Full wwPDB EM Validation Report ⓘ

Sep 27, 2026 – 04:03 AM JST

PDB ID	:	9XE9 / pdb_00009xe9
EMDB ID	:	EMD-66785
Title	:	Crimean-Congo hemorrhagic fever virus RNA polymerase containing a 15-bp RNA product
Authors	:	Xue, L.; Gui, J.; Pan, H.; Chang, T.; Xiong, X.
Deposited on	:	2025-10-27
Resolution	:	2.81 Å(reported)

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:

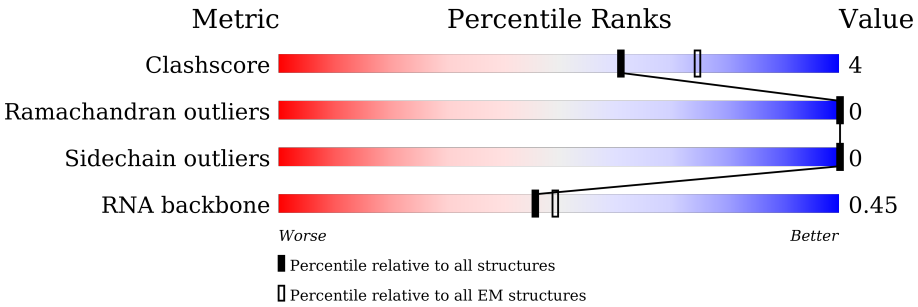
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.50

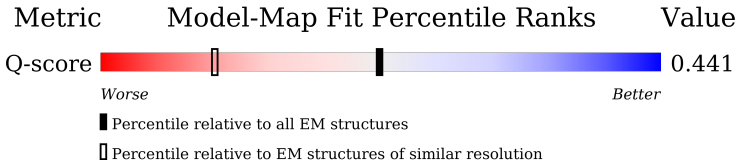
1 Overall quality at a glance

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

The reported resolution of this entry is 2.81 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	11740 (2.31 - 3.31)

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	A	3945	68% 10% 22%
2	B	19	32% 16% 11% 42%
3	C	19	5% 32% 32% 5% 32%

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Mol	Chain	Length	Quality of chain
3	E	19	26% 16% 58%
4	D	15	33% 33% 33%
5	F	3	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 25605 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3074	Total	C	N	O	S	0	0
			24614	15636	4199	4621	158		

- Molecule 2 is a RNA chain called RNA (5'-R(*UP*UP*CP*CP*AP*AP*AP*AP*AP*AP*AP*UP*CP*GP*UP*UP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	11	Total	C	N	O	P	0	0
			231	106	45	70	10		

- Molecule 3 is a RNA chain called RNA (5'-R(P*GP*GP*GP*AP*UP*UP*GP*GP*UP*GP*UP*CP*UP*UP*UP*GP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	13	Total	C	N	O	P	0	0
			280	124	48	95	13		
3	E	8	Total	C	N	O	P	0	0
			170	76	29	57	8		

- Molecule 4 is a RNA chain called RNA (5'-R(*UP*CP*UP*CP*AP*AP*AP*GP*AP*CP*AP*CP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	10	Total	C	N	O	P	0	0
			215	97	44	64	10		

- Molecule 5 is a RNA chain called RNA (5'-R(P*UP*CP*U)-3').

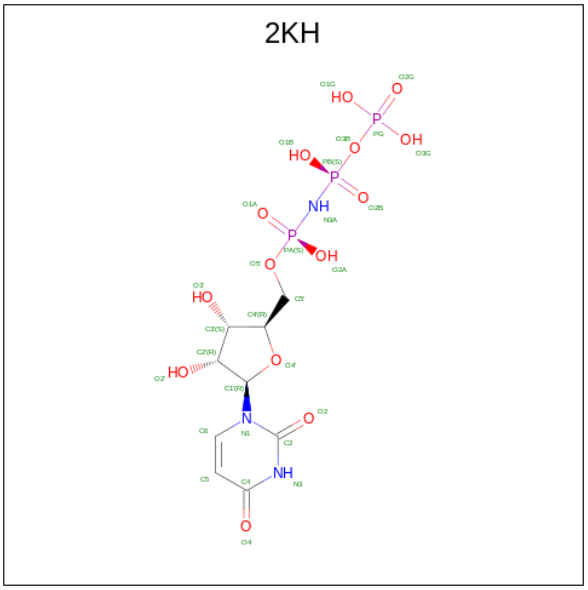
Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	3	Total	C	N	O	P	0	0
			61	27	7	24	3		

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
6	A	4	Total Mn 4 4	0

- Molecule 7 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]uridine (CCD ID: 2KH) (formula: $C_9H_{16}N_3O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O P 29 9 3 14 3	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

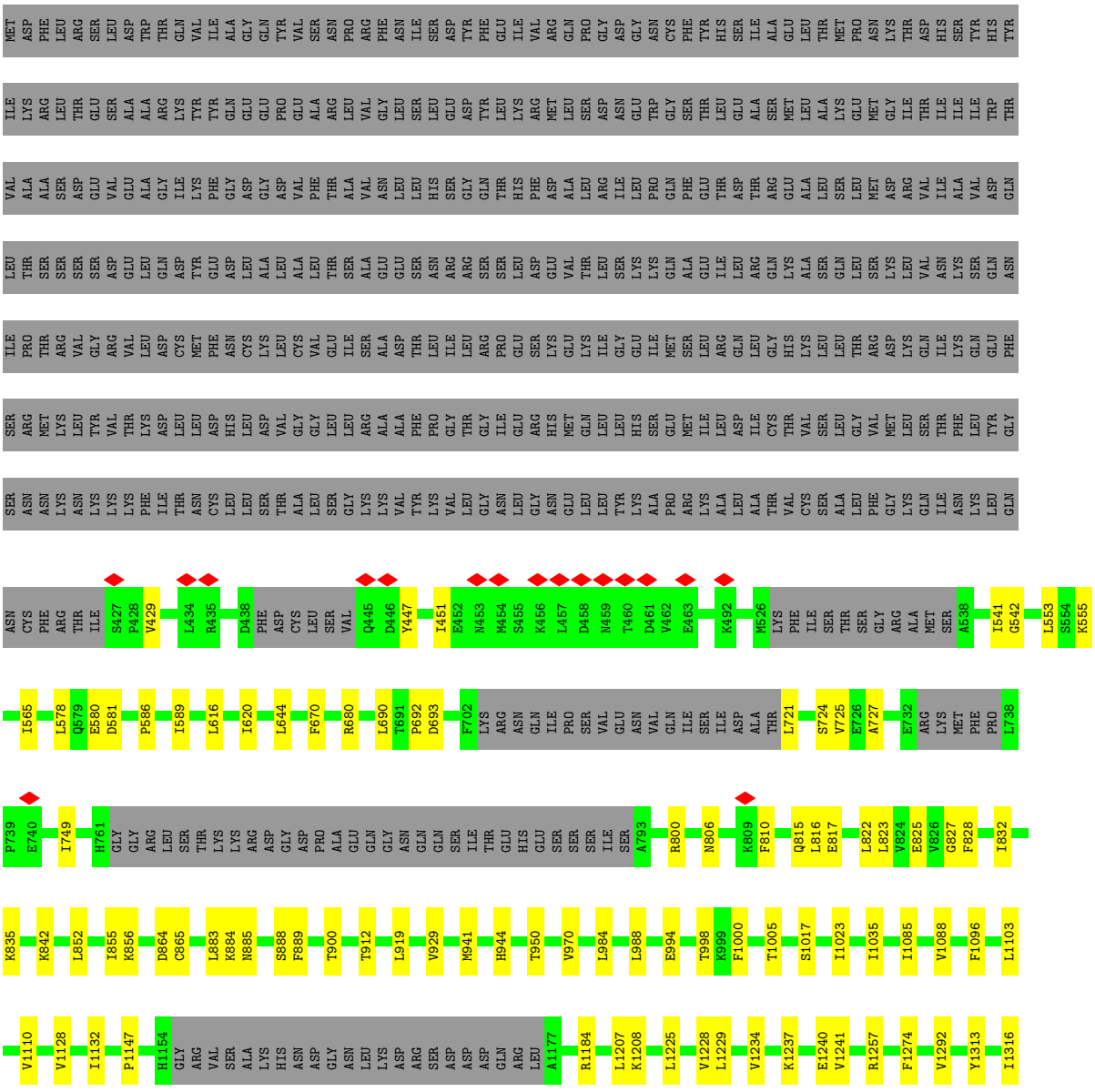
3 Residue-property plots (i)

