Full wwPDB EM Validation Report (i)

May 19, 2024 – 06:49 am BST

PDB ID	:	6Z6G
EMDB ID	:	EMD-11093
Title	:	Cryo-EM structure of La Crosse virus polymerase at pre-initiation stage
Authors	:	Arragain, B.; Effantin, G.; Gerlach, P.; Reguera, J.; Schoehn, G.; Cusack, S.; Malet, H.
Deposited on	:	2020-05-28
Resolution	:	3.06 Å(reported)
Based on initial model	:	5AMQ

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 (i) 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 (i)) were used in the production of this report:

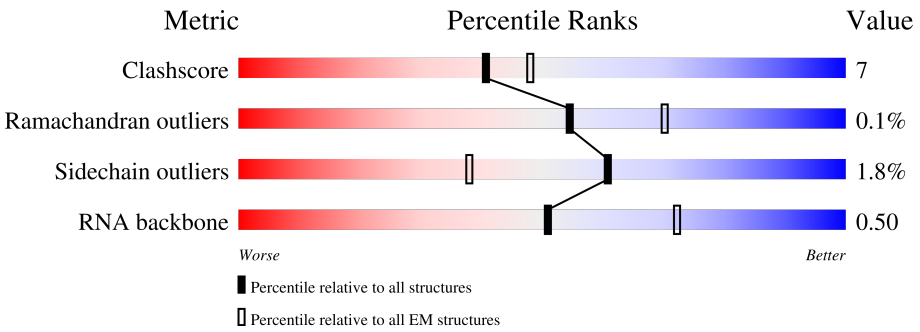
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	U	10	60% 30% 10%
2	X	8	38% 25% 38%
3	H	16	44% 38% 19%
4	A	2285	7% 80% 13% • 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18068 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 RNA chain called 5'vRNA 1-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	U	10	216	96	39	71	10	0	0

- Molecule 2 is a RNA chain called 5'vRNA 9-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	X	5	101	47	18	32	4	0	0

- Molecule 3 is a RNA chain called 3'vRNA 1-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	H	13	274	123	47	91	13	0	0

- Molecule 4 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	2142	17475	11184	2924	3256	111	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A5HC98
A	-20	GLY	-	expression tag	UNP A5HC98
A	-19	HIS	-	expression tag	UNP A5HC98
A	-18	HIS	-	expression tag	UNP A5HC98
A	-17	HIS	-	expression tag	UNP A5HC98
A	-16	HIS	-	expression tag	UNP A5HC98
A	-15	HIS	-	expression tag	UNP A5HC98
A	-14	HIS	-	expression tag	UNP A5HC98
A	-13	ASP	-	expression tag	UNP A5HC98

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	TYR	-	expression tag	UNP A5HC98
A	-11	ASP	-	expression tag	UNP A5HC98
A	-10	ILE	-	expression tag	UNP A5HC98
A	-9	PRO	-	expression tag	UNP A5HC98
A	-8	THR	-	expression tag	UNP A5HC98
A	-7	THR	-	expression tag	UNP A5HC98
A	-6	GLU	-	expression tag	UNP A5HC98
A	-5	ASN	-	expression tag	UNP A5HC98
A	-4	LEU	-	expression tag	UNP A5HC98
A	-3	TYR	-	expression tag	UNP A5HC98
A	-2	PHE	-	expression tag	UNP A5HC98
A	-1	GLN	-	expression tag	UNP A5HC98
A	0	GLY	-	expression tag	UNP A5HC98

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	1	1	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0

3 Residue-property plots (i)

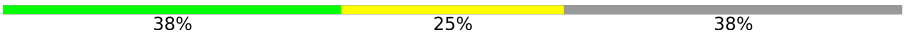
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

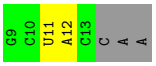
- Molecule 1: 5'vRNA 1-10

Chain U:

- Molecule 2: 5'vRNA 9-16

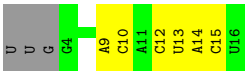
Chain X:





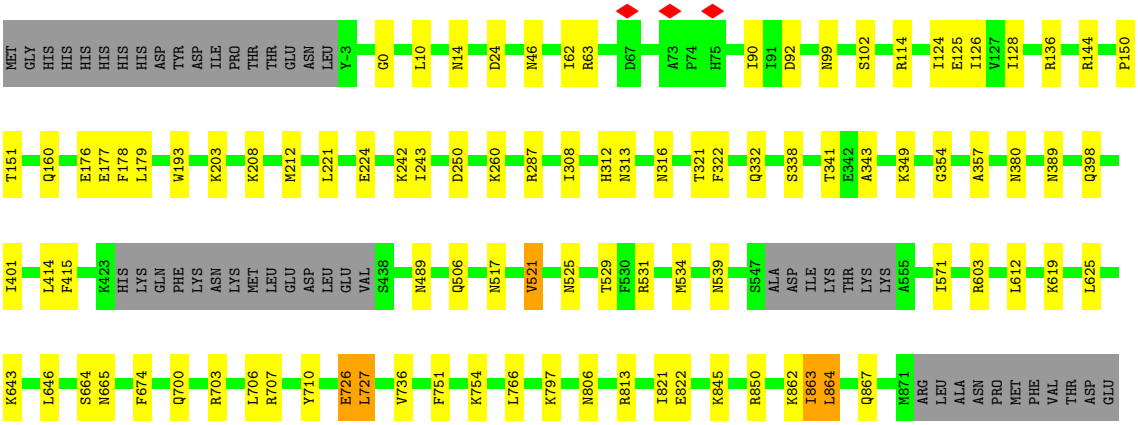
- Molecule 3: 3'vRNA 1-16

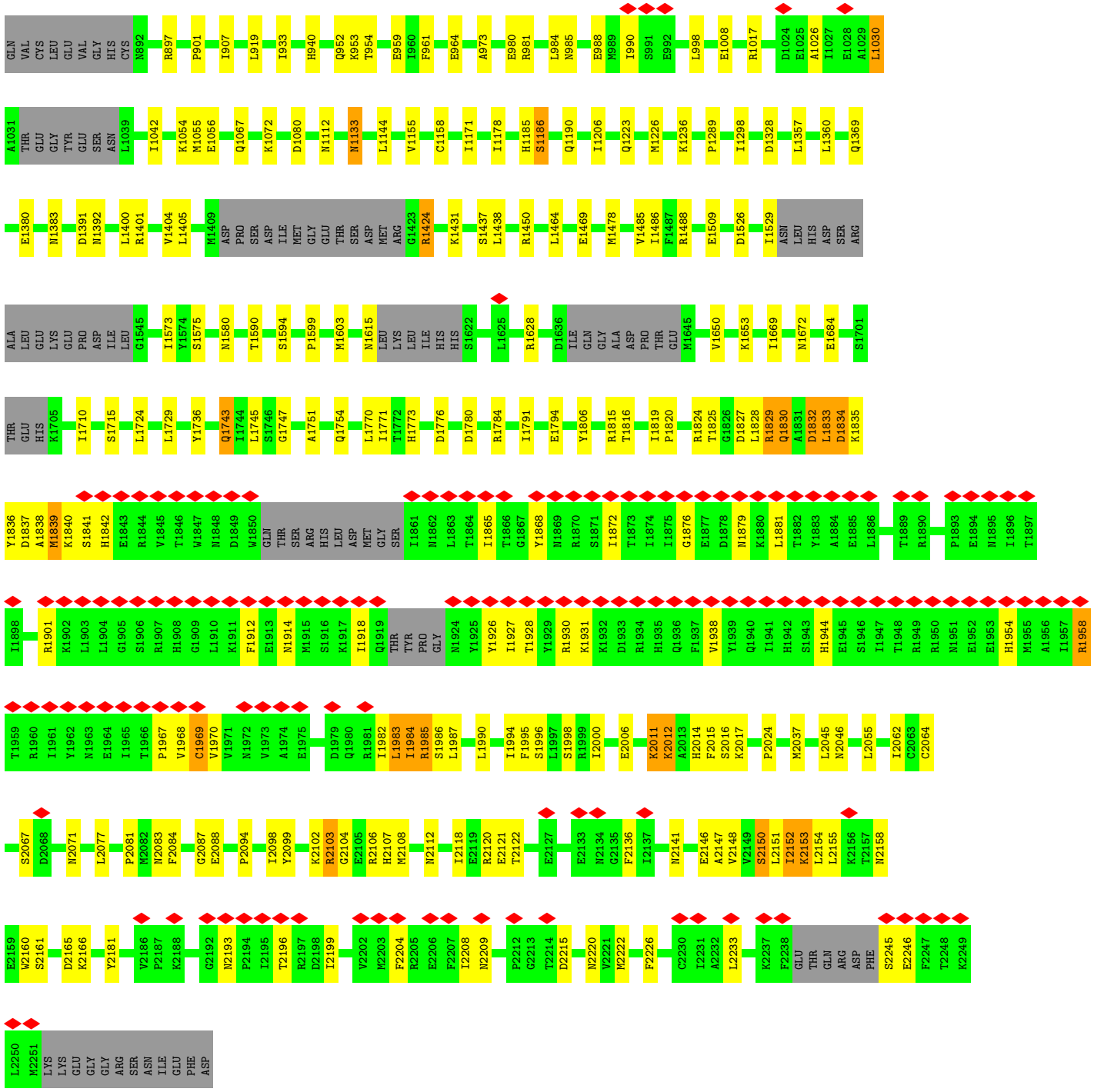
Chain H:



