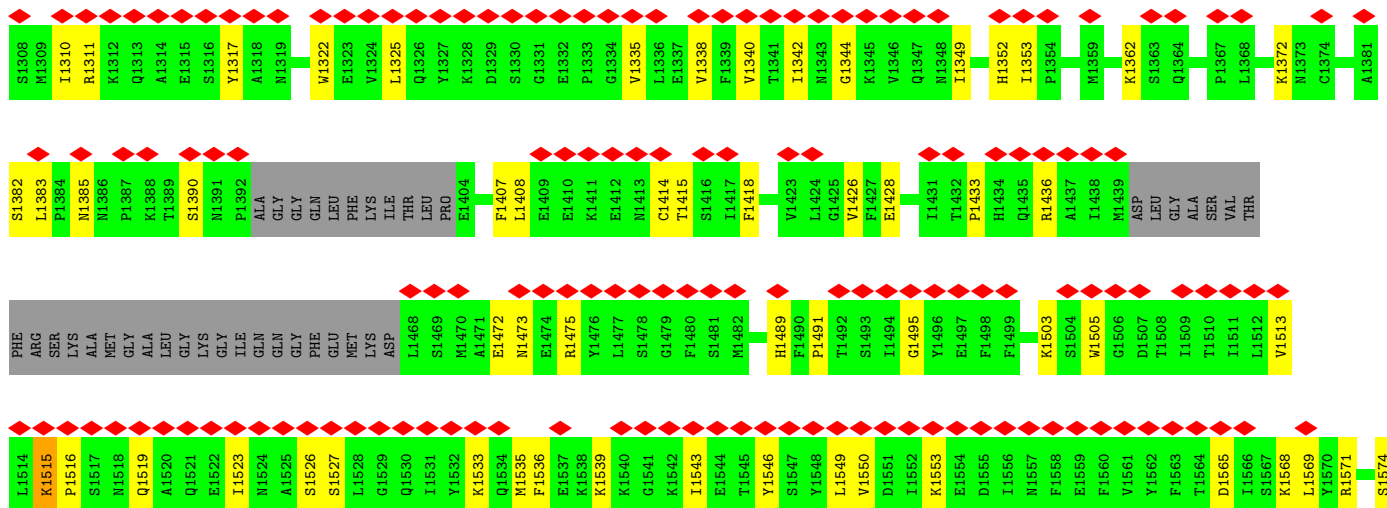


- Molecule 15: DNA polymerase epsilon subunit B





• Molecule 16: DNA polymerase epsilon catalytic subunit



T2159	Q2160	R2163	C2164	S2165	R2166	C2167	H2168	K2169	D2173	Y2174	M2175	S2176	A2177	H2178	C2179	A2182	G2183	A2184	T2188	L2189	P2190	R2191	L2198	K2202	Y2207	D2211	I2212	I2217	A2218	T2221	Q1575	E1576	T1577	T1578	K1579	L1580	K1581	E1582	E1583	R1584	G1585	L1586	Q1587	F1588	L1589	N1637	L1640	G1643	S1644	W1645	I1646	S1647	H1648	L1649	I1650	K1651	L1652	S1653	Q1654	Y1655	S1656	O1657	I1658	P1659	I1660	C1661	N1662	L1663	O1664	L1665	D1666	S1667	M1668	D1669	Y1670	D1673	A1677	R1678	K1679	L1680	K1681	K1682	E1683	N1684	I1685	O1686	L1687	W1688	W1689	N1690	E1691	K1692	A1693	P1696	D1697	H1698	G1699	G1700	I1701	Q1702	L1703	M1703	LYS	ASP	ALA	VAL	ILE	ASN	SER	PRO	GLU	PHE	VAL	HIS	ASP	ALA	PHE	S1784	N1785	D1786	M1722	N1723	S1724	G1725	V1726	Y1727	D1728	N1729	M1730	V1731	L1732	D1733	D1737	M1738	L1739	M1742	T1743	I1744	L1745	L1746	S1747	ALA	LEU	ILE	ASN	ASP	ALA	GLU	SER	ASP	LEU	VAL	ASN	ASN	MET	GLY	ILE	ASP	ASP	L1834	H1835	N1838	A1843	L1847	V1848	N1849	E1850	F1851	S1852	A1853	L1854	G1855	T1857	L1858	V1859	Y1860	D1862	R1863	A1861	Q1865	I1866	L1867	I1868	K1869	T1870	N1871	K1872	Y1873	S1874	P1875	Y1879	A1880	Y1881	Y1884	M1885	M1886	K1887	R1890	T1891	N1892	P1893	M1894	F1895	S1896	Y1897	L1898	D1899	L1900	N1901	I1902	K1903	R1904	Y1905	W1906	D1907	L1908	L1909	T1910	W1911	M1912	D1913	N1914	F1915	N1916	F1917	S1918	G1919	A1921	C1922	I1923	E1924	I1925	E1926	E1927	N1928	E1929	N1930	Q1931	D1932	Y1933	T1934	Q1938	W1939	K1942	M1964	L1965	K1966	T1967	K1968	Y1971	L1972	K1973	L1974	N1975	SER	GLY	THR	GLN	ARG	PRO	THR	GLN	ILE	VAL	ASN	VAL	LYS	LYS	GLN	ASP	K1993	E1994	D1995	S1996	R2015	V2016	E2025	F2026	D2029	P2030	A2034	ASP	TYR	VAL	ILE	PRO	VAL	LEU	PRO	GLY	S2043	H2044	V2047	K2048	N2049	E2053	K2056	S2057	L2058	C2059	H2060	V2061	N2062	S2065	K2066	S2067	T2068	I2069	L2070	E2071	I2072	ARG	THR	LEU	ARG	LYS	GLU	LEU	L2100	L2101	V2102	D2105	F2106	L2107	C2108	E2109	Y2110	C2111	S2115	K2121	ALA	PRO	GLU	ILE	F2128	S2129	C2130	V2131	R2132	K2135	A2136	Q2139	V2140	L2141	L2142	K2149	L2150	R2151	L2158	L1592	L1592	Q1593	S1594	P1595	F1596	I1597	T1598	K1599	L1600	L1601	G1602	R1605	L1606	L1607	N1608	Q1609	M1610	P1611	I1612	V1613	K1614	L1615	S1616	L1617	N1618	E1619	V1620	L1621	L1622	P1623	Q1624	L1625	N1626	W1627	W1628	P1629	T1630	L1631	L1632	K1633	L1635	V1636	N1637	L1640	G1643	S1644	W1645	I1646	S1647	H1648	L1649	I1650	K1651	L1652	S1653	Q1654	Y1655	S1656	O1657	I1658	P1659	I1660	C1661	N1662	L1663	O1664	L1665	D1666	S1667	M1668	D1669	Y1670	D1673	A1677	R1678	K1679	L1680	K1681	K1682	E1683	N1684	I1685	O1686	L1687	W1688	W1689	N1690	E1691	K1692	A1693	P1696	D1697	H1698	G1699	G1700	I1701	Q1702	L1703	M1703	LYS	ASP	ALA	VAL	ILE	ASN	SER	PRO	GLU	PHE	VAL	HIS	ASP	ALA	PHE	S1784	N1785	D1786	M1722	N1723	S1724	G1725	V1726	Y1727	D1728	N1729	M1730	V1731	L1732	D1733	D1737	M1738	L1739	M1742	T1743	I1744	L1745	L1746	S1747	ALA	LEU	ILE	ASN	ASP	ALA	GLU	SER	ASP	LEU	VAL	ASN	ASN	MET	GLY	ILE	ASP	ASP	L1834	H1835	N1838	A1843	L1847	V1848	N1849	E1850	F1851	S1852	A1853	L1854	G1855	T1857	L1858	V1859	Y1860	D1862	R1863	A1861	Q1865	I1866	L1867	I1868	K1869	T1870	N1871	K1872	Y1873	S1874	P1875	Y1879	A1880	Y1881	Y1884	M1885	M1886	K1887	R1890	T1891	N1892	P1893	M1894	F1895	S1896	Y1897	L1898	D1899	L1900	N1901	I1902	K1903	R1904	Y1905	W1906	D1907	L1908	L1909	T1910	W1911	M1912	D1913	N1914	F1915	N1916	F1917	S1918	G1919	A1921	C1922	I1923	E1924	I1925	E1926	E1927	N1928	E1929	N1930	Q1931	D1932	Y1933	T1934	Q1938	W1939	K1942	M1964	L1965	K1966	T1967	K1968	Y1971	L1972	K1973	L1974	N1975	SER	GLY	THR	GLN	ARG	PRO	THR	GLN	ILE	VAL	ASN	VAL	LYS	LYS	GLN	ASP	K1993	E1994	D1995	S1996	R2015	V2016	E2025	F2026	D2029	P2030	A2034	ASP	TYR	VAL	ILE	PRO	VAL	LEU	PRO	GLY	S2043	H2044	V2047	K2048	N2049	E2053	K2056	S2057	L2058	C2059	H2060	V2061	N2062	S2065	K2066	S2067	T2068	I2069	L2070	E2071	I2072	ARG	THR	LEU	ARG	LYS	GLU	LEU	L2100	L2101	V2102	D2105	F2106	L2107	C2108	E2109	Y2110	C2111	S2115	K2121	ALA	PRO	GLU	ILE	F2128	S2129	C2130	V2131	R2132	K2135	A2136	Q2139	V2140	L2141	L2142	K2149	L2150	R2151	L2158	L1592	L1592	Q1593	S1594	P1595	F1596	I1597	T1598	K1599	L1600	L1601	G1602	R1605	L1606	L1607	N1608	Q1609	M1610	P1611	I1612	V1613	K1614	L1615	S1616	L1617	N1618	