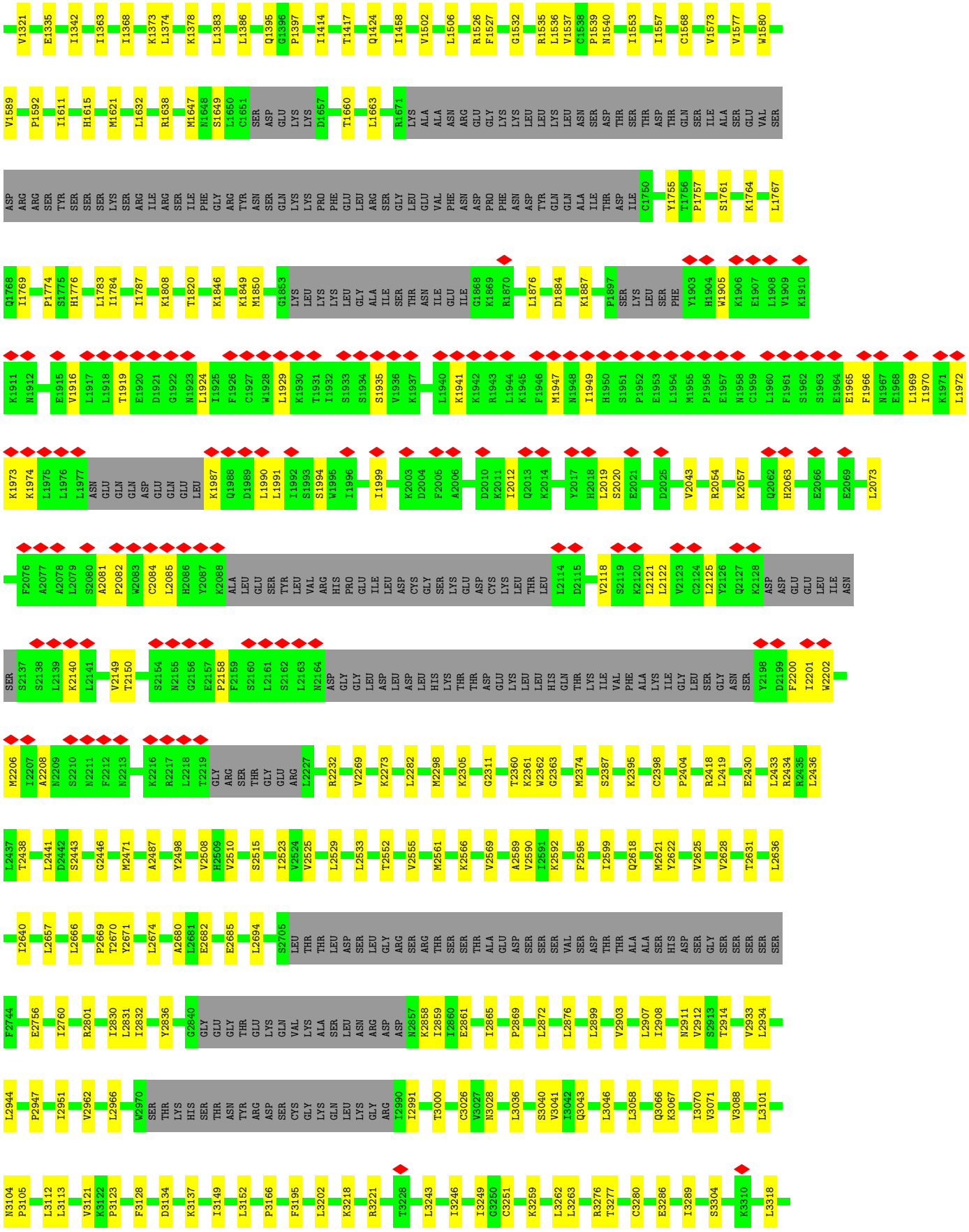
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

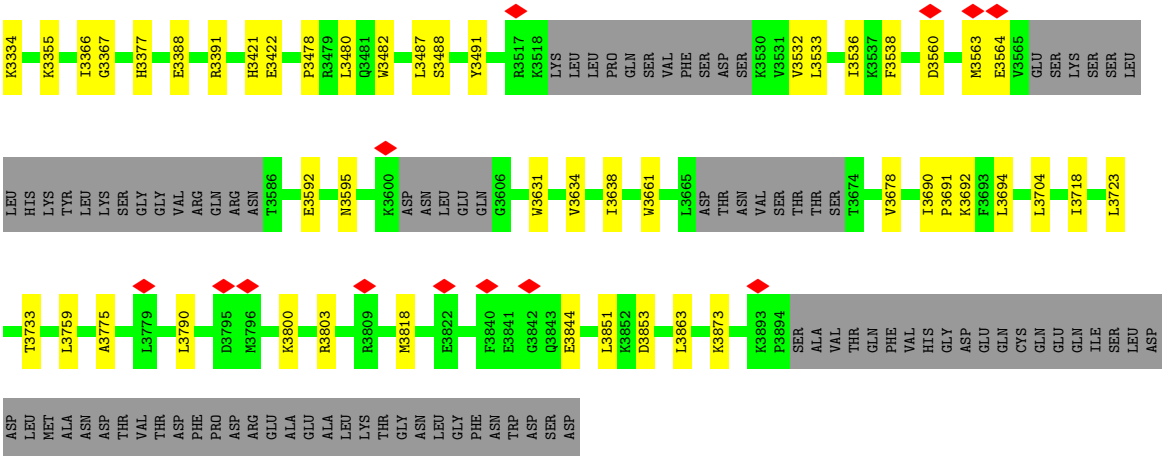
- Molecule 1: RNA-directed RNA polymerase L

Chain A:

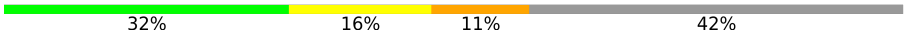


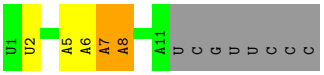



V1321 E1335 I1342 I1363 I1368 K1373 L1374 K1378 L1383 L1386 Q1395 G1396 P1397 I1414 T1417 Q1424 I1458 V1502 L1506 R1526 F1527 G1532 R1535 L1536 V1537 C1538 P1539 N1540 I1553 I1557 C1568 V1573 V1577 W1580
V1589 P1592 I1611 H1615 M1621 L1632 R1638 M1647 N1648 S1649 L1650 C1651 SER ASP GLU LYS LYS D1657 T1660 L1663 R1671 LYS ALA ALA ASN ARG GLU GLY LYS LYS LEU LEU LYS LEU ASN SER ASP THR SER THR ASP THR GLN SER ILE ALA SER GLU VAL SER
ASP ARG ARG SER TYR SER SER SER LYS SER ARG ILE ARG SER ILE PHE GLY ARG TYR ASN SER GLN LYS LYS PRO PHE GLU LEU ARG SER GLY LEU GLU VAL PHE ASN ASP PRO PHE ASN ASP TYR GLN GLN ALA ILE THR ASP ILE C1750 Y1755 T1756 P1757 S1761 K1764 L1767
Q1768 I1769 P1774 S1775 H1776 L1783 I1784 I1787 K1808 T1820 K1846 K1849 M1850 G1853 LYS LEU LYS LYS LEU GLY ALA ILE SER THR ASN ILE GLU ILE G1868 K1869 R1870 L1876 D1884 K1887 P1897 SER LYS LEU SER PHE Y1903 H1904 W1905 K1906 E1907 L1908 V1909 K1910
K1911 N1912 E1915 V1916 L1917 L1918 T1919 E1920 D1921 G1922 N1923 L1924 I1925 F1926 C1927 W1928 L1929 K1930 T1931 I1932 S1933 S1934 S1935 V1936 K1937 L1940 K1941 K1942 R1943 L1944 K1945 F1946 M1947 N1948 I1949 H1950 S1951 P1952 E1953 L1954 M1955 P1956 E1957 N1958 C1959 L1960 F1961 S1962 S1963 E1964 E1965 F1966 N1967 E1968 L1969 I1970 K1971 L1972
K1973 K1974 L1975 L1976 L1977 ASN GLU GLN GLN ASP GLU GLN GLU LEU K1987 Q1988 D1989 L1990 L1991 I1992 S1993 S1994 W1995 I1996 I1999 K2003 D2004 F2005 A2006 D2010 K2011 I2012 Q2013 K2014 Y2017 H2018 L2019 S2020 E2021 D2025 V2043 R2054 K2057 Q2062 H2063 E2066 E2069 L2073
F2076 A2077 A2078 L2079 S2080 A2081 P2082 W2083 C2084 L2085 H2086 Y2087 K2088 ALA LEU GLU SER TYR LEU VAL ARG HIS PRO GLU ILE LEU ASP CYS GLY SER LYS GLU ASP CYS LYS LEU THR LEU L2114 D2115 V2118 S2119 K2120 L2121 L2122 V2123 C2124 L2125 Y2126 Q2127 K2128 ASP ASP GLU GLU LEU ILE ASN
SER S2137 S2138 L2139 K2140 L2141 V2149 T2150 S2154 N2155 G2156 E2157 P2158 F2159 S2160 L2161 S2162 L2163 N2164 ASP GLY GLY LEU ASP LEU ASP LEU HIS LYS THR THR ASP GLU LYS LEU LEU HIS GLN THR LYS ILE VAL PHE ALA LYS ILE GLY LEU SER GLY ASN SER Y2198 D2199 F2200 I2201 W2202
M2206 I2207 A2208 N2209 S2210 N2211 F2212 N2213 K2216 R2217 L2218 T2219 GLY ARG SER THR GLY GLU ARG L2227 R2232 V2269 K2273 L2282 M2298 K2305 G2311 T2360 K2361 W2362 G2363 M2374 S2387 K2395 C2398 P2404 R2418 L2419 E2430 L2433 R2434 R2435 L2436
L2437 T2438 L2441 D2442 S2443 G2446 M2471 A2487 Y2498 V2508 H2509 V2510 S2515 I2523 V2524 V2525 L2529 L2533 T2552 V2555 M2561 K2566 V2569 A2589 V2590 I2591 K2592 F2595 I2599 Q2618 M2621 Y2622 V2625 V2628 T2631 L2636
I2640 L2657 L2666 P2669 T2670 Y2671 L2674 A2680 L2681 E2682 E2685 L2694 S2705 LEU THR THR LEU ASP SER LEU LEU GLY ARG SER ARG THR SER SER SER THR ALA GLU ASP SER SER SER VAL SER ASP THR THR ALA ALA SER HIS ASP SER GLY SER SER SER SER SER
F2744 E2756 I2760 R2801 I2830 L2831 I2832 Y2836 G2840 GLY GLU GLY THR GLU LYS GLN VAL LYS ALA SER LEU ASN ARG ASP ASP N2857 K2858 I2859 I2860 E2861 I2865 P2869 L2872 L2876 L2899 V2903 L2907 I2908 N2911 V2912 S2913 T2914 V2933 L2934
L2944 P2947 I2951 V2962 L2966 W2970 SER THR LYS HIS SER THR ASN TYR ARG ASP SER CYS GLY LYS GLN LEU LYS GLY ARG I2990 I2991 T3000 C3026 V3027 N3028 L3036 S3040 V3041 I3042 Q3043 L3046 L3058 Q3066 K3067 I3070 V3071 V3088 L3101
N3104 P3105 L3112 L3113 V3121 K3122 P3123 F3128 D3134 K3137 I3149 L3152 P3166 F3195 L3202 K3218 R3221 T3228 L3243 I3246 I3249 G3250 C3251 K3259 L3262 L3263 R3276 T3277 C3280 E3286 I3289 S3304 K3310 L3318

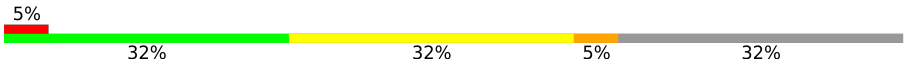


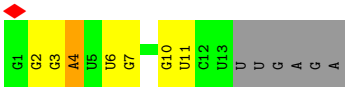
• Molecule 2: RNA (5'-R(*UP*UP*CP*CP*AP*AP*AP*AP*AP*AP*AP*UP*CP*GP*UP*UP *CP*CP*C)-3')

Chain B: 