- Molecule 4: RNA-directed RNA polymerase L

Chain A:




GLN VAL CYS LEU GLU VAL GLY HIS CYS N892 R897 P901 I907 L919 I933 H940 Q952 K953 T954 E959 I960 F961 E964 A973 E980 R981 L984 N985 E988 M989 I990 S991 E992 L998 E1008 R1017 D1024 E1025 A1026 I1027 E1028 A1029 L1030
A1031 THR GLU GLY TYR GLU SER ASN L1039 I1042 K1054 M1055 E1056 Q1067 K1072 D1080 N1112 N1133 L1144 V1155 C1158 I1171 I1178 H1185 S1186 Q1190 I1206 Q1223 M1226 K1236 P1289 T1298 D1328 L1357 L1360 Q1369
E1380 N1383 D1391 N1392 L1400 R1401 V1404 L1405 M1409 ASP PRO SER ASP ILE MET GLY GLU THR SER ASP MET ARG G1423 R1424 K1431 S1437 L1438 R1450 L1464 E1469 M1478 V1485 I1486 F1487 R1488 E1509 D1526 I1529 ASN LEU HIS ASP SER ARG
ALA LEU GLU LYS GLU PRO ASP ILE LEU G1545 I1573 Y1574 S1575 N1580 T1590 S1594 P1599 M1603 N1615 LEU LYS LEU ILE HIS HIS S1622 L1625 R1628 D1636 ILE GLN GLY ALA ASP PRO THR GLU M1645 V1650 K1653 I1669 N1672 E1684 S1701
THR GLU HIS K1705 I1710 S1715 L1724 L1729 Y1736 Q1743 I1744 L1745 S1746 G1747 A1751 Q1754 L1770 I1771 T1772 H1773 D1776 D1780 R1784 I1791 E1794 Y1806 R1815 T1816 I1819 P1820 R1824 T1825 G1826 D1827 L1828 R1829 Q1830 A1831 D1832 L1833 D1834 K1835
Y1836 D1837 A1838 M1839 K1840 S1841 H1842 E1843 R1844 V1845 T1846 W1847 N1848 D1849 W1850 GLN THR SER ARG HIS LEU ASP MET GLY SER I1861 N1862 L1863 T1864 I1865 T1866 G1867 Y1868 N1869 R1870 S1871 I1872 T1873 I1874 I1875 G1876 E1877 D1878 N1879 K1880 L1881 T1882 Y1883 A1884 E1885 L1886 T1889 R1890 P1893 E1894 N1895 I1896 T1897
I1898 R1901 K1902 L1903 L1904 G1905 S1906 R1907 H1908 G1909 L1910 K1911 F1912 E1913 N1914 M1915 S1916 K1917 I1918 Q1919 THR TYR PRO GLY N1924 Y1925 Y1926 I1927 T1928 Y1929 R1930 K1931 K1932 D1933 R1934 H1935 Q1936 F1937 V1938 Y1939 Q1940 I1941 H1942 S1943 H1944 E1945 S1946 I1947 T1948 R1949 R1950 N1951 E1952 E1953 H1954 M1955 A1956 I1957 R1958
T1959 R1960 I1961 Y1962 N1963 E1964 I1965 T1966 P1967 V1968 C1969 V1970 V1971 N1972 V1973 A1974 E1975 D1979 Q1980 R1981 I1982 L1983 I1984 R1985 S1986 L1987 L1990 I1994 F1995 S1996 L1997 S1998 R1999 I2000 E2006 K2011 K2012 A2013 H2014 F2015 S2016 K2017 P2024 M2037 L2045 N2046 L2055 I2062 C2063 C2064
S2067 D2068 N2071 L2077 P2081 M2082 N2083 F2084 G2087 E2088 P2094 I2098 Y2099 K2102 R2103 G2104 E2105 R2106 H2107 M2108 N2112 I2118 E2119 R2120 E2121 T2122 E2127 E2133 N2134 G2135 F2136 I2137 N2141 E2146 A2147 V2148 W2149 S2150 L2151 I2152 K2153 L2154 L2155 K2156 T2157 N2158
E2159 W2160 S2161 D2165 K2166 Y2181 V2186 P2187 K2188 G2192 N2193 P2194 I2195 T2196 R2197 D2198 I2199 V2202 M2203 F2204 R2205 E2206 F2207 I2208 N2209 P2212 G2213 T2214 D2215 N2220 V2221 M2222 F2226 C2230 I2231 A2232 L2233 K2237 F2238 GLU THR GLN ARG ASP PHE S2245 E2246 F2247 T2248 K2249
L2250 M2251 LYS LYS GLU GLY GLY ARG SER ASN ILE GLU PHE ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57660	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 ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	247.79999, 247.79999, 247.79999	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	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: MG, 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	U	0.95	0/241	1.26	5/374 (1.3%)
2	X	0.50	0/112	1.11	0/173
3	H	0.93	0/305	1.00	2/472 (0.4%)
4	A	0.47	0/17824	0.57	1/24023 (0.0%)
All	All	0.49	0/18482	0.60	8/25042 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	8	U	N3-C2-O2	-8.67	116.13	122.20
1	U	8	U	N1-C2-O2	8.36	128.65	122.80
1	U	8	U	C6-N1-C2	-6.24	117.25	121.00
3	H	12	C	N1-C2-O2	6.04	122.53	118.90
1	U	8	U	C5-C6-N1	5.96	125.68	122.70
1	U	8	U	C2-N1-C1'	5.85	124.72	117.70
3	H	12	C	N3-C2-O2	-5.64	117.95	121.90
4	A	1464	LEU	CB-CG-CD1	-5.15	102.24	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	216	0	108	0	0
2	X	101	0	53	2	0
3	H	274	0	140	1	0
4	A	17475	0	17524	266	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
All	All	18068	0	17825	268	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 7.