E1619	V1620	L1621	L1622	P1623	Q1624	L1625	N1626	W1627	W1628	P1629	T1630	L1631	L1632	K1633	L1635	V1636	N1637	L1640	G1643	S1644	W1645	I1646	S1647	H1648	L1649	I1650	K1651	L1652	S1653	Q1654	Y1655	S1656	O1657	I1658	P1659	I1660	C1661	N1662	L1663	O1664	L1665	D1666	S1667	M1668	D1669	Y1670	D1673	A1677	R1678	K1679	L1680	K1681	K1682	E1683	N1684	I1685	O1686	L1687	W1688	W1689	N1690	E1691	K1692	A1693	P1696	D1697	H1698	G1699	G1700	I1701	Q1702	L1703	M1703	LYS	ASP	ALA	VAL	ILE	ASN	SER	PRO	GLU	PHE	VAL	HIS	ASP	ALA	PHE	S1784	N1785	D1786	M1722	N1723	S1724	G1725	V1726	Y1727	D1728	N1729	M1730	V1731	L1732	D1733	D1737	M1738	L1739	M1742	T1743	I1744	L1745	L1746	S1747	ALA	LEU	ILE	ASN	ASP	ALA	GLU	SER	ASP	LEU	VAL	ASN	ASN	MET	GLY	ILE	ASP	ASP	L1834	H1835	N1838	A1843	L1847	V1848	N1849	E1850	F1851	S1852	A1853	L1854	G1855	T1857	L1858	V1859	Y1860	D1862	R1863	A1861	Q1865	I1866	L1867	I1868	K1869	T1870	N1871	K1872	Y1873	S1874	P1875	Y1879	A1880	Y1881	Y1884	M1885	M1886	K1887	R1890	T1891	N1892	P1893	M1894	F1895	S1896	Y1897	L1898	D1899	L1900	N1901	I1902	K1903	R1904	Y1905	W1906	D1907	L1908	L1909	T1910	W1911	M1912	D1913	N1914	F1915	N1916	F1917	S1918	G1919	A1921	C1922	I1923	E1924	I1925	E1926	E1927	N1928	E1929	N1930	Q1931	D1932	Y1933	T1934	Q1938	W1939	K1942	M1964	L1965	K1966	T1967	K1968	Y1971	L1972	K1973	L1974	N1975	SER	GLY	THR	GLN	ARG	PRO	THR	GLN	ILE	VAL	ASN	VAL	LYS	LYS	GLN	ASP	K1993	E1994	D1995	S1996	R2015	V2016	E2025	F2026	D2029	P2030	A2034	ASP	TYR	VAL	ILE	PRO	VAL	LEU	PRO	GLY	S2043	H2044	V2047	K2048	N2049	E2053	K2056	S2057	L2058	C2059	H2060	V2061	N2062	S2065	K2066	S2067	T2068	I2069	L2070	E2071	I2072	ARG	THR	LEU	ARG	LYS	GLU	LEU	L2100	L2101	V2102	D2105	F2106	L2107	C2108	E2109	Y2110	C2111	S2115	K2121	ALA	PRO	GLU	ILE	F2128	S2129	C2130	V2131	R2132	K2135	A2136	Q2139	V2140	L2141	L2142	K2149	L2150	R2151	L2158	L1592	L1592	Q1593	S1594	P1595	F1596	I1597	T1598	K1599	L1600	L1601	G1602	R1605	L1606	L1607	N1608	Q1609	M1610	P1611	I1612	V1613	K1614	L1615	S1616	L1617	N1618	E1619	V1620	L1621	L1622	P1623	Q1624	L1625	N1626	W1627	W1628	P1629	T1630	L1631	L1632	K1633	L1635	V1636	N1637	L1640	G1643	S1644	W1645	I1646	S1647	H1648	L1649	I1650	K1651	L1652	S1653	Q1654	Y1655	S1656	O1657	I1658	P1659	I1660	C1661	N1662	L1663	O1664	L1665	D1666	S1667	M1668	D1669	Y1670	D1673	A1677	R1678	K1679	L1680	K1681	K1682	E1683	N1684	I1685	O1686	L1687	W1688	W1689	N1690	E1691	K1692	A1693	P1696	D1697	H1698	G1699	G1700	I1701	Q1702	L1703	M1703	LYS	ASP	ALA	VAL	ILE	ASN	SER	PRO	GLU	PHE	VAL	HIS	ASP	ALA	PHE	S1784	N1785	D1786	M1722	N1723	S1724	G1725	V1726	Y1727	D1728	N1729	M1730	V1731	L1732	D1733	D1737	M1738	L1739	M1742	T1743	I1744	L1745	L1746	S1747	ALA	LEU	ILE	ASN	ASP	ALA	GLU	SER	ASP	LEU	VAL	ASN	ASN	MET	GLY	ILE	ASP	ASP	L1834	H1835	N1838	A1843	L1847	V1848	N1849	E1850	F1851	S1852	A1853	L1854	G1855	T1857	L1858	V1859	Y1860	D1862	R1863	A1861	Q1865	I1866	L1867	I1868	K1869	T1870	N1871	K1872	Y1873	S1874	P1875	Y1879	A1880	Y1881	Y1884	M1885	M1886	K1887	R1890	T1891	N1892	P1893	M1894	F1895	S1896	Y1897	L1898	D1899	L1900	N1901	I1902	K1903	R1904	Y1905	W1906	D1907	L1908	L1909	T1910	W1911	M1912	D1913	N1914	F1915	N1916	F1917	S1918	G1919	A1921	C1922	I1923	E1924	I1925	E1926	E1927	N1928	E1929	N1930	Q1931	D1932	Y1933	T1934	Q1938	W1939	K1942	M1964	L1965	K1966	T1967	K1968	Y1971	L1972	K1973	L1974	N1975	SER	GLY	THR	GLN	ARG	PRO	THR	GLN	ILE	VAL	ASN	VAL	LYS	LYS	GLN	ASP	K1993	E1994	D1995	S1996	R2015	V2016	E2025	F2026	D2029	P2030	A2034	ASP	TYR	VAL	ILE	PRO	VAL	LEU	PRO	GLY	S2043	H2044	V2047	K2048	N2049	E2053	K2056	S2057	L2058	C2059	H2060	V2061	N2062	S2065	K2066	S2067	T2068	I2069	L2070	E2071	I2072	ARG	THR	LEU	ARG	LYS	GLU	LEU	L2100	L2101	V2102	D2105	F2106	L2107	C2108	E2109	Y2110	C2111	S2115	K2121	ALA	PRO	GLU	ILE	F2128	S2129	C2130	V2131	R2132	K2135	A2136	Q2139	V2140	L2141	L2142	K2149	L2150	R2151	L2158	L1592	L1592	Q1593	S1594	P1595	F1596	I1597	T1598	K1599	L1600	L1601	G1602	R1605	L1606	L1607	N1608	Q1609	M1610	P1611	I1612	V1613	K1614	L1615	S1616	L1617	N1618	E1619	V1620	L1621	L1622	P1623	Q1624	L1625	N1626	W1627	W1628	P1629	T1630	L1631	L
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.270	Depositor
Minimum map value	-2.822	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.184	Depositor
Recommended contour level	1.01	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality

5.1 Standard geometry

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

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	3	0.60	0/4330	1.12	19/5872 (0.3%)
2	4	0.40	0/4594	0.89	6/6203 (0.1%)
3	5	0.75	0/4741	1.31	24/6405 (0.4%)
4	6	0.49	0/4359	0.97	3/5882 (0.1%)
5	2	0.65	0/4241	1.16	12/5720 (0.2%)
6	7	0.40	0/4853	0.84	2/6553 (0.0%)
7	C	0.61	0/1511	1.30	15/2039 (0.7%)
8	D	0.63	0/1489	1.29	8/2016 (0.4%)
9	E	0.63	0/1294	1.14	2/1750 (0.1%)
10	F	0.55	0/1771	1.22	15/2386 (0.6%)
11	G	0.52	0/4311	1.18	28/5832 (0.5%)
12	X	0.41	0/475	0.76	0/731
13	Y	0.40	0/486	0.71	0/748
14	J	0.79	0/153	1.16	0/234
15	B	0.47	0/3727	0.98	3/5041 (0.1%)
16	A	0.45	0/6029	1.09	23/8179 (0.3%)
All	All	0.54	0/48364	1.09	160/65591 (0.2%)

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
10	F	0	4
11	G	0	3
All	All	0	7

There are no bond length outliers.

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	216	VAL	CA-C-N	11.38	143.44	122.84
10	F	216	VAL	C-N-CA	11.38	143.44	122.84
11	G	98	ILE	CA-C-N	10.85	148.27	121.80
11	G	98	ILE	C-N-CA	10.85	148.27	121.80
10	F	200	LYS	CA-C-N	9.54	138.87	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	F	212	THR	Mainchain,Peptide
10	F	216	VAL	Mainchain,Peptide
11	G	523	ARG	Sidechain
11	G	98	ILE	Mainchain,Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	4270	0	4259	79	0
2	4	4543	0	4517	78	0
3	5	4690	0	4526	105	0
4	6	4307	0	4166	88	0
5	2	4184	0	4126	85	0
6	7	4785	0	4761	83	0
7	C	1492	0	1394	36	0
8	D	1461	0	1445	46	0
9	E	1262	0	1240	32	0
10	F	1743	0	1672	41	0
11	G	4239	0	4083	51	0
12	X	425	0	238	18	0
13	Y	433	0	235	20	0
14	J	140	0	85	7	0
15	B	3661	0	3656	56	0
16	A	5918	0	5682	121	0
17	5	62	0	24	8	0
18	A	2	0	0	0	0
All	All	47617	0	46109	871	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 9.

The worst 5 of 871 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)
6:7:460:GLY:HA3	6:7:600:MET:HB2	1.62	0.81
5:2:617:ARG:O	5:2:621:HIS:HB2	1.84	0.77
9:E:48:LEU:O	9:E:52:ARG:HB2	1.85	0.76
11:G:244:GLY:HA3	11:G:603:ASN:HB2	1.67	0.76
3:5:447:ALA:HA	5:2:637:VAL:HA	1.69	0.73

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	3	542/971 (56%)	500 (92%)	40 (7%)	2 (0%)	30	67
2	4	569/933 (61%)	508 (89%)	60 (10%)	1 (0%)	43	77
3	5	598/775 (77%)	547 (92%)	51 (8%)	0	100	100
4	6	551/1017 (54%)	496 (90%)	55 (10%)	0	100	100
5	2	527/868 (61%)	483 (92%)	44 (8%)	0	100	100
6	7	588/845 (70%)	539 (92%)	48 (8%)	1 (0%)	43	77
7	C	188/208 (90%)	177 (94%)	10 (5%)	1 (0%)	24	63
8	D	177/213 (83%)	164 (93%)	10 (6%)	3 (2%)	7	34
9	E	151/194 (78%)	143 (95%)	8 (5%)	0	100	100
10	F	206/294 (70%)	184 (89%)	21 (10%)	1 (0%)	24	63
11	G	525/650 (81%)	478 (91%)	44 (8%)	3 (1%)	21	58
15	B	441/689 (64%)	390 (88%)	50 (11%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	A	751/914 (82%)	553 (74%)	193 (26%)	5 (1%)	18	55
All	All	5814/8571 (68%)	5162 (89%)	634 (11%)	18 (0%)	37	72

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	374	ILE
8	D	54	THR
8	D	113	SER
8	D	171	ASP
11	G	284	TYR

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	3	458/835 (55%)	456 (100%)	2 (0%)	84	83
2	4	493/848 (58%)	490 (99%)	3 (1%)	78	81
3	5	488/688 (71%)	486 (100%)	2 (0%)	84	83
4	6	435/886 (49%)	433 (100%)	2 (0%)	81	82
5	2	435/770 (56%)	435 (100%)	0	100	100
6	7	524/753 (70%)	522 (100%)	2 (0%)	84	83
7	C	149/193 (77%)	149 (100%)	0	100	100
8	D	156/198 (79%)	155 (99%)	1 (1%)	78	81
9	E	135/173 (78%)	135 (100%)	0	100	100
10	F	194/279 (70%)	194 (100%)	0	100	100
11	G	443/586 (76%)	442 (100%)	1 (0%)	87	86
15	B	409/629 (65%)	408 (100%)	1 (0%)	87	86
16	A	624/837 (75%)	614 (98%)	10 (2%)	55	69
All	All	4943/7675 (64%)	4919 (100%)	24 (0%)	78	82

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	A	1325	LEU
16	A	1592	LEU
16	A	1408	LEU
16	A	1658	ILE
3	5	573	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
15	B	553	HIS
16	A	1385	ASN
16	A	2143	GLN
4	6	730	HIS
4	6	698	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
17	AGS	5	801	-	32,33,33	1.48	4 (12%)	45,52,52	1.30	4 (8%)
17	AGS	5	802	-	32,33,33	1.17	3 (9%)	45,52,52	1.51	7 (15%)

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
17	AGS	5	801	-	-	9/21/38/38	0/3/3/3
17	AGS	5	802	-	-	5/21/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	801	AGS	PB-O3A	-5.00	1.54	1.59
17	5	801	AGS	PA-O3A	-4.69	1.54	1.59
17	5	802	AGS	PB-O3B	-4.37	1.54	1.59
17	5	801	AGS	PB-O3B	-3.82	1.55	1.59
17	5	802	AGS	PA-O3A	-2.50	1.56	1.59