• Molecule 3: RNA (5'-R(P*GP*GP*GP*AP*UP*UP*GP*GP*UP*GP*UP*CP*UP*UP*UP*G P*AP*GP*A)-3')

Chain C: 

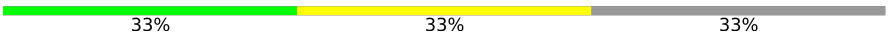


• Molecule 3: RNA (5'-R(P*GP*GP*GP*AP*UP*UP*GP*GP*UP*GP*UP*CP*UP*UP*UP*G P*AP*GP*A)-3')

Chain E: 

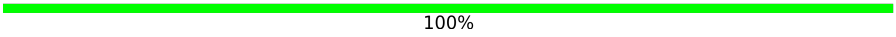


• Molecule 4: RNA (5'-R(*UP*CP*UP*CP*AP*AP*AP*GP*AP*CP*AP*CP*CP*AP*A)-3')

Chain D: 



• Molecule 5: RNA (5'-R(P*UP*CP*U)-3')

Chain F: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51896	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.417	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	262.44, 262.44, 262.44	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8748, 0.8748, 0.8748	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 2KH, 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	A	0.15	0/25034	0.32	0/33767
2	B	0.13	0/259	0.27	0/401
3	C	0.15	0/312	0.25	0/485
3	E	0.16	0/189	0.36	0/292
4	D	0.15	0/241	0.19	0/373
5	F	0.18	0/66	0.49	0/98
All	All	0.15	0/26101	0.32	0/35416

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24614	0	25007	217	0
2	B	231	0	121	1	0
3	C	280	0	139	4	0
3	E	170	0	86	0	0
4	D	215	0	111	4	0
5	F	61	0	32	0	0
6	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	29	0	13	0	0
8	A	1	0	0	0	0
All	All	25605	0	25509	224	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 4.