All (268) 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)
4:A:2151:LEU:HD13	4:A:2204:PHE:CE2	1.35	1.57
4:A:1838:ALA:HA	4:A:1868:TYR:CE1	1.47	1.50
4:A:2151:LEU:HD13	4:A:2204:PHE:CZ	1.50	1.46
4:A:2151:LEU:CD1	4:A:2204:PHE:CE2	1.99	1.44
4:A:1838:ALA:HA	4:A:1868:TYR:CZ	1.60	1.33
4:A:1829:ARG:O	4:A:1832:ASP:OD2	1.61	1.18
4:A:2151:LEU:CD2	4:A:2204:PHE:HE2	1.57	1.17
4:A:1829:ARG:HH11	4:A:1829:ARG:HB2	1.13	1.06
4:A:1838:ALA:CA	4:A:1868:TYR:CZ	2.40	1.05
4:A:1838:ALA:CA	4:A:1868:TYR:CE1	2.41	1.04
4:A:2151:LEU:CD2	4:A:2204:PHE:CE2	2.46	0.99
4:A:710:TYR:CD1	4:A:2099:TYR:HB2	1.97	0.98
4:A:2151:LEU:HD22	4:A:2204:PHE:CE2	1.99	0.97
4:A:1185:HIS:O	4:A:1186:SER:OG	1.87	0.92
4:A:1833:LEU:O	4:A:1836:TYR:HB3	1.71	0.91
4:A:710:TYR:CE1	4:A:2099:TYR:HB2	2.07	0.89
4:A:1838:ALA:HB1	4:A:1868:TYR:OH	1.72	0.89
4:A:1985:ARG:HG2	4:A:1985:ARG:HH11	1.36	0.89
4:A:1838:ALA:CB	4:A:1868:TYR:OH	2.22	0.88
4:A:2151:LEU:HD11	4:A:2204:PHE:CE2	2.10	0.85
4:A:2151:LEU:CG	4:A:2204:PHE:HE2	1.89	0.85
4:A:2084:PHE:HB3	4:A:2108:MET:CE	2.08	0.84
4:A:1983:LEU:HD12	4:A:1983:LEU:H	1.43	0.83
4:A:1743:GLN:NE2	4:A:1745:LEU:HB2	1.92	0.83
4:A:2151:LEU:CG	4:A:2204:PHE:CE2	2.62	0.82
4:A:1841:SER:O	4:A:1842:HIS:CD2	2.32	0.82
4:A:1837:ASP:O	4:A:1868:TYR:CD1	2.32	0.82
4:A:1838:ALA:CA	4:A:1868:TYR:OH	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2151:LEU:CD1	4:A:2204:PHE:CZ	2.44	0.79
4:A:1743:GLN:HE22	4:A:1745:LEU:HB2	1.45	0.79
4:A:1838:ALA:O	4:A:1868:TYR:CE2	2.35	0.79
4:A:1829:ARG:C	4:A:1832:ASP:OD2	2.22	0.78
4:A:1829:ARG:HH11	4:A:1829:ARG:CB	1.96	0.77
4:A:1829:ARG:HB2	4:A:1829:ARG:NH1	1.98	0.77
4:A:1833:LEU:HG	4:A:1982:ILE:HG22	1.65	0.77
4:A:1842:HIS:HB2	4:A:2006:GLU:OE2	1.84	0.77
4:A:2084:PHE:CE1	4:A:2104:GLY:HA2	2.19	0.77
4:A:1833:LEU:HG	4:A:1982:ILE:CG2	2.15	0.77
4:A:1838:ALA:HA	4:A:1868:TYR:HE1	1.44	0.76
4:A:2084:PHE:HE1	4:A:2104:GLY:HA2	1.51	0.75
4:A:710:TYR:HD1	4:A:2099:TYR:HB2	1.50	0.75
4:A:710:TYR:CE1	4:A:2099:TYR:CB	2.70	0.74
4:A:1838:ALA:HA	4:A:1868:TYR:OH	1.84	0.74
4:A:2084:PHE:HB3	4:A:2108:MET:HE1	1.70	0.74
4:A:177:GLU:OE2	4:A:1954:HIS:CE1	2.41	0.74
4:A:1983:LEU:HD12	4:A:1983:LEU:N	2.02	0.74
4:A:176:GLU:HB2	4:A:1958:ARG:NH2	2.04	0.71
4:A:1838:ALA:O	4:A:1868:TYR:CZ	2.43	0.71
4:A:1832:ASP:OD2	4:A:1832:ASP:N	2.24	0.69
4:A:2152:ILE:HG22	4:A:2153:LYS:N	2.08	0.69
4:A:338:SER:HG	4:A:341:THR:HG1	1.38	0.68
4:A:1017:ARG:NE	4:A:2088:GLU:OE2	2.26	0.68
4:A:176:GLU:HB2	4:A:1958:ARG:HH22	1.59	0.67
4:A:1841:SER:O	4:A:1842:HIS:CG	2.47	0.67
4:A:1791:ILE:HD11	4:A:2037:MET:HE3	1.76	0.67
4:A:2103:ARG:O	4:A:2103:ARG:HG3	1.94	0.67
4:A:1828:LEU:HD21	4:A:1833:LEU:HD22	1.78	0.66
4:A:1830:GLN:O	4:A:1830:GLN:NE2	2.30	0.65
4:A:1030:LEU:HD12	4:A:1042:ILE:HG13	1.78	0.64
4:A:1927:ILE:HG23	4:A:1968:VAL:HG23	1.79	0.64
4:A:1983:LEU:H	4:A:1983:LEU:CD1	2.11	0.64
4:A:1833:LEU:HD21	4:A:1987:LEU:HD11	1.80	0.63
4:A:312:HIS:HD2	4:A:506:GLN:HE22	1.45	0.63
4:A:1833:LEU:HD23	4:A:1984:ILE:CD1	2.28	0.63
4:A:710:TYR:HE1	4:A:2099:TYR:CB	2.12	0.63
4:A:2151:LEU:CD1	4:A:2204:PHE:HE2	1.71	0.63
4:A:1837:ASP:O	4:A:1868:TYR:CE1	2.52	0.62
4:A:707:ARG:NH1	4:A:1603:MET:O	2.33	0.62
4:A:517:ASN:ND2	4:A:534:MET:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1985:ARG:HG2	4:A:1985:ARG:NH1	2.08	0.61
4:A:1328:ASP:HB3	4:A:1392:ASN:HD21	1.65	0.61
4:A:1784:ARG:NH2	4:A:1995:PHE:O	2.34	0.60
4:A:1824:ARG:HH21	4:A:1996:SER:H	1.50	0.60
4:A:813:ARG:NH2	4:A:984:LEU:O	2.33	0.59
4:A:710:TYR:HE1	4:A:2099:TYR:CG	2.20	0.59
4:A:114:ARG:HH22	4:A:124:ILE:H	1.50	0.59
4:A:2046:ASN:HA	4:A:2083:ASN:O	2.03	0.58
4:A:2062:ILE:HG23	4:A:2166:LYS:HD2	1.85	0.58
4:A:521:VAL:HG22	4:A:531:ARG:HE	1.68	0.58
4:A:2055:LEU:HB2	4:A:2121:GLU:HB3	1.86	0.58
4:A:102:SER:HB2	4:A:128:ILE:HD13	1.86	0.58
4:A:1791:ILE:HD11	4:A:2037:MET:CE	2.33	0.58
4:A:703:ARG:HD2	4:A:726:GLU:HB3	1.85	0.57
4:A:981:ARG:NH1	4:A:1080:ASP:OD1	2.36	0.57
4:A:1380:GLU:OE1	4:A:1383:ASN:ND2	2.37	0.57
4:A:1469:GLU:HG3	4:A:1628:ARG:HG2	1.86	0.57
4:A:1828:LEU:HD21	4:A:1833:LEU:CD2	2.35	0.57
4:A:2084:PHE:CB	4:A:2108:MET:CE	2.83	0.57
4:A:221:LEU:HD13	4:A:243:ILE:HG23	1.88	0.56
4:A:1838:ALA:C	4:A:1868:TYR:CZ	2.78	0.56
4:A:2148:VAL:O	4:A:2152:ILE:HD12	2.06	0.56
4:A:1986:SER:O	4:A:1990:LEU:HD12	2.05	0.55
4:A:1815:ARG:NH1	4:A:1827:ASP:O	2.40	0.55
4:A:1575:SER:O	4:A:1580:ASN:ND2	2.40	0.54
4:A:1830:GLN:HA	4:A:1984:ILE:HG12	1.89	0.54
4:A:2152:ILE:HG13	4:A:2161:SER:OG	2.06	0.54
4:A:136:ARG:O	4:A:1615:ASN:ND2	2.39	0.54
4:A:2015:PHE:CE2	4:A:2045:LEU:HD11	2.41	0.54
4:A:2084:PHE:CD1	4:A:2108:MET:HE1	2.42	0.54
4:A:2147:ALA:O	4:A:2151:LEU:HB2	2.08	0.54
4:A:2152:ILE:CG1	4:A:2161:SER:OG	2.56	0.54
4:A:2084:PHE:CD1	4:A:2108:MET:CE	2.91	0.54
4:A:62:ILE:HD12	4:A:63:ARG:HG2	1.90	0.54
4:A:250:ASP:OD2	4:A:797:LYS:NZ	2.30	0.54
4:A:1879:ASN:O	4:A:1914:ASN:ND2	2.41	0.54
4:A:864:LEU:O	4:A:867:GLN:HG3	2.08	0.54
4:A:2084:PHE:CB	4:A:2108:MET:HE3	2.38	0.54
4:A:92:ASP:HB3	4:A:128:ILE:HG22	1.88	0.54
4:A:2150:SER:O	4:A:2154:LEU:HB2	2.07	0.53
4:A:2120:ARG:NH1	4:A:2121:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1401:ARG:HB2	4:A:1573:ILE:HD11	1.91	0.53
4:A:603:ARG:NH1	4:A:751:PHE:O	2.42	0.53
4:A:706:LEU:HD11	4:A:2094:PRO:HB2	1.91	0.53
4:A:2087:GLY:HA2	4:A:2098:ILE:O	2.09	0.53
4:A:2151:LEU:CD2	4:A:2208:ILE:HD11	2.39	0.53
4:A:177:GLU:OE1	4:A:1954:HIS:CE1	2.61	0.53
4:A:2151:LEU:HD22	4:A:2208:ILE:HD11	1.89	0.53
4:A:2152:ILE:C	4:A:2154:LEU:H	2.12	0.53
4:A:2152:ILE:O	4:A:2154:LEU:N	2.41	0.53
4:A:2155:LEU:HD13	4:A:2233:LEU:HD23	1.90	0.52
4:A:1590:THR:O	4:A:1594:SER:OG	2.26	0.52
4:A:850:ARG:HD3	4:A:897:ARG:HH21	1.74	0.52
4:A:665:ASN:HD22	4:A:1226:MET:HB3	1.74	0.52
4:A:1008:GLU:OE1	4:A:1054:LYS:NZ	2.42	0.52
4:A:1773:HIS:NE2	4:A:2011:LYS:O	2.42	0.52
4:A:727:LEU:N	4:A:727:LEU:CD2	2.73	0.52
4:A:525:ASN:OD1	4:A:529:THR:OG1	2.27	0.52
4:A:952:GLN:NE2	4:A:954:THR:OG1	2.43	0.51
4:A:1404:VAL:O	4:A:1424:ARG:NH1	2.43	0.51
4:A:2165:ASP:OD1	4:A:2181:TYR:OH	2.27	0.51
3:H:13:U:H5”	3:H:14:A:H5’	1.93	0.51
4:A:2064:CYS:SG	4:A:2067:SER:N	2.81	0.51
4:A:2146:GLU:O	4:A:2150:SER:HB2	2.10	0.51
4:A:2154:LEU:HD11	4:A:2199:ILE:HD13	1.92	0.51
4:A:919:LEU:HD13	4:A:1478:MET:HG3	1.93	0.51
4:A:1833:LEU:HG	4:A:1982:ILE:HG21	1.90	0.51
4:A:1485:VAL:HG23	4:A:1488:ARG:HH21	1.76	0.51
4:A:1834:ASP:C	4:A:1836:TYR:N	2.61	0.51