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	801	AGS	PB-O3B-PG	-6.16	110.64	133.17
17	5	802	AGS	C4'-O4'-C1'	-5.10	98.21	109.47
17	5	802	AGS	PB-O3B-PG	-4.42	116.98	133.17
17	5	802	AGS	O4'-C1'-C2'	-3.76	98.58	106.62
17	5	802	AGS	C1'-N9-C8	-2.96	120.53	127.09

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

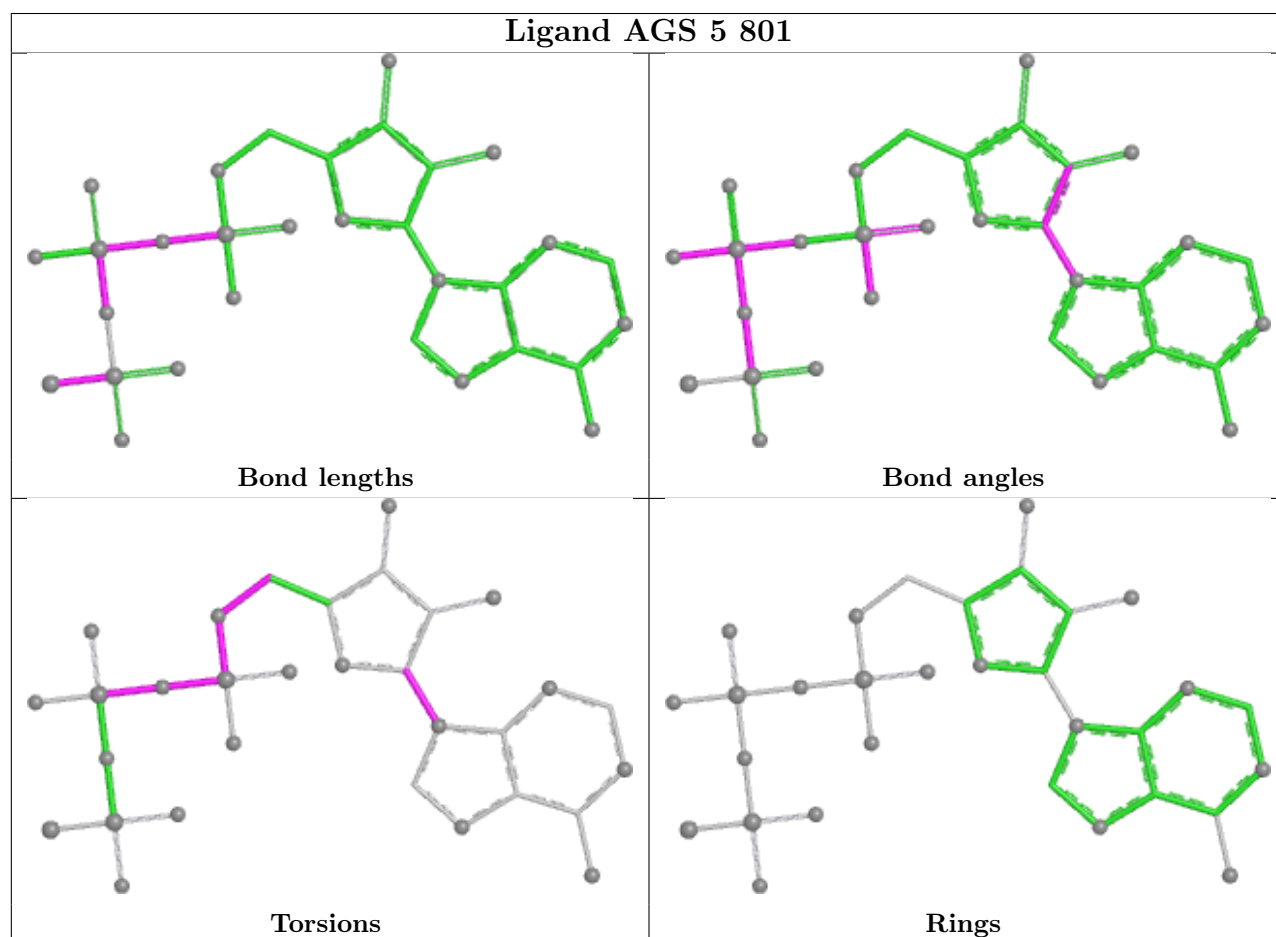
Mol	Chain	Res	Type	Atoms
17	5	801	AGS	C5'-O5'-PA-O1A
17	5	801	AGS	C5'-O5'-PA-O2A
17	5	801	AGS	C5'-O5'-PA-O3A
17	5	801	AGS	O4'-C1'-N9-C4
17	5	802	AGS	C5'-O5'-PA-O1A

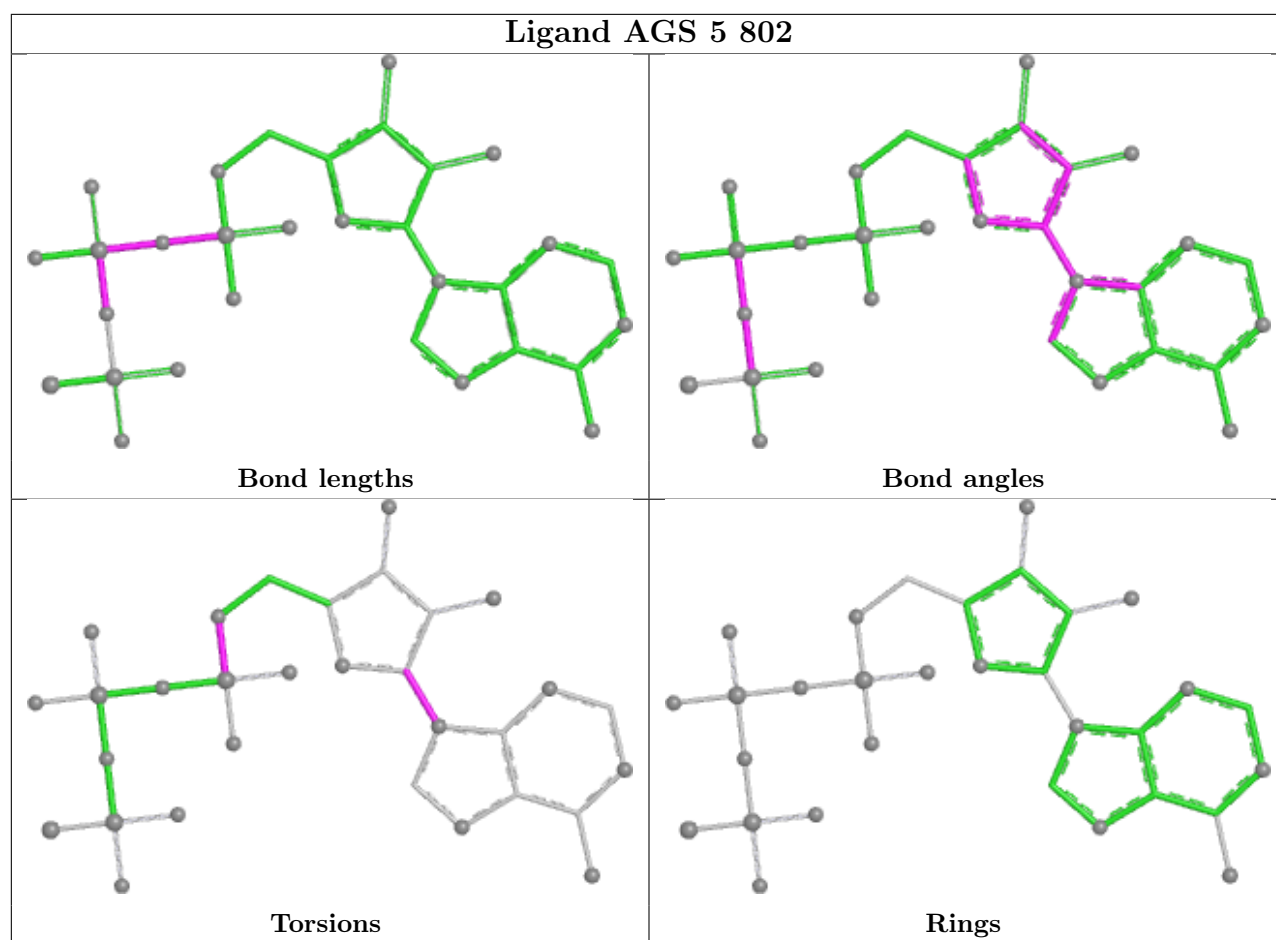
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	5	801	AGS	5	0
17	5	802	AGS	3	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	A	1
15	B	1
3	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2060:HIS	C	2061:VAL	N	14.58
1	B	280:GLN	C	281:ASN	N	5.05
1	5	269:GLU	C	270:MET	N	1.09