All (224) 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:1535:ARG:HD3	1:A:1577:VAL:HG11	1.71	0.72
1:A:542:GLY:HA3	1:A:900:THR:HG21	1.74	0.69
1:A:3113:LEU:HD21	1:A:3152:LEU:HD13	1.75	0.69
1:A:586:PRO:HD2	1:A:589:ILE:HD13	1.75	0.69
1:A:1638:ARG:HH21	1:A:2361:LYS:HG3	1.58	0.68
1:A:2657:LEU:HD22	1:A:2666:LEU:HB2	1.75	0.68
1:A:912:THR:HG21	1:A:3128:PHE:HB3	1.77	0.66
1:A:1096:PHE:HB3	1:A:1103:LEU:HD11	1.77	0.66
1:A:1532:GLY:HA2	1:A:1573:VAL:HG12	1.79	0.64
1:A:1536:LEU:HB2	1:A:2569:VAL:HB	1.81	0.63
1:A:3718:ILE:HG12	1:A:3723:LEU:HD12	1.81	0.62
1:A:2311:GLY:H	1:A:2515:SER:HB2	1.65	0.61
1:A:2801:ARG:HH12	1:A:3036:LEU:HD13	1.65	0.61
1:A:2122:LEU:HD23	1:A:2125:LEU:HD12	1.83	0.61
1:A:885:ASN:O	1:A:889:PHE:HB2	2.01	0.60
1:A:1916:VAL:HG23	1:A:1924:LEU:HD13	1.83	0.60
1:A:2831:LEU:HD11	1:A:2962:VAL:HG21	1.83	0.60
1:A:3388:GLU:HG3	1:A:3391:ARG:HH21	1.67	0.59
1:A:884:LYS:O	1:A:888:SER:HB2	2.03	0.58
1:A:994:GLU:HG3	1:A:1767:LEU:HD22	1.86	0.58
1:A:2232:ARG:HE	1:A:2269:VAL:HG11	1.69	0.58
1:A:2801:ARG:HH22	1:A:3036:LEU:HB3	1.68	0.58
1:A:827:GLY:HA2	1:A:835:LYS:HE3	1.86	0.57
1:A:998:THR:HG23	1:A:1000:PHE:H	1.69	0.57
1:A:1929:LEU:HD12	1:A:2208:ALA:HB2	1.85	0.57
1:A:1110:VAL:HG12	1:A:1147:PRO:HD3	1.87	0.57
1:A:941:MET:HE2	1:A:2395:LYS:HG2	1.86	0.56
1:A:2912:VAL:HG21	1:A:3123:PRO:HB3	1.87	0.56
1:A:680:ARG:HB3	1:A:2043:VAL:HG13	1.88	0.56
1:A:1919:THR:HG21	1:A:1924:LEU:HD21	1.88	0.56
1:A:2869:PRO:HD2	1:A:2872:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2589:ALA:HB3	1:A:2592:LYS:HD3	1.88	0.55
1:A:2622:TYR:HA	1:A:3195:PHE:HB2	1.88	0.55
1:A:692:PRO:HG3	1:A:823:LEU:HD22	1.89	0.55
1:A:1632:LEU:HD22	1:A:2404:PRO:HD2	1.88	0.55
1:A:3276:ARG:HG3	1:A:3286:GLU:HG3	1.89	0.54
1:A:1663:LEU:HD22	1:A:1769:ILE:HD11	1.89	0.54
1:A:919:LEU:HD11	1:A:3128:PHE:HE2	1.72	0.54
1:A:3101:LEU:HD12	1:A:3105:PRO:HG3	1.88	0.54
1:A:1526:ARG:HA	1:A:1611:ILE:HB	1.89	0.53
1:A:3112:LEU:HD23	1:A:3149:ILE:HD13	1.90	0.53
1:A:810:PHE:HE2	1:A:815:GLN:HG2	1.73	0.53
1:A:3482:TRP:HB2	1:A:3487:LEU:HA	1.91	0.53
1:A:2760:ILE:HD11	1:A:3058:LEU:HD22	1.91	0.53
1:A:2363:GLY:HA2	1:A:2471:MET:HE2	1.91	0.53
1:A:1965:GLU:HG3	1:A:1994:SER:HB2	1.91	0.52
1:A:3367:GLY:H	1:A:3631:TRP:HZ2	1.57	0.52
1:A:1820:THR:HB	3:C:4:A:H5"	1.92	0.52
1:A:2438:THR:HA	1:A:2441:LEU:HD23	1.90	0.52
1:A:2933:VAL:HG22	4:D:8:A:H4'	1.92	0.51
1:A:2510:VAL:HG22	1:A:2523:ILE:HG23	1.92	0.51
1:A:749:ILE:HG23	1:A:822:LEU:HD22	1.92	0.51
1:A:1386:LEU:HD12	1:A:1395:GLN:HB3	1.92	0.51
4:D:9:C:H2'	4:D:10:A:H8	1.75	0.51
3:C:6:U:H2'	3:C:7:G:H8	1.76	0.51
1:A:680:ARG:HE	1:A:852:LEU:HD21	1.76	0.51
1:A:541:ILE:HD13	1:A:578:LEU:HB3	1.92	0.51
1:A:806:ASN:HD21	1:A:856:LYS:HA	1.75	0.51
1:A:725:VAL:HG11	1:A:1757:PRO:HA	1.93	0.51
1:A:1292:VAL:HG11	1:A:1321:VAL:HG13	1.93	0.51
1:A:2621:MET:HE2	1:A:2671:TYR:HD1	1.76	0.51
1:A:1313:TYR:HE2	1:A:2670:THR:HG23	1.76	0.50
1:A:1884:ASP:HA	1:A:1887:LYS:HE3	1.92	0.50
1:A:970:VAL:HB	1:A:1755:TYR:HE1	1.77	0.50
1:A:3043:GLN:HA	1:A:3046:LEU:HD12	1.94	0.50
1:A:2858:LYS:HE2	1:A:2861:GLU:HA	1.92	0.50
1:A:3066:GLN:O	1:A:3070:ILE:HG12	2.11	0.50
1:A:2012:ILE:HG13	1:A:2073:LEU:HD22	1.93	0.49
1:A:3733:THR:HG23	1:A:3775:ALA:HB2	1.94	0.49
1:A:1537:VAL:HG13	1:A:1539:PRO:HD3	1.93	0.49
1:A:832:ILE:HD11	1:A:865:CYS:HB3	1.94	0.49
1:A:555:LYS:HD2	1:A:565:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:LEU:HD22	1:A:842:LYS:HE3	1.95	0.49
1:A:1941:LYS:HG3	1:A:2085:LEU:HD21	1.95	0.49
1:A:800:ARG:HG2	1:A:832:ILE:HG21	1.95	0.49
1:A:3243:LEU:HD21	1:A:3318:LEU:HD11	1.94	0.49
1:A:693:ASP:HB2	1:A:825:GLU:HA	1.94	0.48
1:A:1966:PHE:HA	1:A:1969:LEU:HD12	1.95	0.48
1:A:2682:GLU:O	1:A:2685:GLU:HG2	2.13	0.48
1:A:1342:ILE:HA	1:A:1363:ILE:HD12	1.94	0.48
1:A:1316:ILE:HG23	1:A:2628:VAL:HG13	1.96	0.48
1:A:2911:ASN:HB3	1:A:3104:ASN:HD21	1.78	0.48
1:A:3592:GLU:HA	1:A:3595:ASN:HB2	1.95	0.48
1:A:3634:VAL:O	1:A:3638:ILE:HG12	2.13	0.48
1:A:1846:LYS:HA	1:A:1849:LYS:HE2	1.96	0.47
1:A:1987:LYS:HD2	1:A:1990:LEU:HD12	1.94	0.47
1:A:2360:THR:HG22	1:A:2361:LYS:HG2	1.95	0.47
4:D:9:C:H2'	4:D:10:A:C8	2.50	0.47
1:A:1502:VAL:HA	1:A:1506:LEU:HB2	1.96	0.47
1:A:644:LEU:HD12	1:A:883:LEU:HD22	1.96	0.47
1:A:1417:THR:HB	1:A:2595:PHE:HE1	1.80	0.47
1:A:670:PHE:HE2	1:A:855:ILE:HG23	1.80	0.46
1:A:2273:LYS:HB2	1:A:2282:LEU:HD11	1.96	0.46
1:A:2020:SER:HB2	1:A:2140:LYS:HB3	1.98	0.46
1:A:2694:LEU:HD12	1:A:2830:ILE:HG13	1.97	0.46
1:A:1414:ILE:HD11	1:A:2599:ILE:HD11	1.98	0.46
1:A:1970:ILE:HG22	1:A:1974:LYS:HE3	1.97	0.46
1:A:2419:LEU:HD11	1:A:2436:LEU:HD13	1.98	0.46
1:A:3277:THR:HG23	1:A:3280:CYS:HB2	1.98	0.46
1:A:2914:THR:HG22	1:A:3123:PRO:HA	1.98	0.46
1:A:2966:LEU:HD22	1:A:3000:THR:HG21	1.98	0.46
1:A:1947:MET:HE2	1:A:2082:PRO:HB2	1.98	0.46
1:A:3218:LYS:HB2	1:A:3221:ARG:HB2	1.96	0.46
1:A:2118:VAL:HG13	1:A:2201:ILE:HD11	1.98	0.46
1:A:2899:LEU:HB3	1:A:3166:PRO:HB3	1.98	0.46
3:C:6:U:H2'	3:C:7:G:C8	2.51	0.46
1:A:1784:ILE:HA	1:A:1787:ILE:HG22	1.98	0.45
1:A:2636:LEU:O	1:A:2640:ILE:HG13	2.16	0.45
1:A:1649:SER:HB2	1:A:1660:THR:HB	1.98	0.45
1:A:1017:SER:OG	1:A:1540:ASN:HA	2.16	0.45
1:A:2081:ALA:HB3	1:A:2084:CYS:HB2	1.99	0.45
1:A:988:LEU:HD21	1:A:2498:TYR:HD1	1.81	0.44
1:A:1237:LYS:HG3	1:A:1240:GLU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1621:MET:HE2	1:A:1621:MET:HB3	1.85	0.44
1:A:1808:LYS:HB3	1:A:2298:MET:HE2	2.00	0.44
1:A:3480:LEU:HB3	1:A:3482:TRP:HZ3	1.82	0.44
1:A:1374:LEU:HD13	1:A:1378:LYS:HE3	1.98	0.44
1:A:2529:LEU:HD22	1:A:2533:LEU:HD23	1.98	0.44
1:A:2912:VAL:HG13	1:A:3104:ASN:HD22	1.83	0.44
1:A:3790:LEU:HB2	1:A:3844:GLU:HG3	2.00	0.44
1:A:941:MET:HE3	1:A:2398:CYS:HB3	1.99	0.44
1:A:3560:ASP:HA	1:A:3563:MET:HE2	2.00	0.44
1:A:1615:HIS:NE2	1:A:2592:LYS:HG2	2.33	0.44
1:A:2418:ARG:HD2	1:A:2443:SER:OG	2.18	0.44
1:A:2552:THR:HA	1:A:2555:VAL:HG12	1.99	0.44
1:A:3286:GLU:HA	1:A:3289:ILE:HG22	2.00	0.44
1:A:1088:VAL:HG22	1:A:1368:ILE:HD11	2.00	0.44
1:A:1876:LEU:HB3	1:A:1887:LYS:HG2	2.00	0.44
1:A:1424:GLN:HE22	1:A:2628:VAL:HB	1.82	0.43
1:A:984:LEU:HD11	1:A:1783:LEU:HD11	2.00	0.43
1:A:988:LEU:HD21	1:A:2498:TYR:CD1	2.52	0.43
1:A:2680:ALA:HB1	1:A:2859:ILE:HG13	2.01	0.43
1:A:2869:PRO:HG2	1:A:2944:LEU:HD13	2.00	0.43
1:A:3634:VAL:HG21	1:A:3661:TRP:HZ3	1.82	0.43
1:A:1999:ILE:HG12	1:A:2121:LEU:HD21	2.00	0.43
1:A:800:ARG:HD3	1:A:832:ILE:HD13	2.00	0.43
1:A:1241:VAL:HG13	1:A:1850:MET:HE2	2.00	0.43
1:A:3249:ILE:HG23	1:A:3262:LEU:HD23	2.00	0.43
1:A:447:TYR:O	1:A:451:ILE:HG12	2.19	0.43
1:A:3478:PRO:HG3	1:A:3491:TYR:CZ	2.53	0.43
1:A:1580:TRP:HE3	1:A:1589:VAL:HG11	1.84	0.43
1:A:2433:LEU:HD23	1:A:2433:LEU:HA	1.90	0.43
1:A:3851:LEU:HD23	1:A:3853:ASP:H	1.84	0.43
1:A:816:LEU:HD12	1:A:817:GLU:HG2	2.01	0.43
1:A:2202:TRP:O	1:A:2206:MET:HG2	2.18	0.43
1:A:2908:ILE:HD11	1:A:3121:VAL:HB	2.00	0.43
1:A:3028:ASN:HB2	1:A:3040:SER:HB3	2.01	0.43
1:A:721:LEU:HB2	1:A:724:SER:HB3	1.99	0.43
1:A:828:PHE:HA	1:A:864:ASP:O	2.18	0.43
1:A:2150:THR:HG21	1:A:2158:PRO:HA	2.00	0.43
1:A:2832:ILE:O	1:A:2836:TYR:HB2	2.18	0.43
1:A:3800:LYS:HA	1:A:3803:ARG:HE	1.82	0.43
2:B:7:A:H5"	2:B:8:A:C8	2.54	0.43
3:C:10:G:H2'	3:C:11:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:LEU:HB2	1:A:3304:SER:OG	2.19	0.42
1:A:1257:ARG:NH1	1:A:2446:GLY:HA3	2.34	0.42
1:A:1568:CYS:HB2	1:A:1592:PRO:HG3	2.00	0.42
1:A:3366:ILE:HG12	1:A:3377:HIS:HB2	2.01	0.42
1:A:3480:LEU:HB3	1:A:3482:TRP:CZ3	2.53	0.42
1:A:3487:LEU:HG	1:A:3536:ILE:HB	2.01	0.42
1:A:3818:MET:HG2	1:A:3863:LEU:HD21	2.01	0.42
1:A:2150:THR:HB	1:A:2158:PRO:HG3	2.01	0.42
1:A:3026:CYS:O	1:A:3041:VAL:HA	2.19	0.42
1:A:3101:LEU:HD22	1:A:3134:ASP:HB2	2.01	0.42
1:A:3723:LEU:HD23	1:A:3873:LYS:HD2	2.00	0.42
1:A:950:THR:HB	1:A:1647:MET:HE2	2.01	0.42
1:A:1085:ILE:HD12	1:A:1335:GLU:HG2	2.00	0.42
1:A:1228:VAL:HG13	1:A:1229:LEU:HD12	2.01	0.42
1:A:2054:ARG:HA	1:A:2057:LYS:HE2	2.01	0.42
1:A:1184:ARG:HG2	1:A:1207:LEU:HD22	2.00	0.42
1:A:3690:ILE:HD13	1:A:3704:LEU:HD11	2.01	0.42
1:A:944:HIS:HB2	1:A:2398:CYS:SG	2.60	0.42
1:A:2430:GLU:O	1:A:2434:ARG:HG2	2.20	0.42
1:A:727:ALA:HA	1:A:1755:TYR:HB3	2.02	0.42
1:A:1949:ILE:HA	1:A:1973:LYS:HE3	2.02	0.42
1:A:2947:PRO:O	1:A:2951:ILE:HG13	2.20	0.42
1:A:1787:ILE:HD11	1:A:2487:ALA:HA	2.01	0.42
1:A:2903:VAL:O	1:A:2907:LEU:HB2	2.20	0.42
4:D:10:A:H2'	4:D:11:C:C6	2.55	0.42
1:A:1972:LEU:HD22	1:A:1991:LEU:HD21	2.02	0.41
1:A:3421:HIS:CD2	1:A:3422:GLU:HG3	2.55	0.41
1:A:3491:TYR:HE2	1:A:3533:LEU:HD11	1.85	0.41
1:A:1383:LEU:HD11	1:A:1397:PRO:HB2	2.01	0.41
1:A:3088:VAL:HG21	1:A:3202:LEU:HA	2.01	0.41
1:A:3355:LYS:HB2	1:A:3631:TRP:CH2	2.55	0.41
1:A:2019:LEU:HD13	1:A:2063:HIS:HD2	1.86	0.41
1:A:2149:VAL:HG22	1:A:2200:PHE:HD2	1.85	0.41
1:A:1208:LYS:HE3	1:A:1208:LYS:HB2	1.90	0.41
1:A:1553:ILE:O	1:A:1557:ILE:HG13	2.20	0.41
1:A:3259:LYS:HB2	1:A:3259:LYS:HE3	1.87	0.41
1:A:929:VAL:HG23	1:A:2387:SER:HB2	2.01	0.41
1:A:1905:TRP:HE1	1:A:1935:SER:HB3	1.86	0.41
1:A:2590:VAL:HB	1:A:2625:VAL:HG22	2.03	0.41
1:A:2631:THR:HG23	1:A:2669:PRO:HD2	2.01	0.41
1:A:2756:GLU:O	1:A:2760:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3487:LEU:HD23	1:A:3538:PHE:HE1	1.85	0.41
1:A:2508:VAL:HG22	1:A:2525:VAL:HG22	2.03	0.41
1:A:3678:VAL:HG22	1:A:3759:LEU:HD13	2.01	0.41
1:A:1023:ILE:HD11	1:A:1035:ILE:HD13	2.02	0.41
1:A:1234:VAL:HG22	1:A:1373:LYS:HE3	2.02	0.41
1:A:2618:GLN:HG3	1:A:2674:LEU:HD22	2.03	0.41
1:A:3691:PRO:HD2	1:A:3694:LEU:HD12	2.02	0.41
1:A:2362:TRP:CZ3	1:A:2561:MET:HG2	2.56	0.41
1:A:2374:MET:HE2	1:A:2374:MET:HB3	1.79	0.41
1:A:2865:ILE:HD13	1:A:2991:ILE:HD13	2.03	0.41
1:A:1225:LEU:HA	1:A:1228:VAL:HG12	2.03	0.41
1:A:1274:PHE:HZ	1:A:1458:ILE:HD12	1.86	0.41
1:A:1527:PHE:CE2	1:A:2566:LYS:HD2	2.56	0.41
1:A:1761:SER:HA	1:A:1764:LYS:HE2	2.02	0.41
1:A:2305:LYS:HB2	1:A:2305:LYS:HE3	1.76	0.41
1:A:3246:ILE:HG12	1:A:3263:LEU:HD11	2.03	0.41
1:A:429:VAL:HG11	1:A:3564:GLU:HB3	2.03	0.41
1:A:580:GLU:HG2	1:A:581:ASP:H	1.86	0.41
1:A:1128:VAL:O	1:A:1132:ILE:HG13	2.21	0.41
1:A:1005:THR:HB	1:A:1573:VAL:HG21	2.02	0.40
1:A:3334:LYS:HD3	1:A:3334:LYS:HA	1.94	0.40
1:A:3067:LYS:O	1:A:3071:VAL:HG23	2.22	0.40
1:A:3488:SER:HB3	1:A:3532:VAL:HG13	2.04	0.40
1:A:3134:ASP:HA	1:A:3137:LYS:HB2	2.04	0.40
1:A:616:LEU:O	1:A:620:ILE:HG13	2.21	0.40
1:A:2019:LEU:HD13	1:A:2063:HIS:CD2	2.56	0.40
1:A:3251:CYS:HB3	1:A:3692:LYS:HG3	2.03	0.40
1:A:1774:PRO:HB2	1:A:1776:HIS:CD2	2.57	0.40
1:A:2876:LEU:HD13	1:A:2934:LEU:HD22	2.04	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	3028/3945 (77%)	2926 (97%)	102 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	2828/3601 (78%)	2828 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	622	ASN
1	A	684	HIS
1	A	840	HIS
1	A	913	GLN
1	A	987	ASN
1	A	1057	GLN
1	A	1127	ASN
1	A	1369	ASN
1	A	1381	ASN
1	A	1401	ASN
1	A	1516	GLN
1	A	1776	HIS
1	A	2359	ASN
1	A	2560	GLN
1	A	3098	GLN
1	A	3484	HIS
1	A	3595	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	10/19 (52%)	5 (50%)	0
3	C	12/19 (63%)	3 (25%)	0
3	E	7/19 (36%)	3 (42%)	0
4	D	9/15 (60%)	1 (11%)	0
5	F	2/3 (66%)	0	0
All	All	40/75 (53%)	12 (30%)	0