4:A:1985:ARG:NH1	4:A:1985:ARG:CG	2.73	0.50
4:A:224:GLU:OE2	4:A:242:LYS:NZ	2.42	0.50
4:A:1437:SER:OG	4:A:1438:LEU:N	2.44	0.50
4:A:1912:PHE:HB3	4:A:1968:VAL:HG21	1.94	0.50
4:A:316:ASN:HB3	4:A:322:PHE:HE2	1.77	0.50
4:A:1400:LEU:HD22	4:A:1573:ILE:HG23	1.93	0.50
4:A:1715:SER:HB3	4:A:1724:LEU:HD12	1.94	0.50
4:A:2151:LEU:HB2	4:A:2204:PHE:HZ	1.77	0.49
4:A:354:GLY:HA3	4:A:389:ASN:HD22	1.77	0.49
4:A:1834:ASP:C	4:A:1836:TYR:H	2.15	0.49
4:A:2193:ASN:HB2	4:A:2196:THR:HB	1.94	0.49
4:A:1599:PRO:HB3	4:A:1736:TYR:HE1	1.78	0.49
4:A:177:GLU:OE1	4:A:1954:HIS:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:177:GLU:CD	4:A:1954:HIS:CE1	2.86	0.48
4:A:1026:ALA:O	4:A:1030:LEU:HG	2.13	0.48
4:A:619:LYS:NZ	4:A:625:LEU:O	2.47	0.48
4:A:1918:ILE:HG22	4:A:1944:HIS:HD2	1.79	0.48
4:A:2118:ILE:O	4:A:2122:THR:CB	2.62	0.48
4:A:332:GLN:HE21	4:A:349:LYS:HA	1.76	0.48
4:A:1450:ARG:HD3	4:A:1486:ILE:HG21	1.95	0.48
4:A:1829:ARG:H	4:A:1832:ASP:CG	2.17	0.48
4:A:1837:ASP:HB3	4:A:1982:ILE:HD12	1.95	0.48
4:A:2118:ILE:O	4:A:2122:THR:OG1	2.26	0.48
4:A:2160:TRP:HD1	4:A:2222:MET:HG3	1.78	0.48
4:A:150:PRO:HD2	4:A:1754:GLN:HE22	1.79	0.48
4:A:1930:ARG:HG2	4:A:1938:VAL:HG12	1.96	0.48
4:A:90:ILE:HB	4:A:126:ILE:HG22	1.95	0.48
4:A:99:ASN:O	4:A:102:SER:OG	2.31	0.48
4:A:150:PRO:HG2	4:A:1751:ALA:HB2	1.96	0.47
4:A:1743:GLN:HE21	4:A:1745:LEU:H	1.62	0.47
4:A:1834:ASP:O	4:A:1836:TYR:N	2.48	0.47
4:A:1926:TYR:HE1	4:A:1970:VAL:HG22	1.79	0.47
4:A:401:ILE:HD13	4:A:415:PHE:HZ	1.80	0.47
4:A:1056:GLU:HG2	4:A:1236:LYS:HG2	1.96	0.47
4:A:1876:GLY:HA3	4:A:1881:LEU:HA	1.96	0.47
4:A:1650:VAL:HA	4:A:1653:LYS:HG2	1.96	0.47
4:A:24:ASP:CG	4:A:1901:ARG:NH2	2.67	0.47
4:A:2015:PHE:HE2	4:A:2045:LEU:HD11	1.79	0.47
4:A:176:GLU:OE1	4:A:1958:ARG:NH1	2.48	0.47
4:A:1017:ARG:CZ	4:A:2088:GLU:OE2	2.63	0.47
4:A:2084:PHE:HD1	4:A:2108:MET:HE1	1.79	0.47
4:A:0:GLY:H	4:A:160:GLN:HE22	1.61	0.46
4:A:961:PHE:CD2	4:A:1144:LEU:HB3	2.50	0.46
4:A:2152:ILE:HD11	4:A:2226:PHE:CZ	2.50	0.46
4:A:308:ILE:HD12	4:A:571:ILE:HD11	1.96	0.46
4:A:1833:LEU:HD13	4:A:1833:LEU:HA	1.72	0.46
4:A:1865:ILE:HB	4:A:1872:ILE:HG22	1.97	0.46
4:A:2083:ASN:HA	4:A:2102:LYS:O	2.15	0.46
4:A:1171:ILE:HG13	4:A:1178:ILE:HD12	1.97	0.46
4:A:517:ASN:O	4:A:521:VAL:HB	2.15	0.46
4:A:1780:ASP:CA	4:A:2077:LEU:O	2.64	0.46
4:A:2136:PHE:HA	4:A:2141:ASN:HD22	1.80	0.45
4:A:940:HIS:NE2	4:A:964:GLU:OE2	2.41	0.45
4:A:2151:LEU:HD21	4:A:2204:PHE:HE2	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1824:ARG:NH2	4:A:1994:ILE:O	2.49	0.45
4:A:2158:ASN:HD21	4:A:2160:TRP:HE3	1.64	0.45
4:A:1072:LYS:HD2	4:A:1155:VAL:HG11	1.98	0.45
4:A:1780:ASP:HA	4:A:2077:LEU:O	2.17	0.45
4:A:1770:LEU:HD21	4:A:2014:HIS:O	2.16	0.45
4:A:178:PHE:HD2	4:A:179:LEU:HD12	1.82	0.45
4:A:845:LYS:HB2	4:A:907:ILE:HG22	1.98	0.45
4:A:151:THR:HG21	4:A:1747:GLY:HA3	1.99	0.45
4:A:998:LEU:HD21	4:A:1710:ILE:HD11	1.98	0.45
4:A:1289:PRO:HG3	4:A:1729:LEU:HA	1.98	0.45
4:A:343:ALA:HB1	4:A:414:LEU:HD22	1.99	0.45
4:A:612:LEU:HD23	4:A:1298:ILE:HD11	1.98	0.45
4:A:988:GLU:HG3	4:A:990:ILE:HG12	1.97	0.45
4:A:1369:GLN:H	4:A:1369:GLN:HG2	1.57	0.45
4:A:664:SER:OG	4:A:665:ASN:N	2.50	0.44
4:A:2088:GLU:O	4:A:2088:GLU:HG3	2.16	0.44
4:A:2152:ILE:C	4:A:2154:LEU:N	2.70	0.44
4:A:2014:HIS:CE1	4:A:2016:SER:OG	2.70	0.44
4:A:1391:ASP:OD1	4:A:1391:ASP:N	2.51	0.44
4:A:1830:GLN:N	4:A:1984:ILE:HG12	2.33	0.44
4:A:700:GLN:HB3	4:A:703:ARG:HH21	1.83	0.44
4:A:1881:LEU:HB2	4:A:1969:CYS:HB2	2.00	0.44
4:A:821:ILE:HG12	4:A:980:GLU:HB2	2.00	0.44
4:A:933:ILE:HG21	4:A:973:ALA:HB2	1.99	0.44
4:A:2084:PHE:O	4:A:2084:PHE:CD2	2.70	0.44
4:A:1776:ASP:OD2	4:A:1998:SER:OG	2.27	0.43
4:A:1794:GLU:HG3	4:A:2024:PRO:HG3	2.00	0.43
4:A:1771:ILE:HD13	4:A:1771:ILE:HA	1.82	0.43
4:A:398:GLN:OE1	4:A:531:ARG:NH1	2.51	0.43
4:A:1669:ILE:HD12	4:A:1684:GLU:HG2	1.99	0.43
4:A:1830:GLN:CA	4:A:1984:ILE:HG12	2.49	0.43
4:A:985:ASN:HB3	4:A:988:GLU:HB3	2.01	0.43
4:A:1806:TYR:OH	4:A:1825:THR:OG1	2.26	0.43
4:A:2081:PRO:HG3	4:A:2106:ARG:HH21	1.84	0.43
4:A:313:ASN:HB2	4:A:539:ASN:HD21	1.84	0.43
4:A:1357:LEU:HD23	4:A:1360:LEU:HD12	2.00	0.43
4:A:10:LEU:O	4:A:14:ASN:ND2	2.51	0.43
4:A:1431:LYS:NZ	4:A:1509:GLU:OE1	2.44	0.43
4:A:754:LYS:HE2	4:A:953:LYS:HE3	2.01	0.42
4:A:766:LEU:HD13	4:A:959:GLU:HB3	2.01	0.42
4:A:125:GLU:HG2	4:A:144:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1839:MET:SD	4:A:1839:MET:C	2.97	0.42
4:A:1833:LEU:O	4:A:1836:TYR:CB	2.56	0.42
4:A:863:ILE:HG22	4:A:864:LEU:N	2.35	0.42
4:A:806:ASN:ND2	4:A:1158:CYS:SG	2.92	0.42
4:A:312:HIS:CD2	4:A:506:GLN:HE22	2.32	0.42
4:A:1830:GLN:NE2	4:A:1830:GLN:C	2.73	0.42
4:A:643:LYS:HD2	4:A:646:LEU:HD22	2.02	0.42
4:A:2245:SER:OG	4:A:2246:GLU:N	2.49	0.42
4:A:150:PRO:HD2	4:A:1754:GLN:NE2	2.35	0.41
4:A:203:LYS:HA	4:A:208:LYS:HE3	2.01	0.41
4:A:1526:ASP:HA	4:A:1529:ILE:HG22	2.01	0.41
4:A:193:TRP:NE1	4:A:822:GLU:OE2	2.43	0.41
4:A:1829:ARG:CB	4:A:1829:ARG:NH1	2.73	0.41
4:A:2084:PHE:CG	4:A:2108:MET:HE3	2.55	0.41
4:A:2215:ASP:O	4:A:2220:ASN:ND2	2.53	0.41
4:A:287:ARG:NH2	4:A:674:PHE:O	2.40	0.41
4:A:1816:THR:HG21	4:A:1835:LYS:HG2	2.03	0.41
4:A:1820:PRO:HB3	4:A:2000:ILE:HG23	2.02	0.41
4:A:2136:PHE:HA	4:A:2141:ASN:ND2	2.35	0.41
4:A:863:ILE:CG2	4:A:864:LEU:N	2.81	0.41
4:A:321:THR:HG21	4:A:357:ALA:HB1	2.02	0.41
4:A:1067:GLN:OE1	4:A:1223:GLN:NE2	2.54	0.41
2:X:11:U:H2'	2:X:12:A:C8	2.55	0.41
4:A:521:VAL:HG22	4:A:531:ARG:NE	2.32	0.41
4:A:901:PRO:HD2	4:A:1133:ASN:HD22	1.86	0.41
4:A:1770:LEU:HD11	4:A:2017:LYS:HB2	2.03	0.41
4:A:2107:HIS:O	4:A:2112:ASN:ND2	2.49	0.41
4:A:260:LYS:HE2	4:A:260:LYS:HB3	1.90	0.40
4:A:1928:THR:HG22	4:A:1967:PRO:HB3	2.03	0.40
4:A:1055:MET:HE2	4:A:1206:ILE:HG12	2.03	0.40
4:A:1931:LYS:HE2	4:A:1931:LYS:HB2	1.94	0.40
2:X:11:U:O2	4:A:380:ASN:ND2	2.44	0.40
4:A:1819:ILE:HG22	4:A:2000:ILE:HD11	2.03	0.40
4:A:1839:MET:SD	4:A:1839:MET:O	2.79	0.40
4:A:2012:LYS:HE3	4:A:2012:LYS:HB2	1.25	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
4	A	2116/2285 (93%)	1974 (93%)	139 (7%)	3 (0%)	51 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	2153	LYS
4	A	1186	SER
4	A	1969	CYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	1968/2107 (93%)	1932 (98%)	36 (2%)	59 80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	46	ASN
4	A	212	MET
4	A	489	ASN
4	A	521	VAL
4	A	726	GLU
4	A	727	LEU
4	A	736	VAL
4	A	862	LYS