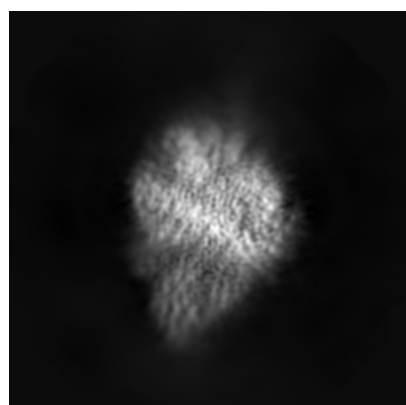
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0288. These allow visual inspection of the internal detail of the map and identification of artifacts.

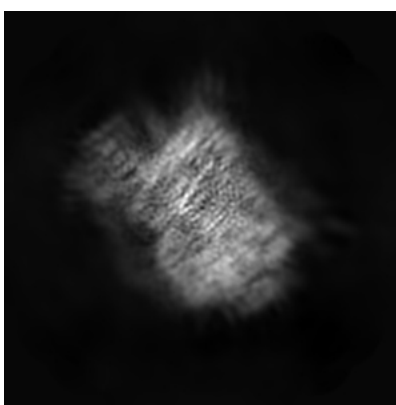
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

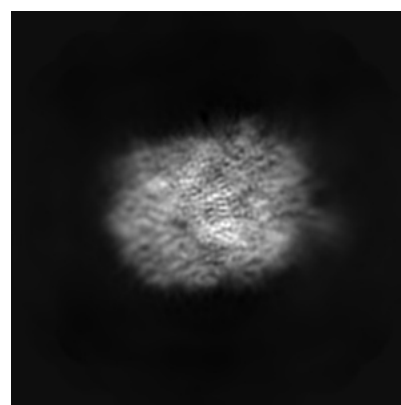
6.1.1 Primary map



X



Y

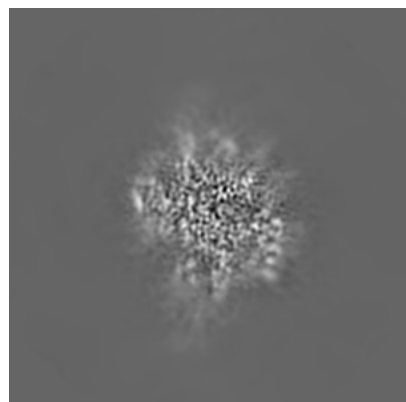


Z

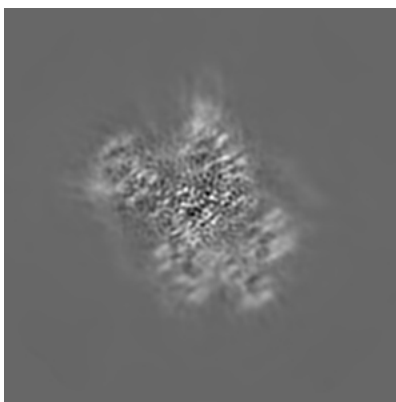
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

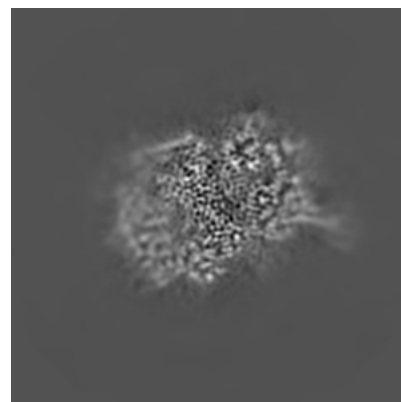
6.2.1 Primary map



X Index: 128



Y Index: 128

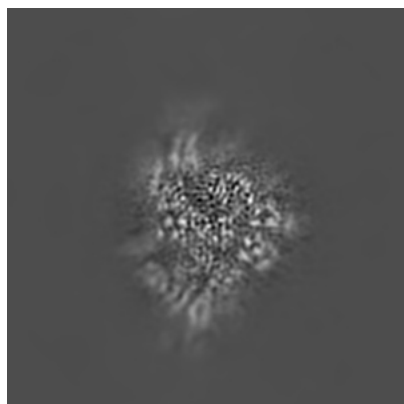


Z Index: 128

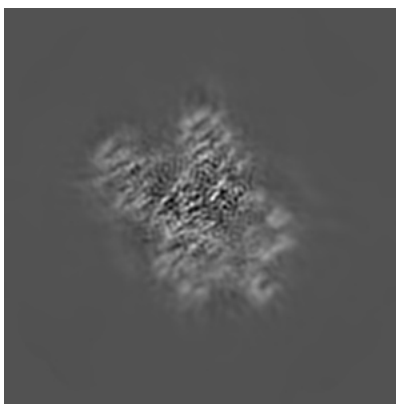
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

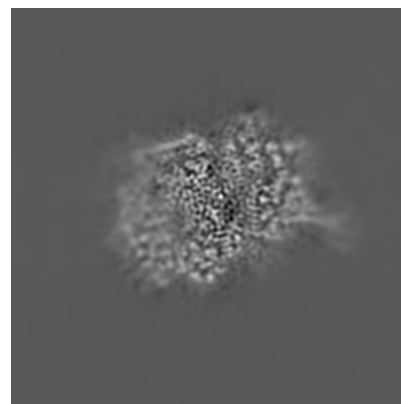
6.3.1 Primary map



X Index: 139



Y Index: 132

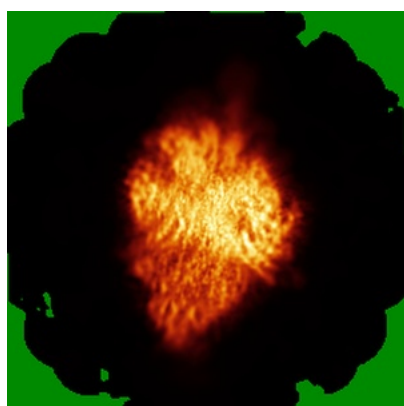


Z Index: 129

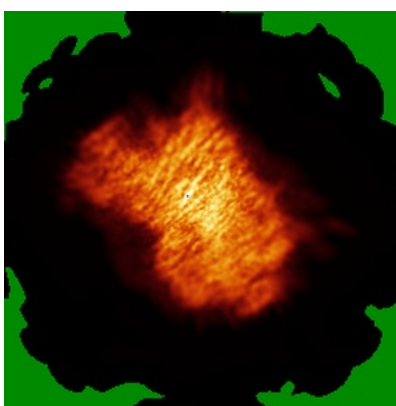
The images above show the largest variance slices of the map in three orthogonal directions.