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	5	A
2	B	6	A
2	B	7	A
2	B	8	A
3	C	2	G
3	C	3	G
3	C	4	A
4	D	6	A
3	E	14	U
3	E	17	A
3	E	19	A

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
7	2KH	A	4005	6	29,30,30	3.95	21 (72%)	42,47,47	1.59	6 (14%)

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
7	2KH	A	4005	6	-	6/19/38/38	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	4005	2KH	C3'-C2'	-8.82	1.29	1.53
7	A	4005	2KH	C2-N3	6.98	1.50	1.38
7	A	4005	2KH	C2-N1	6.46	1.48	1.38
7	A	4005	2KH	C6-C5	6.16	1.49	1.35
7	A	4005	2KH	PB-O3B	6.04	1.66	1.59
7	A	4005	2KH	O4'-C4'	-5.82	1.32	1.45
7	A	4005	2KH	O4'-C1'	5.02	1.53	1.42
7	A	4005	2KH	C1'-N1	-4.84	1.33	1.47
7	A	4005	2KH	C3'-C4'	4.22	1.63	1.53
7	A	4005	2KH	PB-O2B	3.86	1.52	1.46
7	A	4005	2KH	PB-N3A	3.63	1.72	1.63
7	A	4005	2KH	PA-O1A	3.23	1.51	1.46
7	A	4005	2KH	O3'-C3'	3.22	1.50	1.43
7	A	4005	2KH	O4-C4	-3.19	1.18	1.24
7	A	4005	2KH	C5-C4	2.66	1.49	1.43
7	A	4005	2KH	C4-N3	2.57	1.43	1.38
7	A	4005	2KH	PG-O2G	2.56	1.58	1.50
7	A	4005	2KH	C6-N1	2.53	1.44	1.38
7	A	4005	2KH	PA-N3A	2.52	1.70	1.63
7	A	4005	2KH	O2'-C2'	2.25	1.48	1.43
7	A	4005	2KH	PG-O3G	-2.02	1.47	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	4005	2KH	C4-N3-C2	-4.93	120.08	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	4005	2KH	N3-C2-N1	3.94	120.13	114.89
7	A	4005	2KH	C5-C4-N3	3.33	119.83	114.84
7	A	4005	2KH	PB-O3B-PG	-2.99	122.08	132.62
7	A	4005	2KH	O4-C4-C5	-2.65	120.50	125.16
7	A	4005	2KH	C3'-C2'-C1'	2.22	105.65	101.43

There are no chirality outliers.

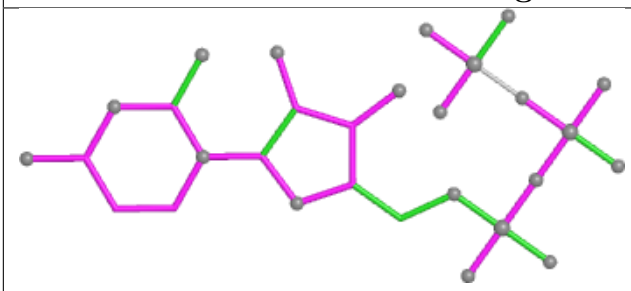
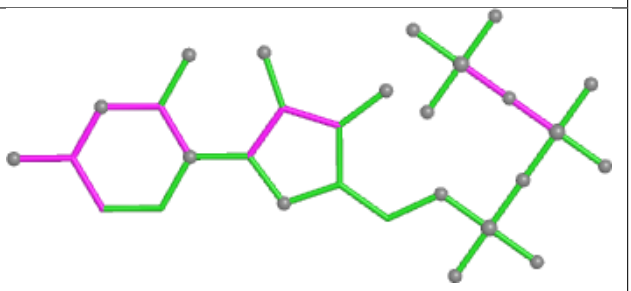
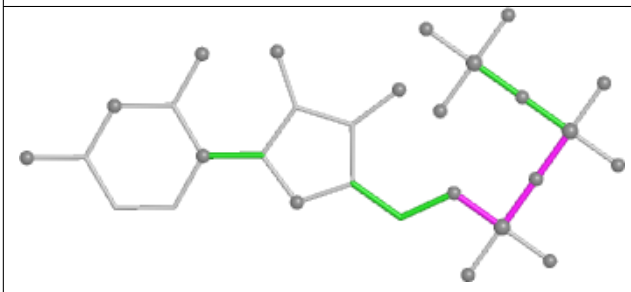
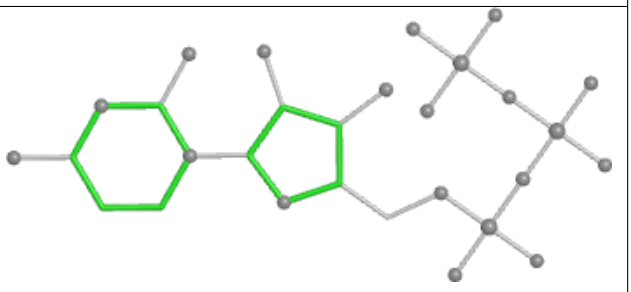
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4005	2KH	PB-N3A-PA-O1A
7	A	4005	2KH	C5'-O5'-PA-O2A
7	A	4005	2KH	PA-N3A-PB-O2B
7	A	4005	2KH	PA-N3A-PB-O3B
7	A	4005	2KH	C5'-O5'-PA-O1A
7	A	4005	2KH	PB-N3A-PA-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand 2KH A 4005	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

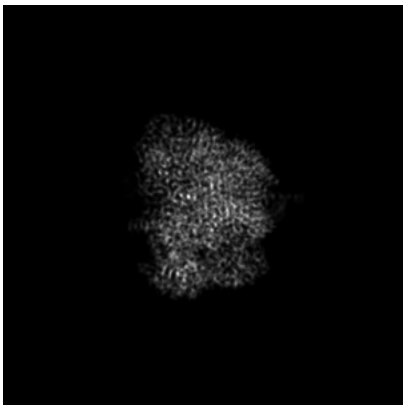
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66785. These allow visual inspection of the internal detail of the map and identification of artifacts.

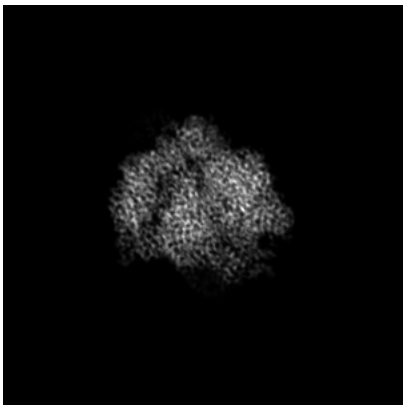
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