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Mol	Chain	Res	Type
4	A	863	ILE
4	A	864	LEU
4	A	1030	LEU
4	A	1112	ASN
4	A	1133	ASN
4	A	1190	GLN
4	A	1405	LEU
4	A	1424	ARG
4	A	1672	ASN
4	A	1743	GLN
4	A	1829	ARG
4	A	1830	GLN
4	A	1832	ASP
4	A	1833	LEU
4	A	1834	ASP
4	A	1839	MET
4	A	1840	LYS
4	A	1958	ARG
4	A	1983	LEU
4	A	1984	ILE
4	A	1985	ARG
4	A	2011	LYS
4	A	2012	LYS
4	A	2071	ASN
4	A	2103	ARG
4	A	2150	SER
4	A	2152	ILE
4	A	2209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	14	ASN
4	A	46	ASN
4	A	160	GLN
4	A	312	HIS
4	A	332	GLN
4	A	389	ASN
4	A	489	ASN
4	A	565	HIS
4	A	602	GLN
4	A	806	ASN

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Mol	Chain	Res	Type
4	A	826	ASN
4	A	952	GLN
4	A	1058	ASN
4	A	1112	ASN
4	A	1133	ASN
4	A	1190	GLN
4	A	1243	ASN
4	A	1392	ASN
4	A	1580	ASN
4	A	1672	ASN
4	A	1726	GLN
4	A	1743	GLN
4	A	1754	GLN
4	A	1830	GLN
4	A	1842	HIS
4	A	1924	ASN
4	A	1944	HIS
4	A	1954	HIS
4	A	2071	ASN
4	A	2141	ASN
4	A	2209	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	9/10 (90%)	4 (44%)	0
2	X	4/8 (50%)	0	0
3	H	12/16 (75%)	3 (25%)	0
All	All	25/34 (73%)	7 (28%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	6	U
1	U	7	G
1	U	8	U
1	U	9	G
3	H	9	A
3	H	10	C
3	H	15	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

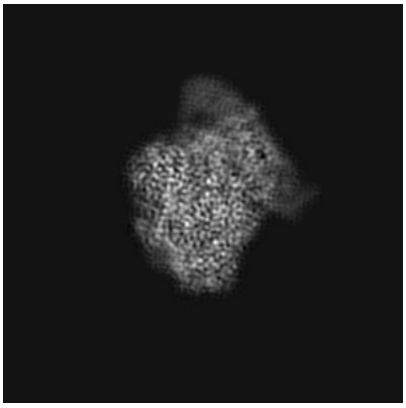
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11093. These allow visual inspection of the internal detail of the map and identification of artifacts.

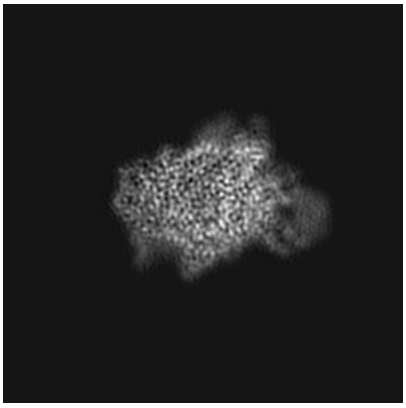
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

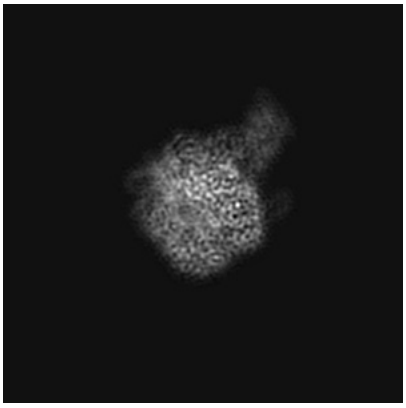
6.1.1 Primary map



X



Y

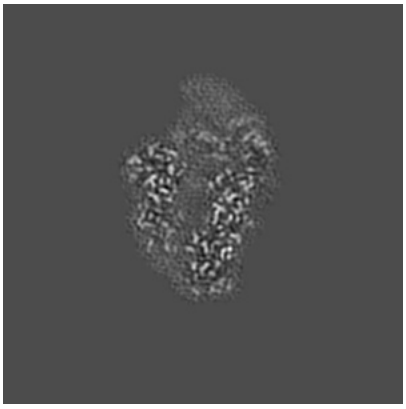


Z

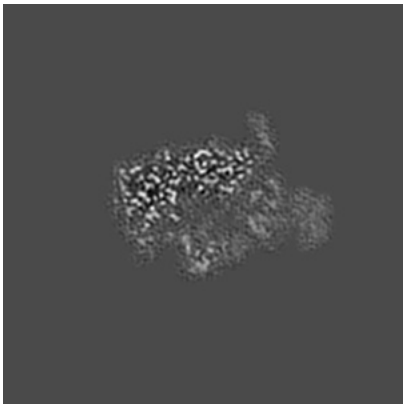
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

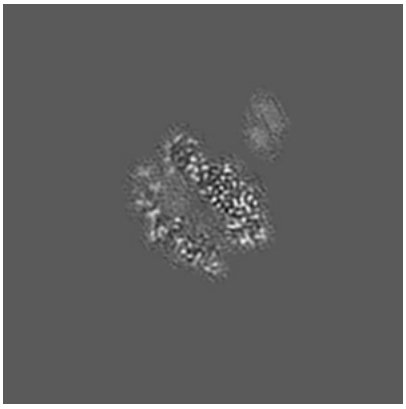
6.2.1 Primary map



X Index: 150



Y Index: 150



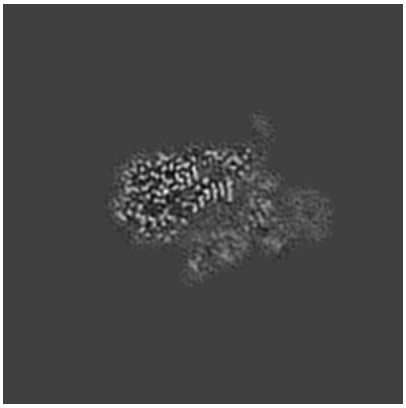
Z Index: 150

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

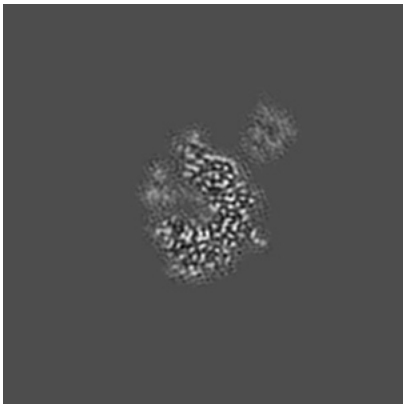
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 170