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

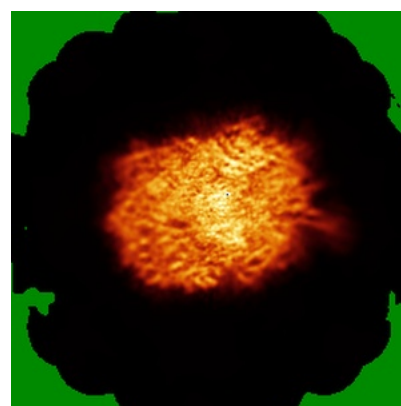
6.4.1 Primary map



X



Y

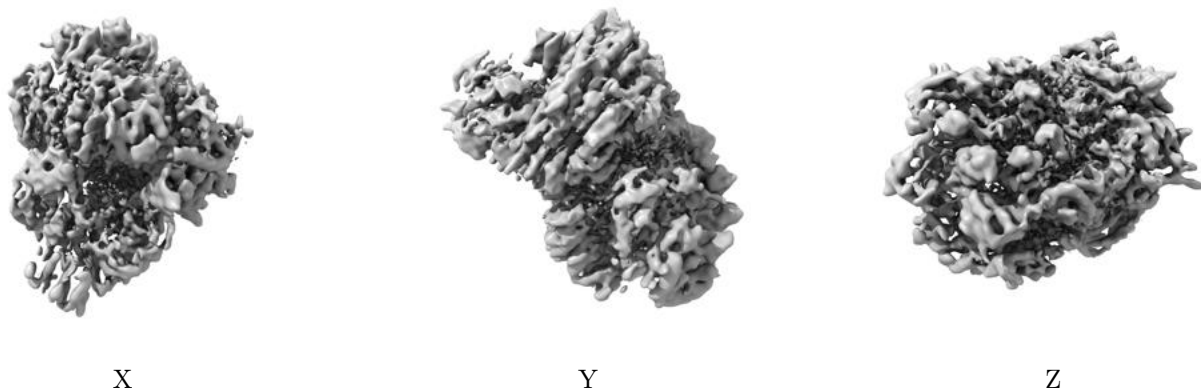


Z

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 1.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

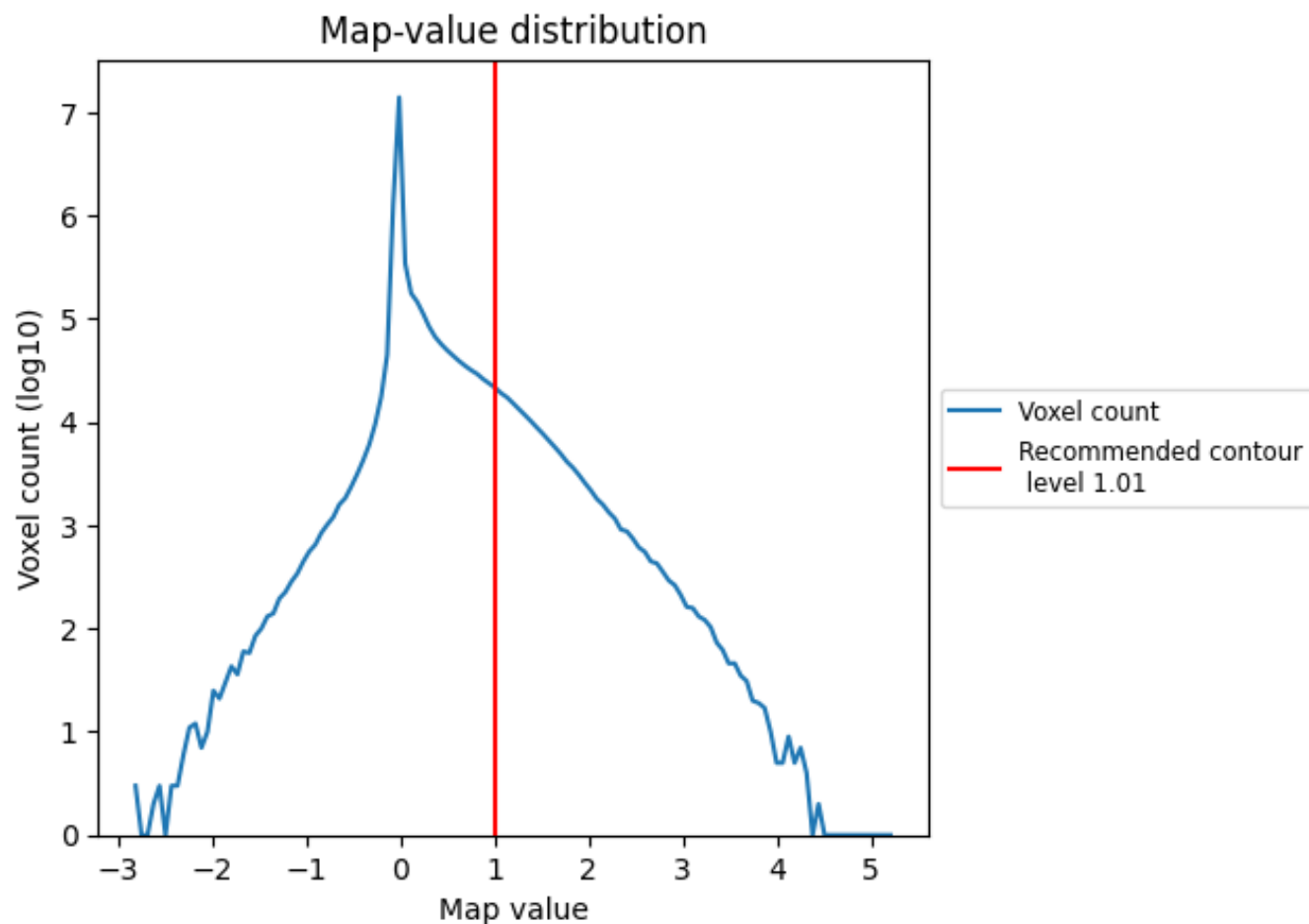
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

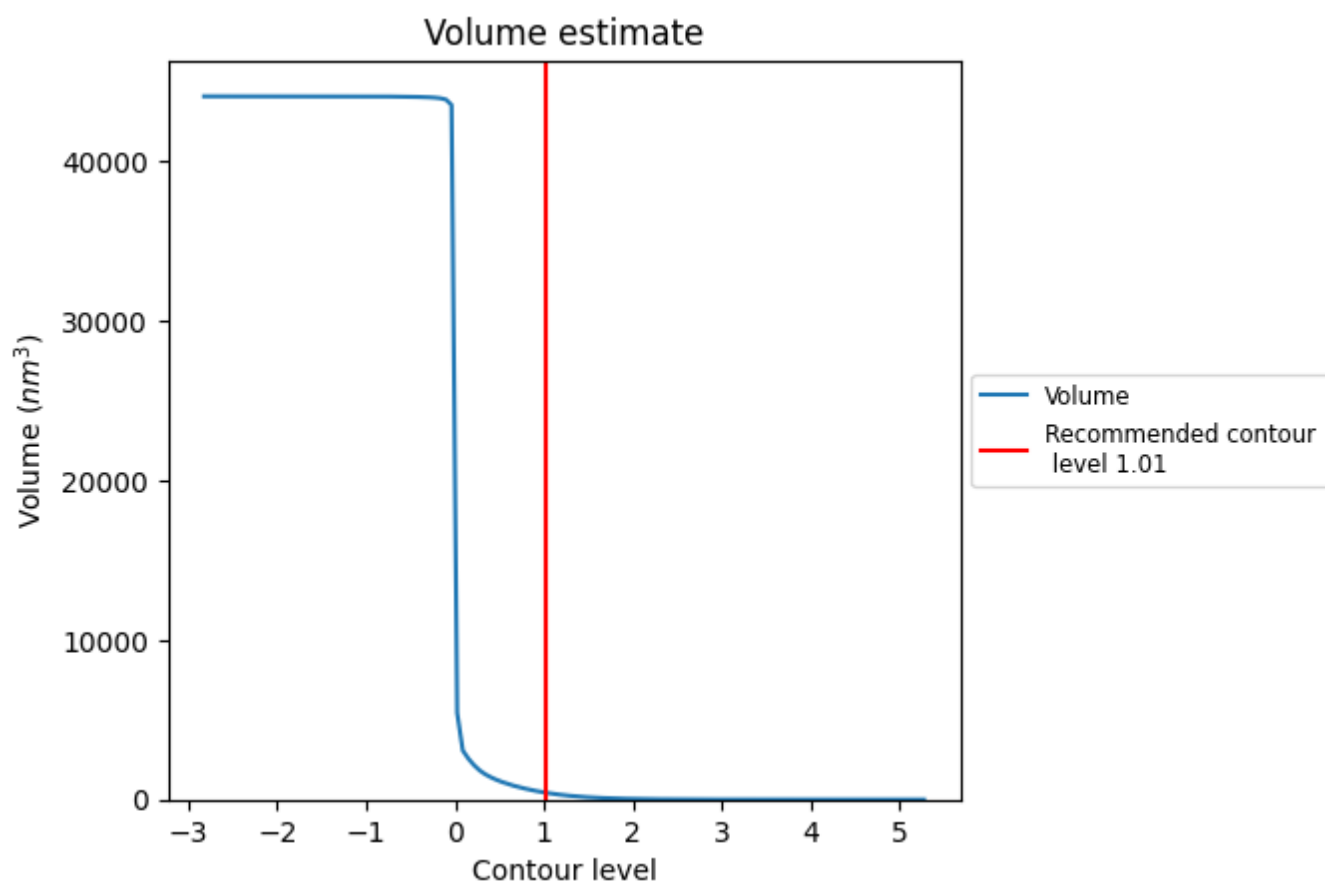
This section contains the results of statistical analysis of the map.