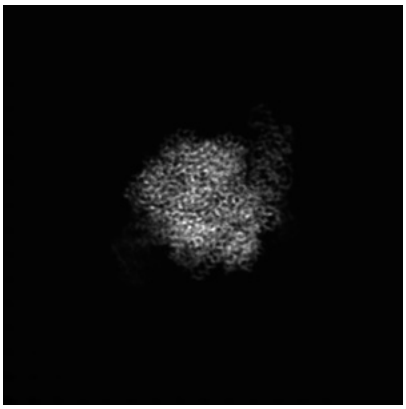
6.1.1 Primary map



X

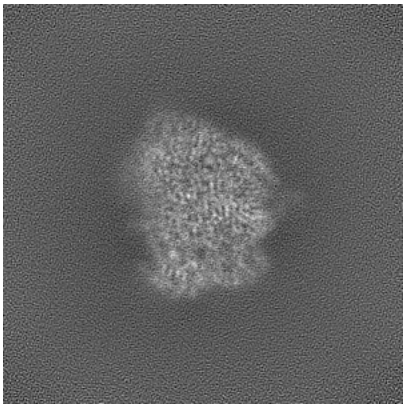


Y

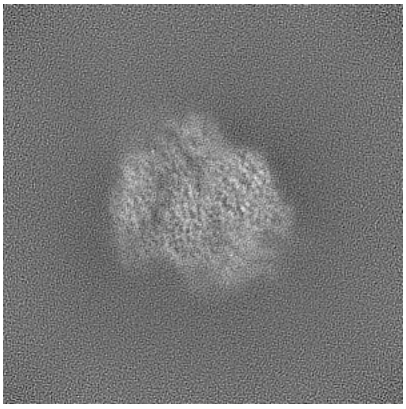


Z

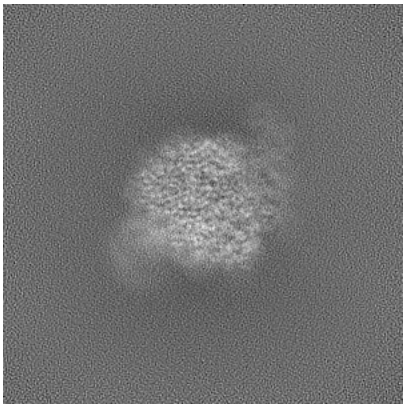
6.1.2 Raw map



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

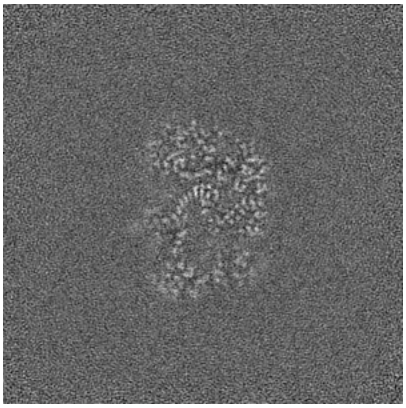


Y Index: 150

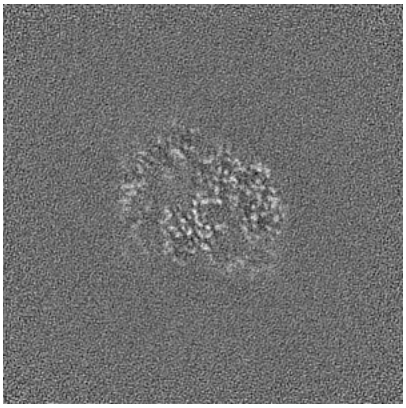


Z Index: 150

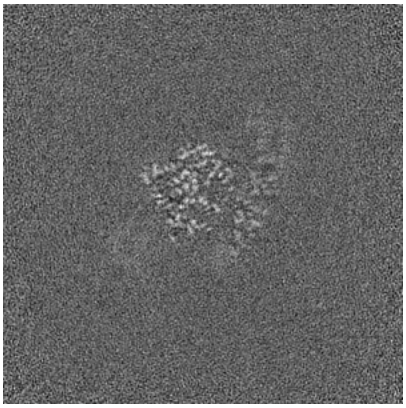
6.2.2 Raw map



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: 142

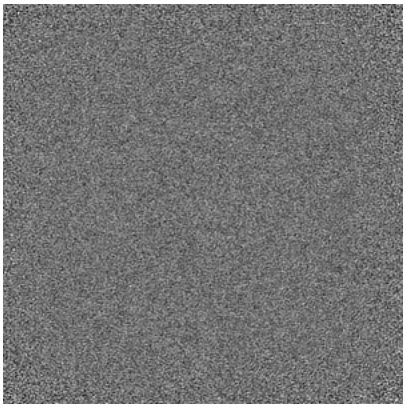


Y Index: 143

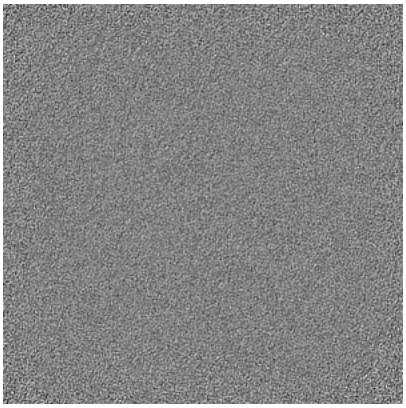


Z Index: 135

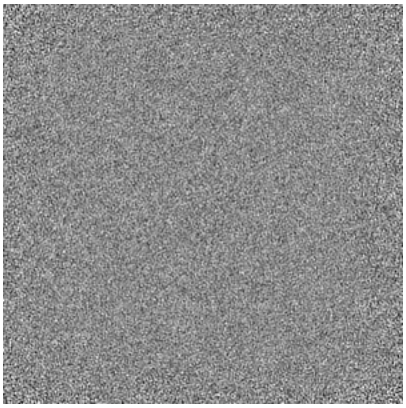
6.3.2 Raw map



X Index: 0



Y Index: 0

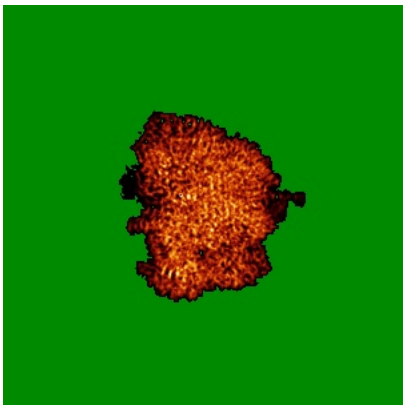


Z Index: 0

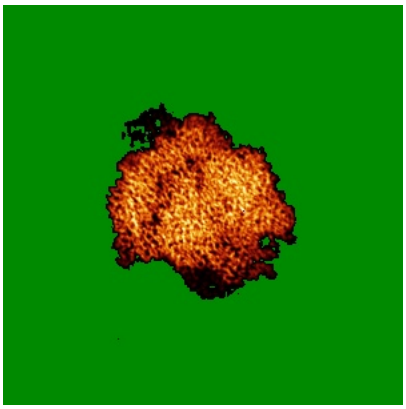
The images above show the largest variance slices of the map in three orthogonal directions.

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

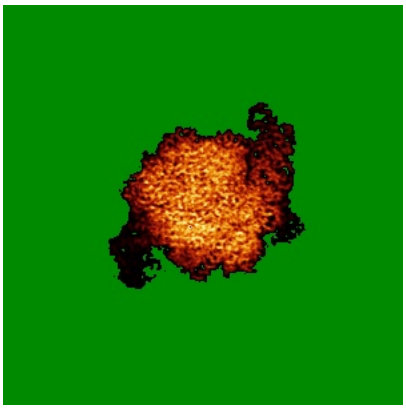
6.4.1 Primary map



X

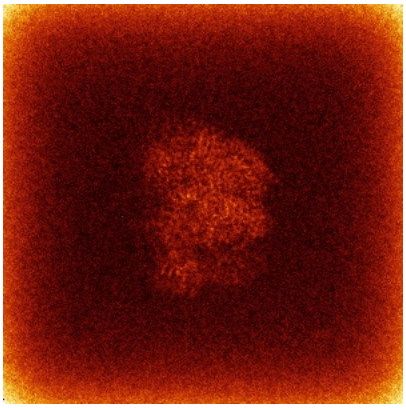


Y

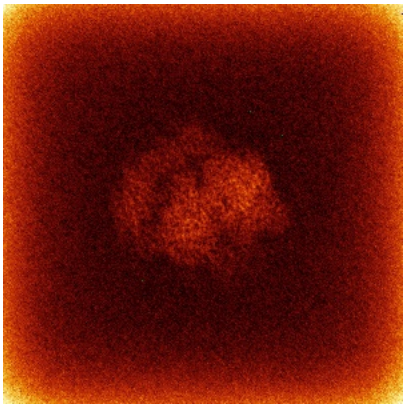


Z

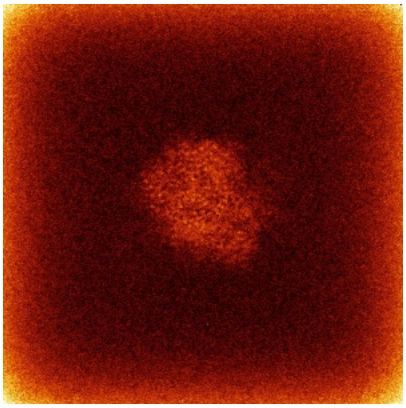
6.4.2 Raw map



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)

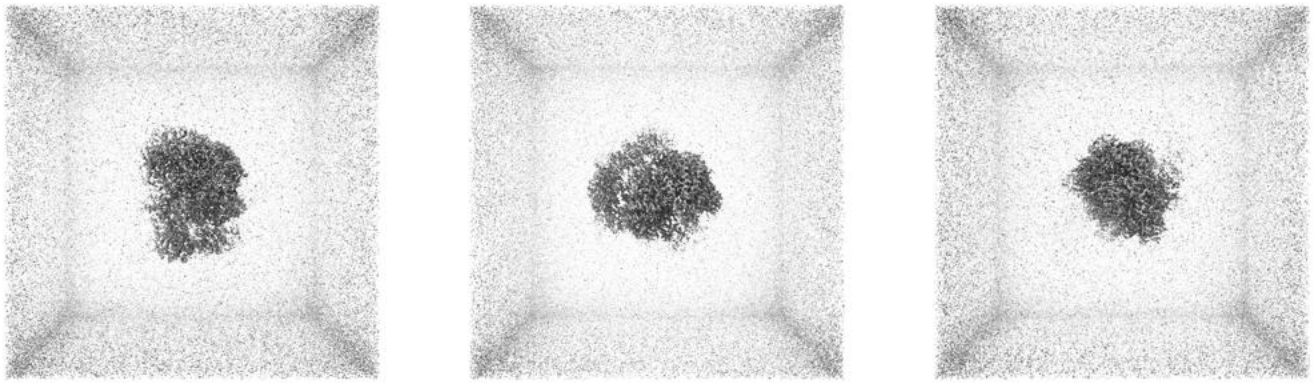
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

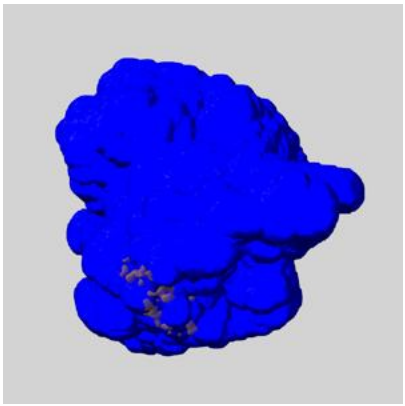
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

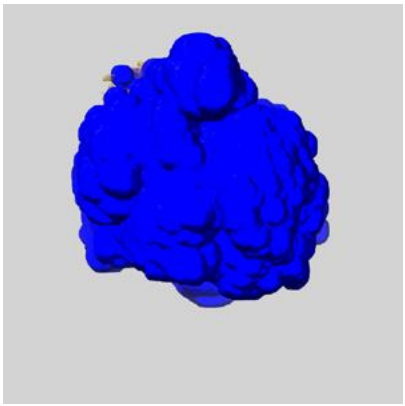
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