Y Index: 158

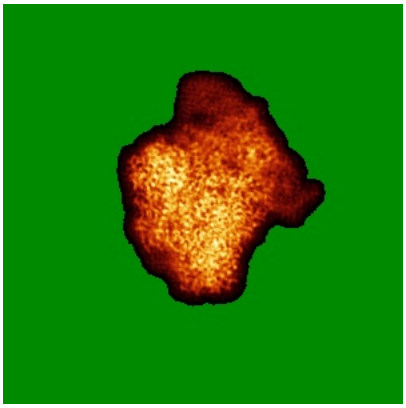


Z Index: 167

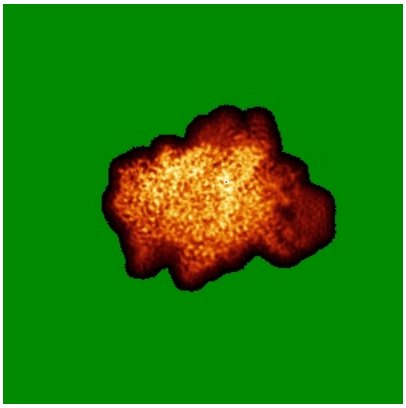
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

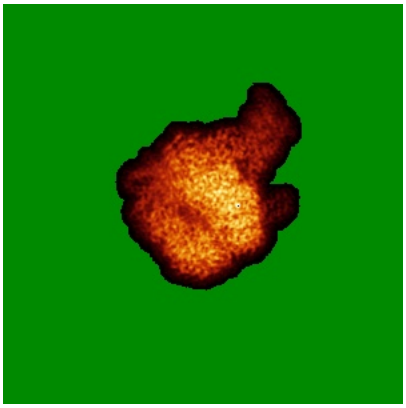
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

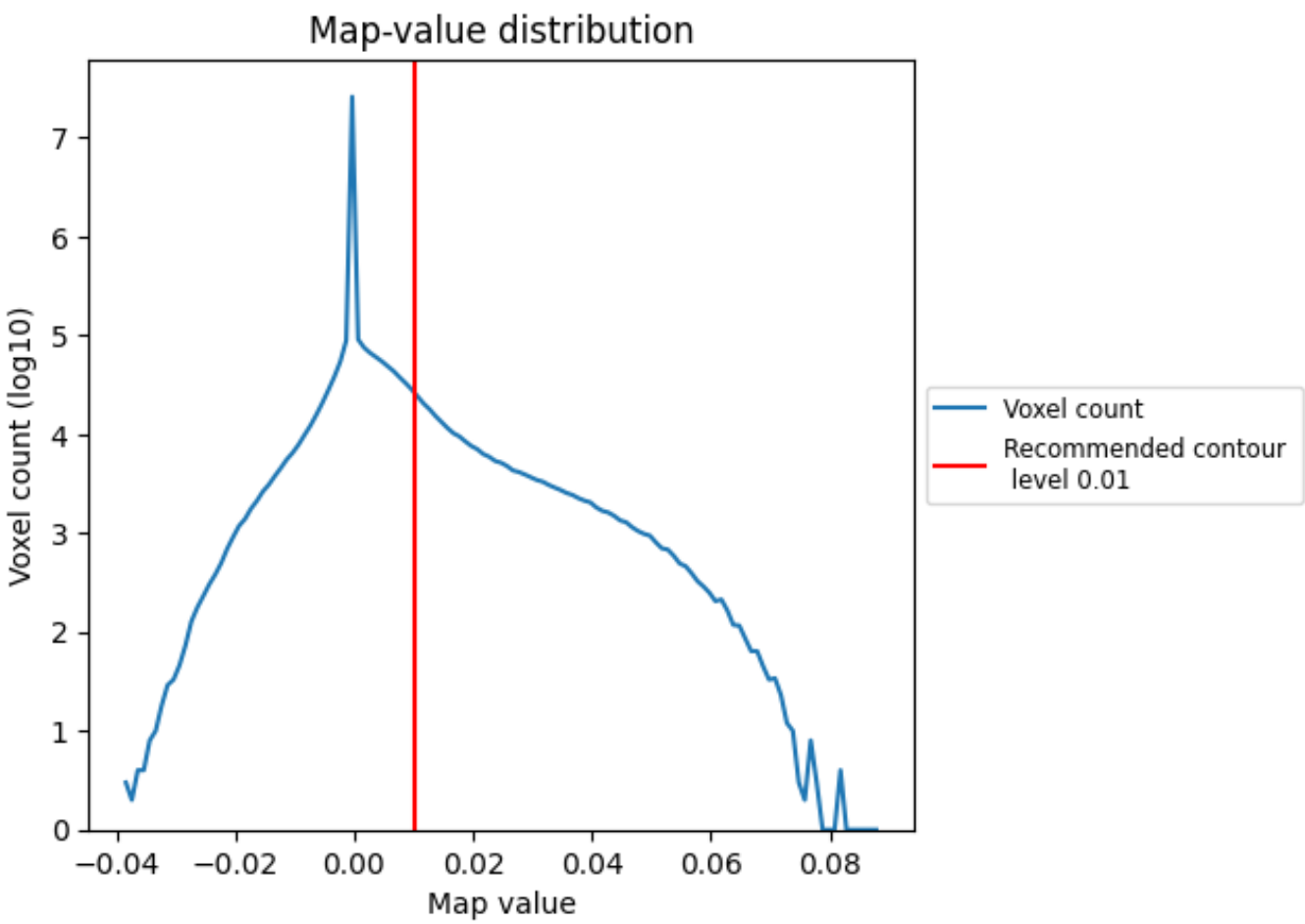
6.6 Mask visualisation (i)

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

7 Map analysis (i)

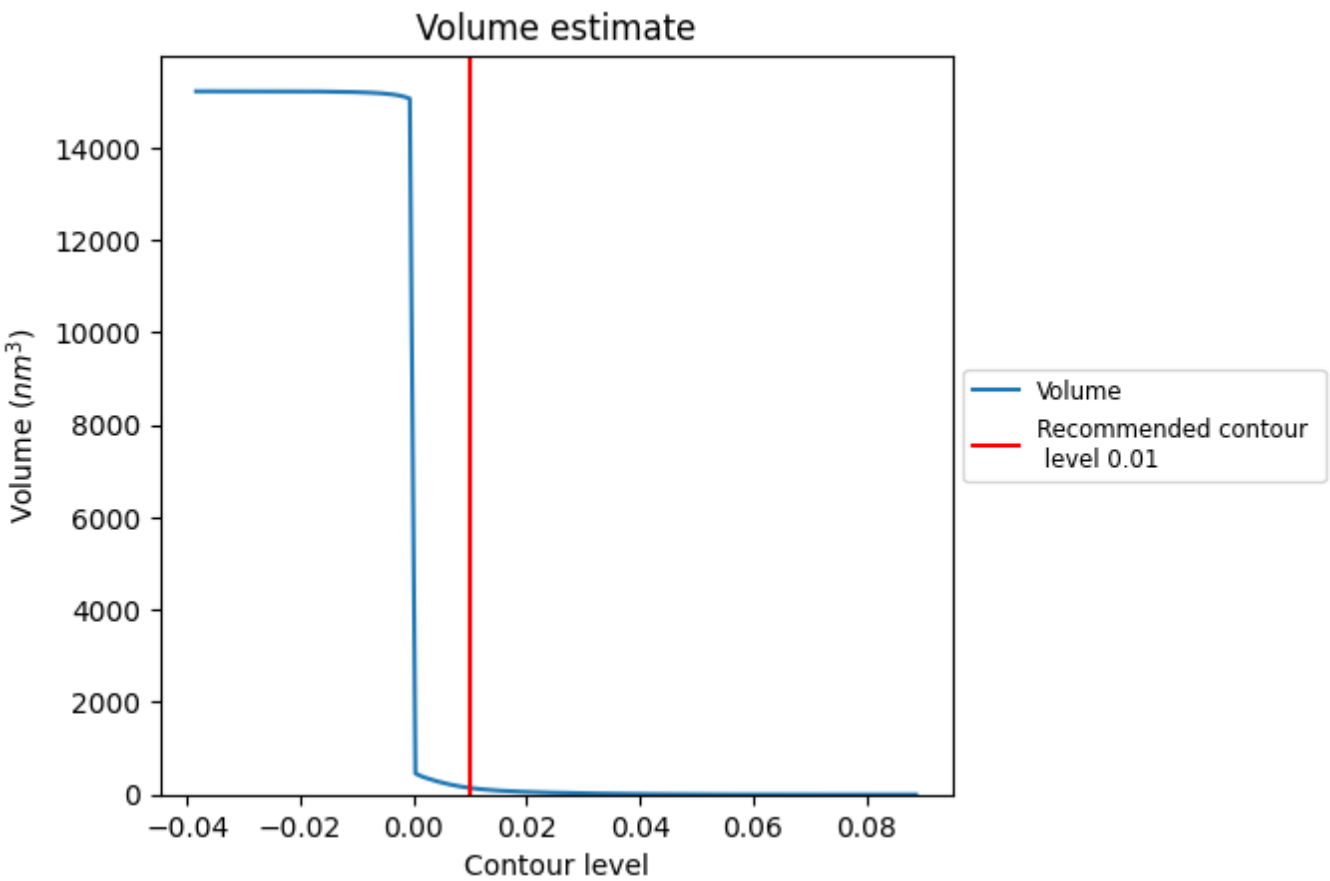
This section contains the results of statistical analysis of the map.