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.

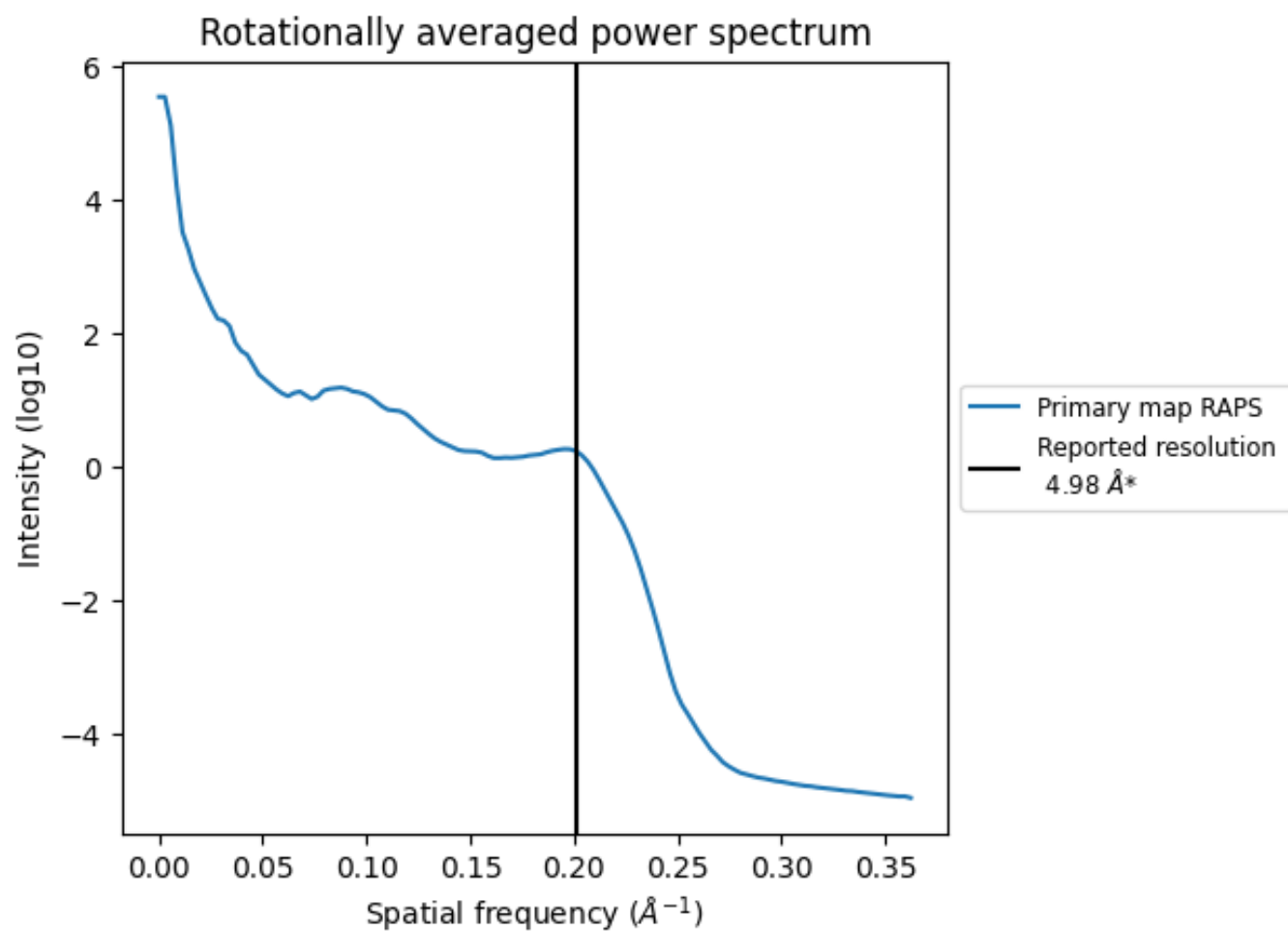
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 440 nm³; this corresponds to an approximate mass of 397 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 0.201 Å⁻¹

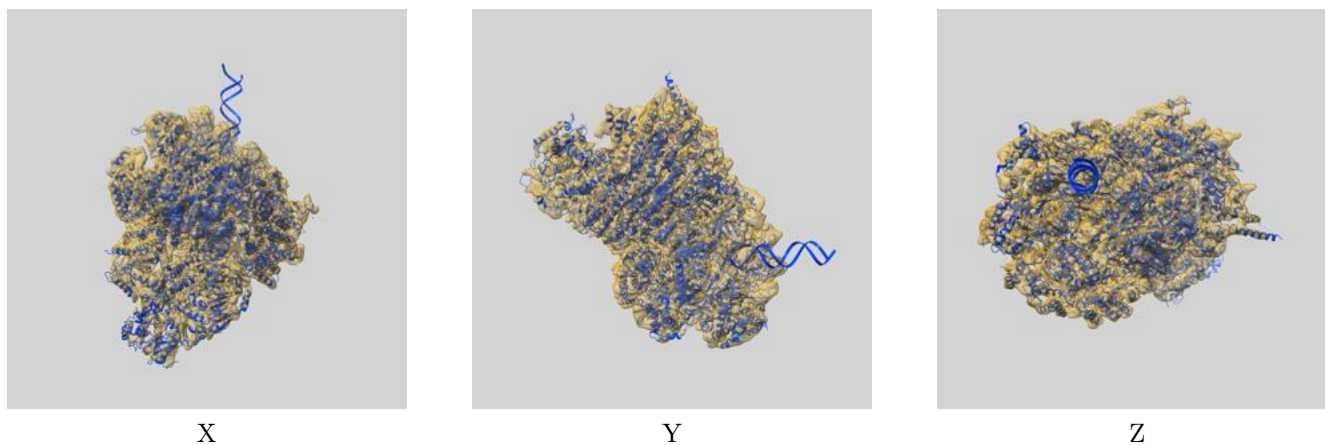
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