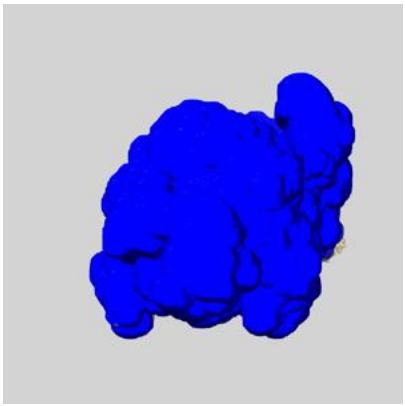
6.6.1 emd_66785_msk_1.map (i)



X



Y

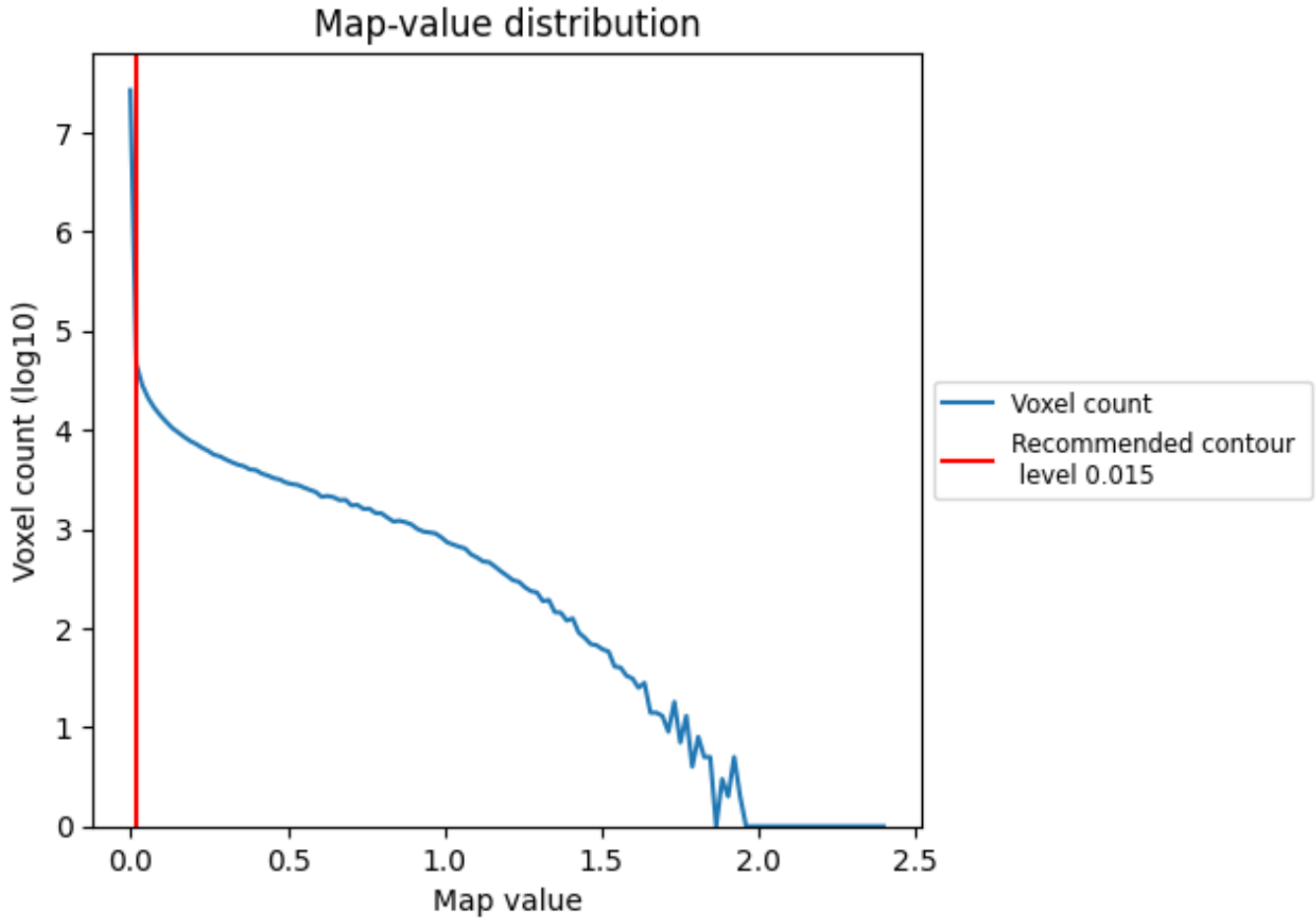


Z

7 Map analysis

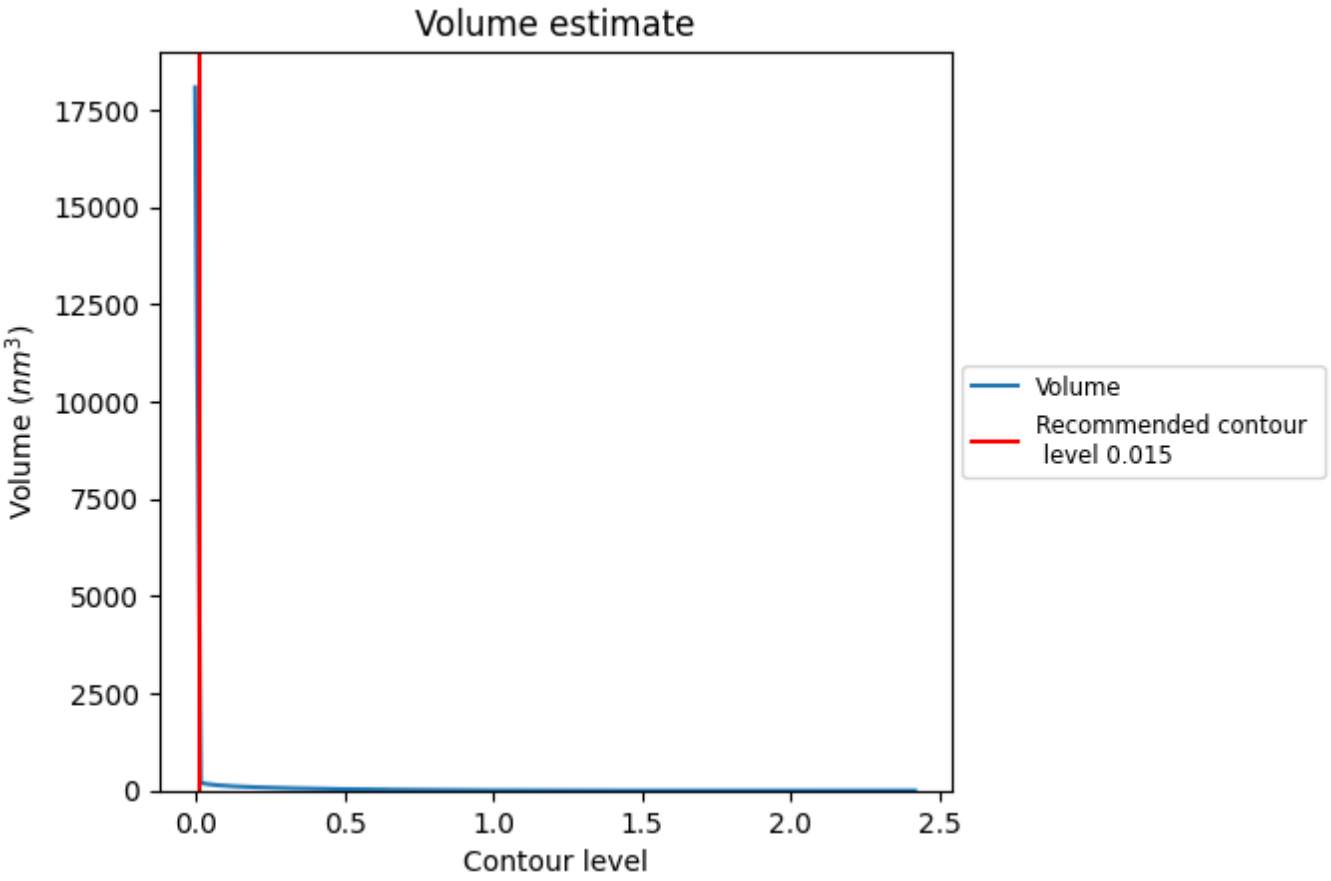
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

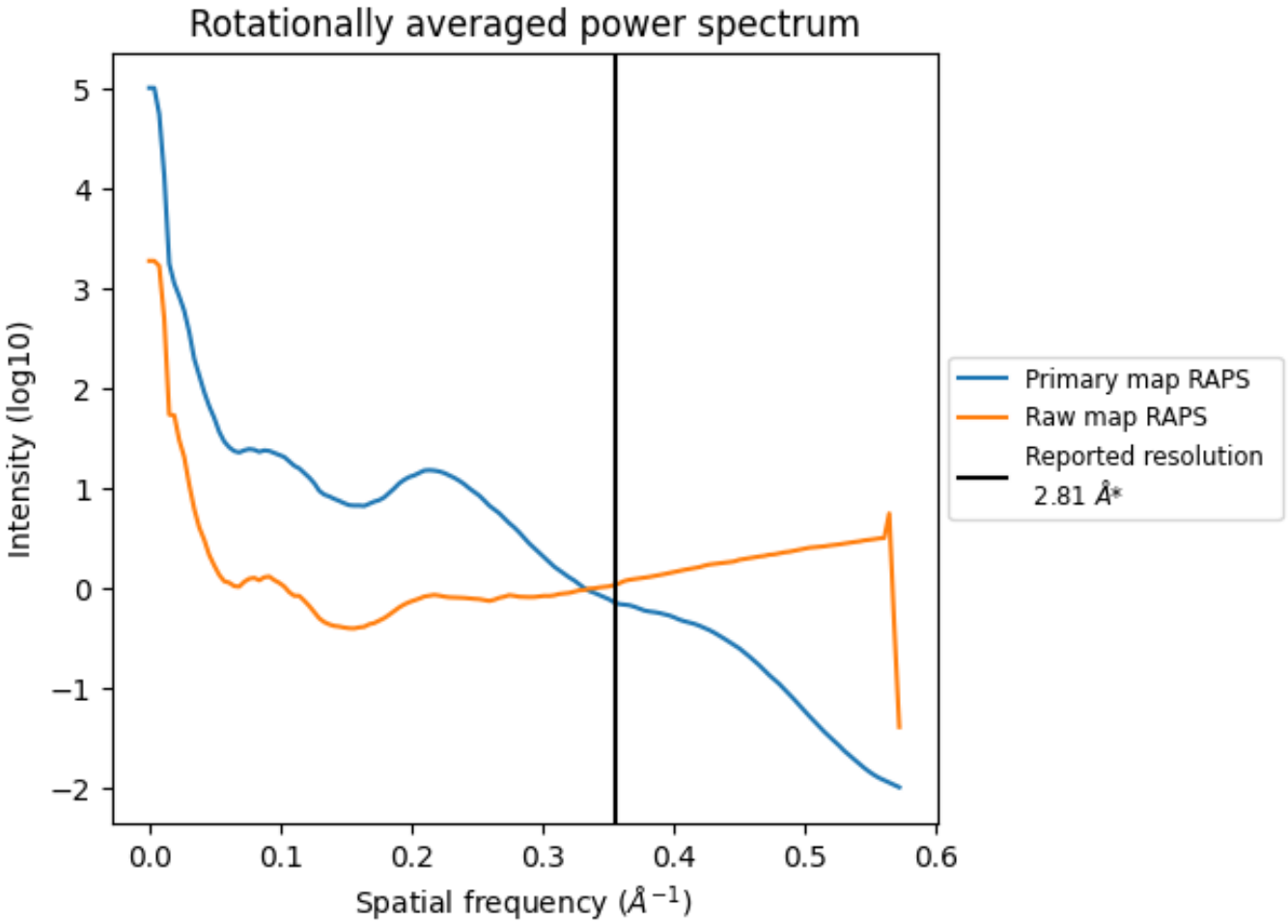
7.2 Volume estimate



The volume at the recommended contour level is 2225 nm^3; this corresponds to an approximate mass of 2010 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)