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.

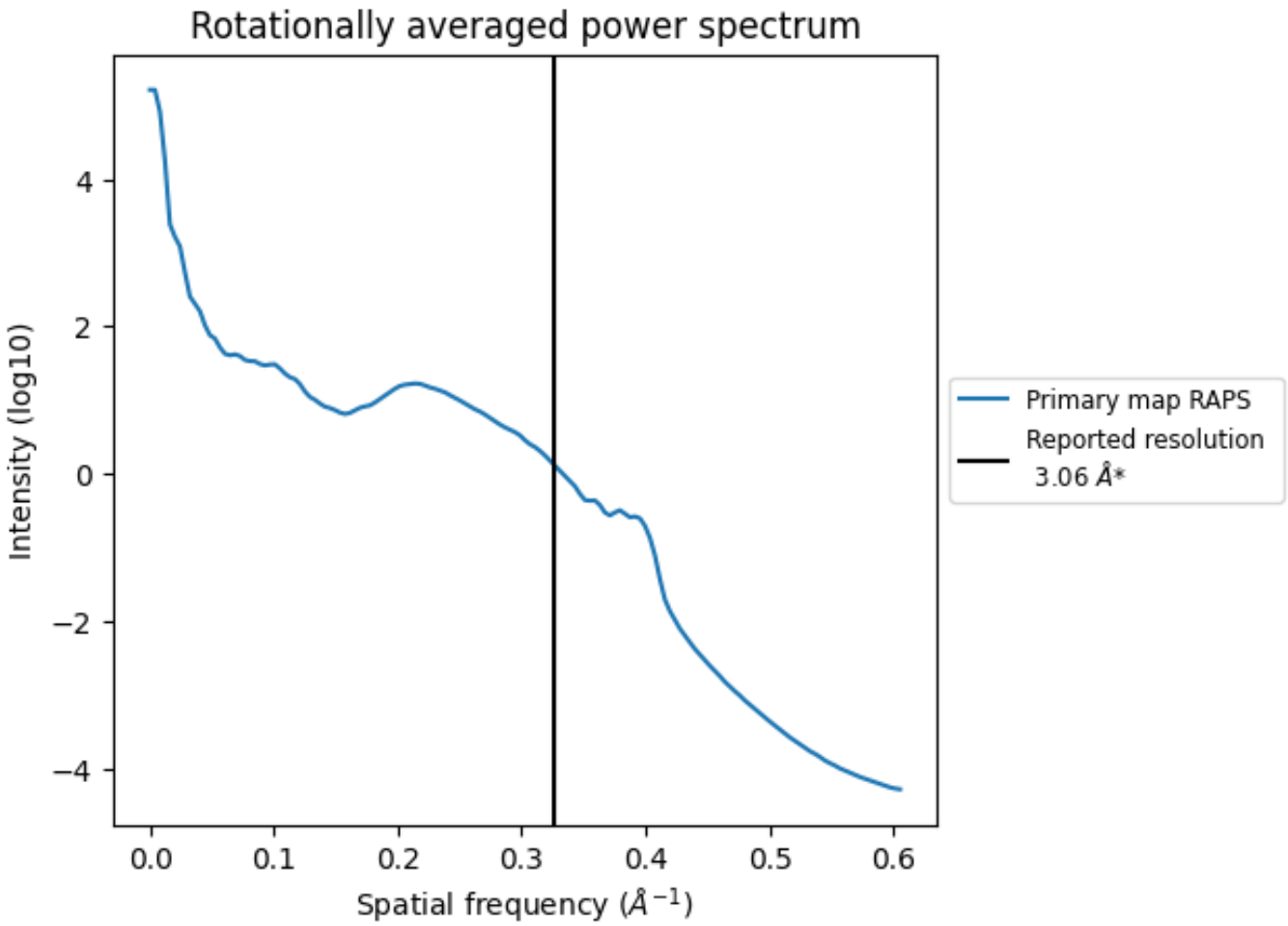
7.2 Volume estimate (i)



The volume at the recommended contour level is 143 nm^3; this corresponds to an approximate mass of 130 kDa.

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

7.3 Rotationally averaged power spectrum (i)

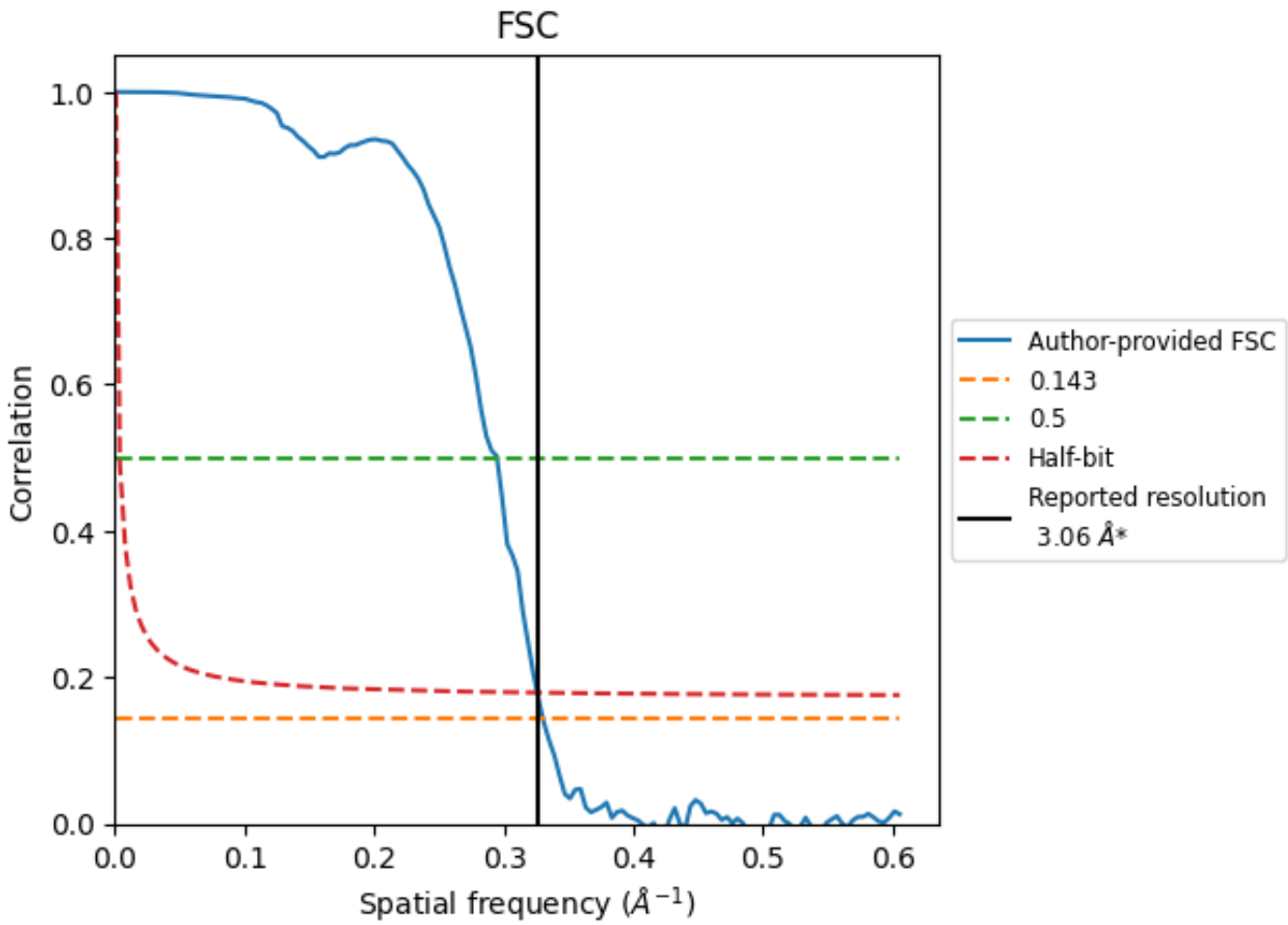


*Reported resolution corresponds to spatial frequency of 0.327 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.327 Å^{-1}