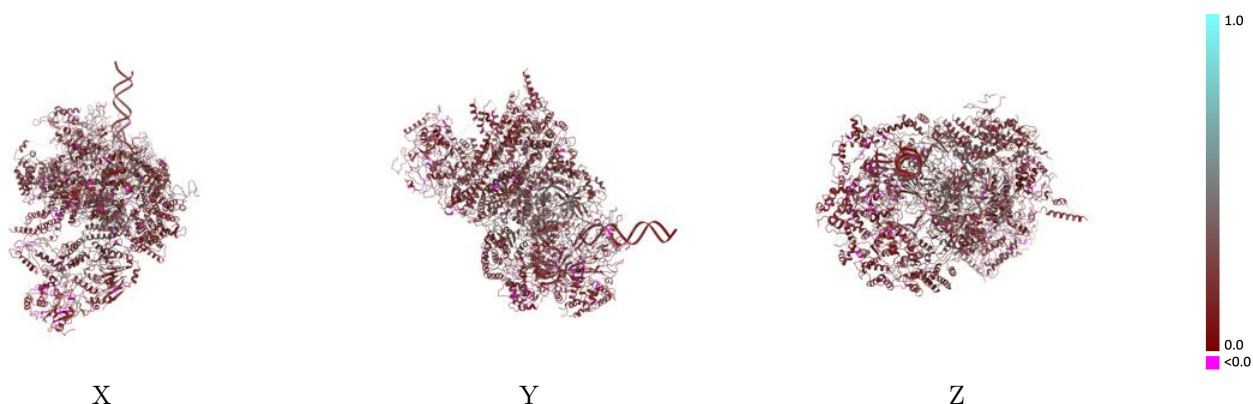
This section contains information regarding the fit between EMDB map EMD-0288 and PDB model 6HV9. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



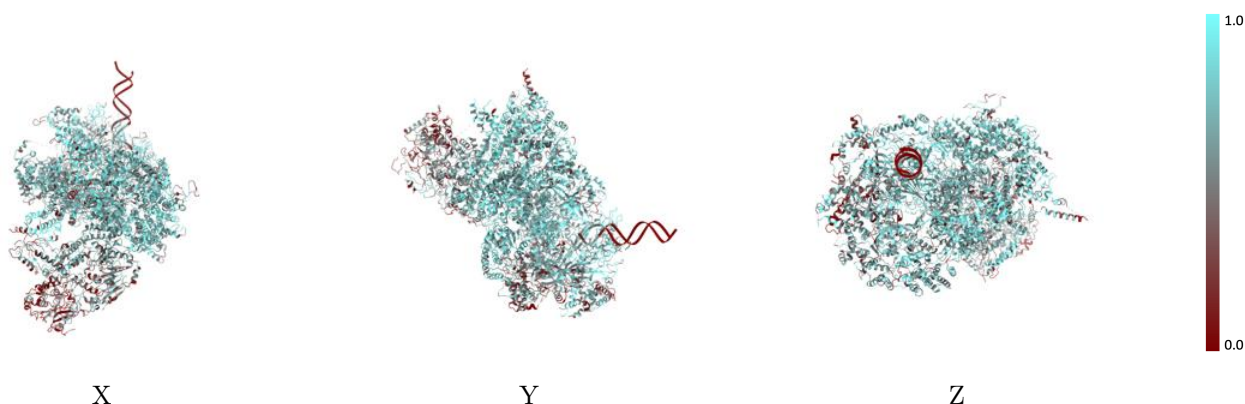
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



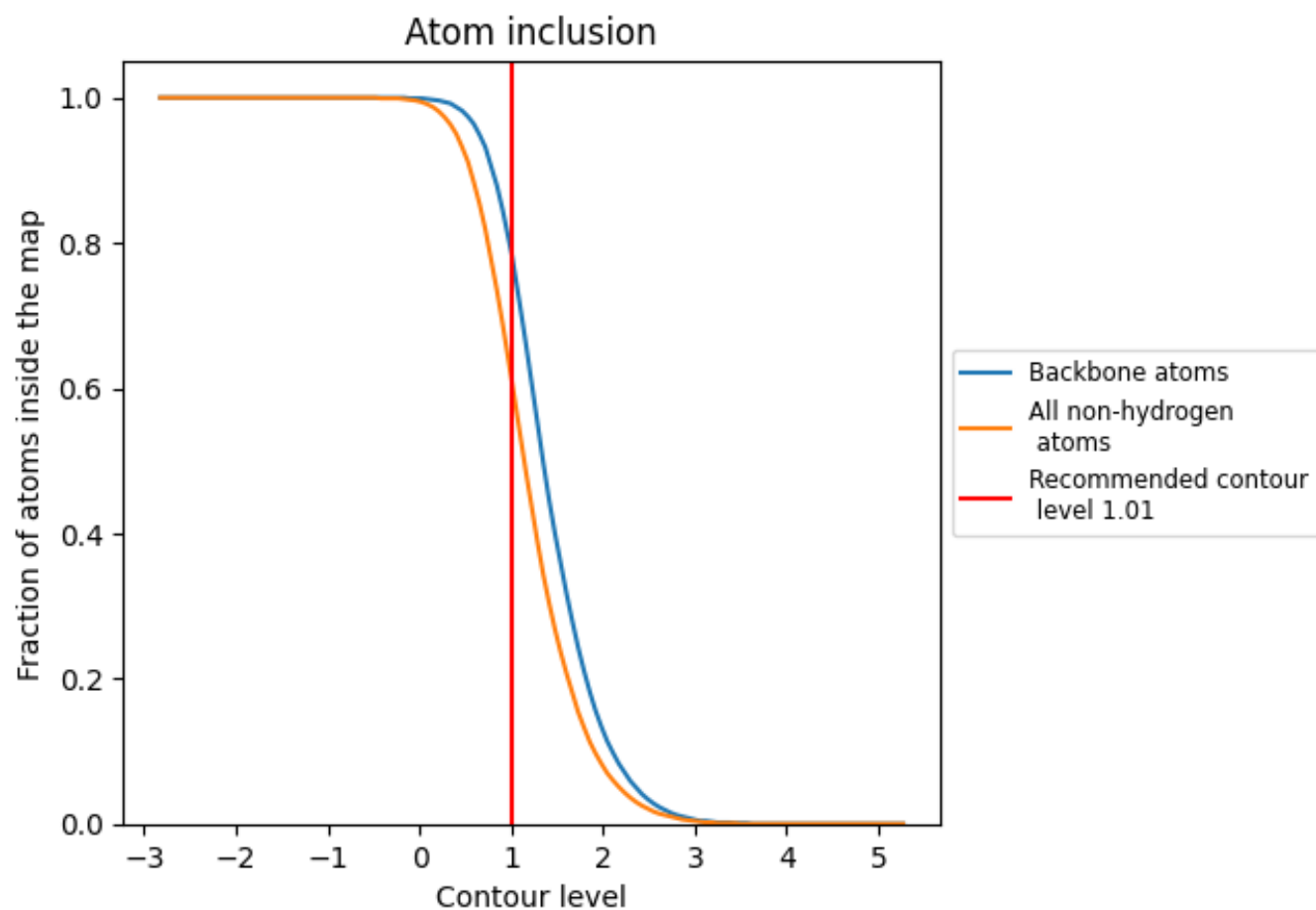
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 61% 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 (1.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6090	 0.2310
2	 0.6910	 0.2780
3	 0.7390	 0.2870
4	 0.5710	 0.1860
5	 0.6920	 0.3050
6	 0.6500	 0.2140
7	 0.5230	 0.1890
A	 0.4210	 0.1710
B	 0.5140	 0.2290
C	 0.7020	 0.2280
D	 0.7350	 0.2480
E	 0.7440	 0.2690
F	 0.6930	 0.2300
G	 0.6860	 0.2410
J	 0.5710	 0.2480
X	 0.1650	 0.1690
Y	 0.1520	 0.1610