8.2 Resolution estimates (i)

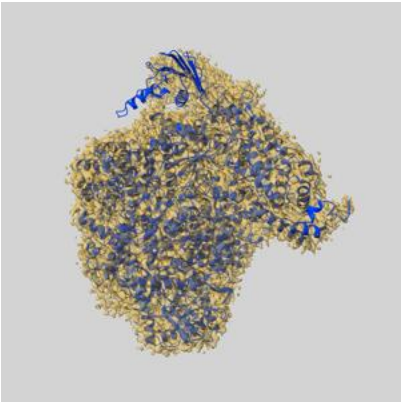
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.03	3.39	3.07
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

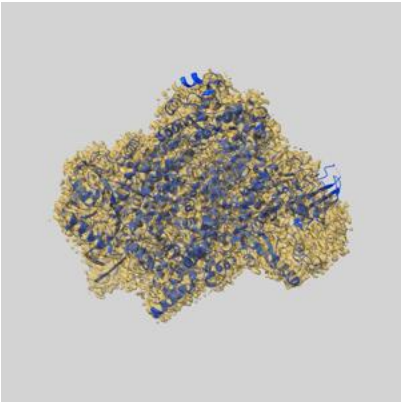
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11093 and PDB model 6Z6G. Per-residue inclusion information can be found in section 3 on page 5.

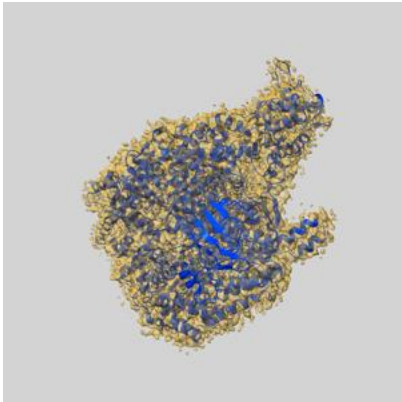
9.1 Map-model overlay (i)



X



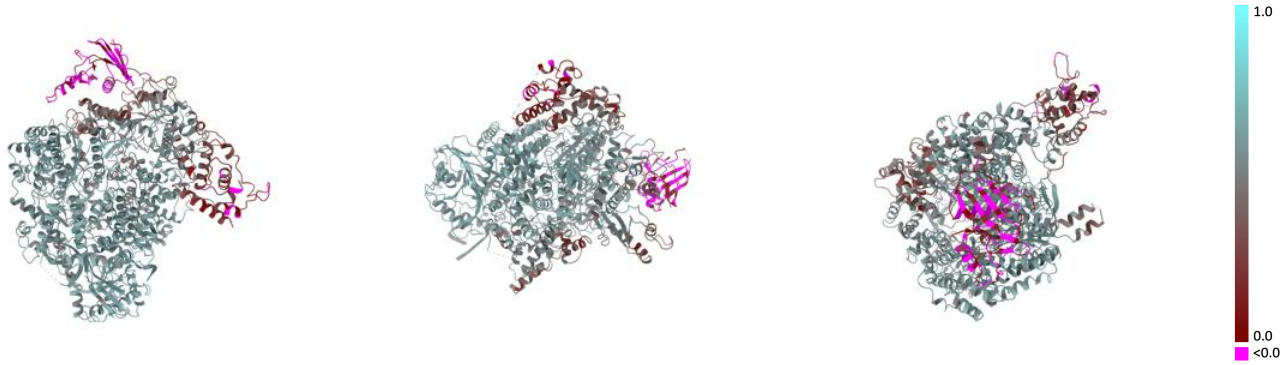
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

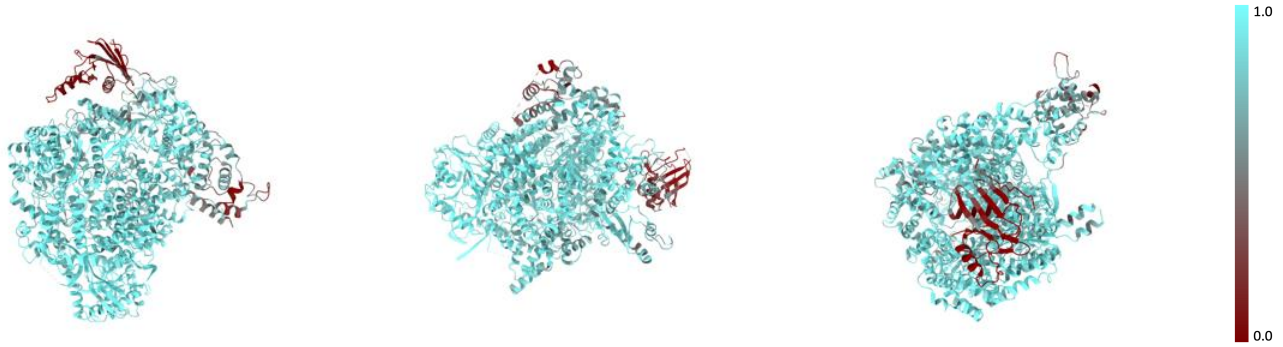
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

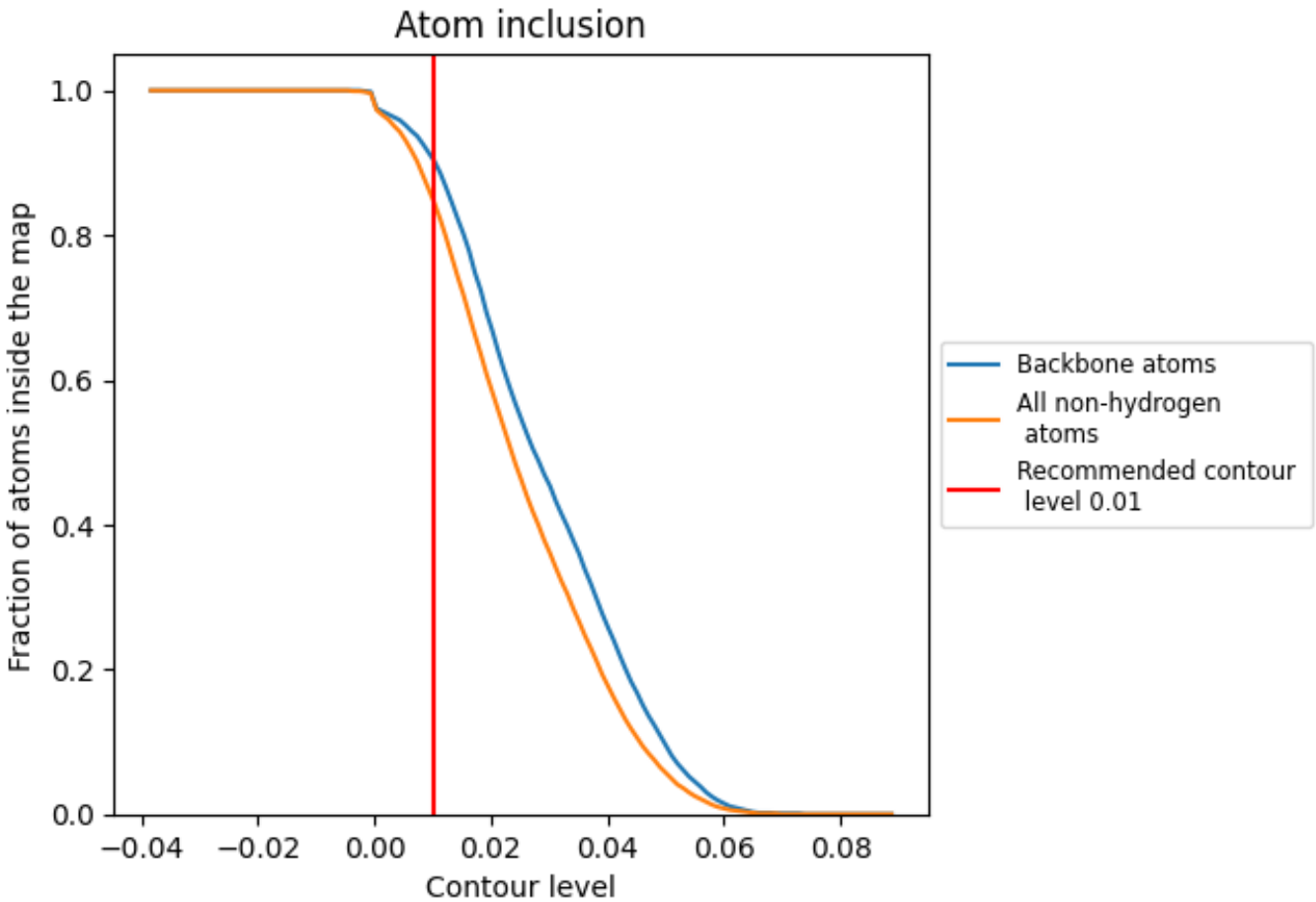
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8500	0.4990
A	0.8460	0.4970
H	0.9820	0.5870
U	0.9860	0.5910
X	0.9800	0.5130