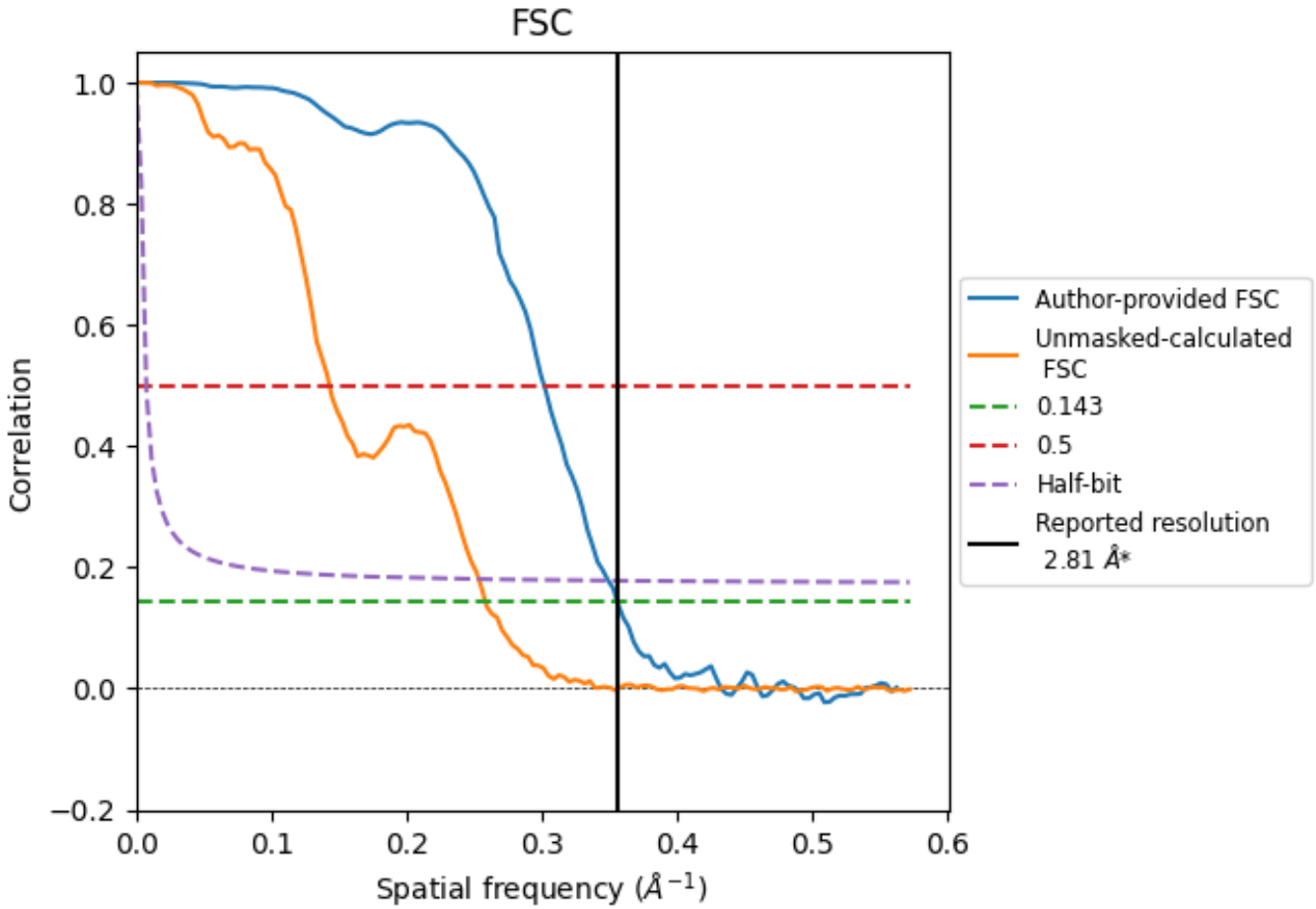


*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8.2 Resolution estimates (i)

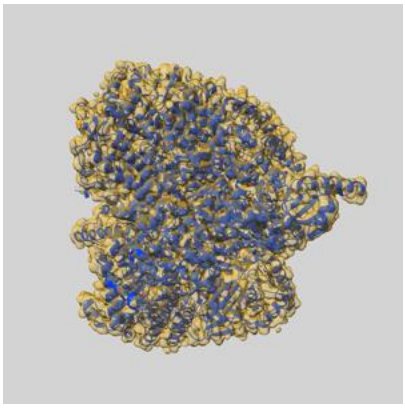
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.32	2.87
Unmasked-calculated*	3.87	7.00	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 2.81 by more than 10 %

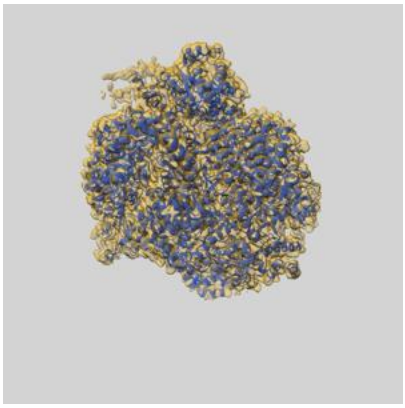
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66785 and PDB model 9XE9. Per-residue inclusion information can be found in section 3 on page 6.

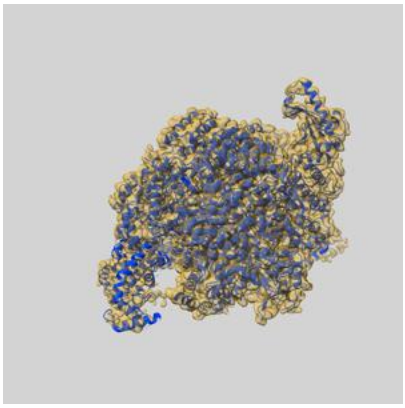
9.1 Map-model overlay



X



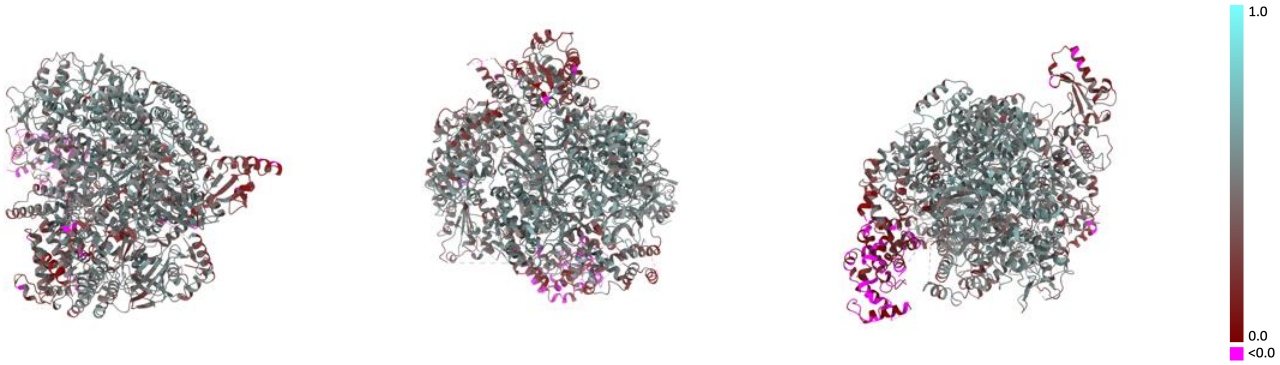
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

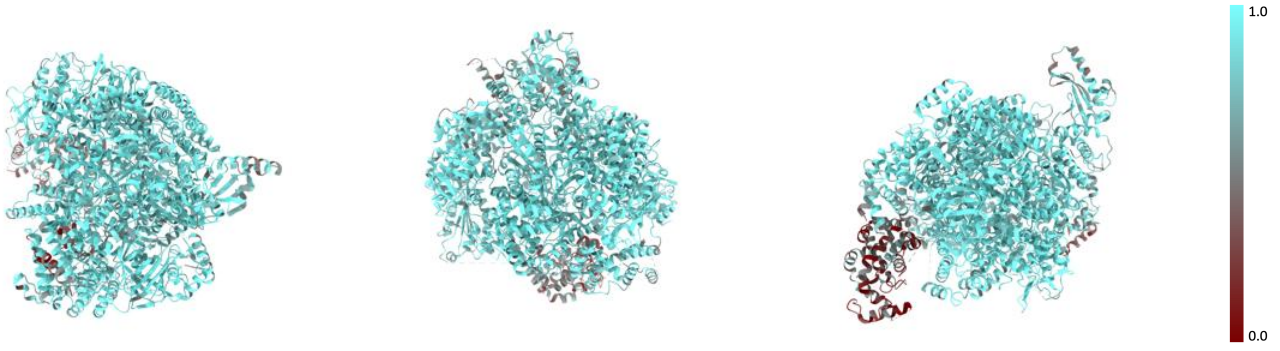
9.2 Q-score mapped to coordinate model (i)



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.

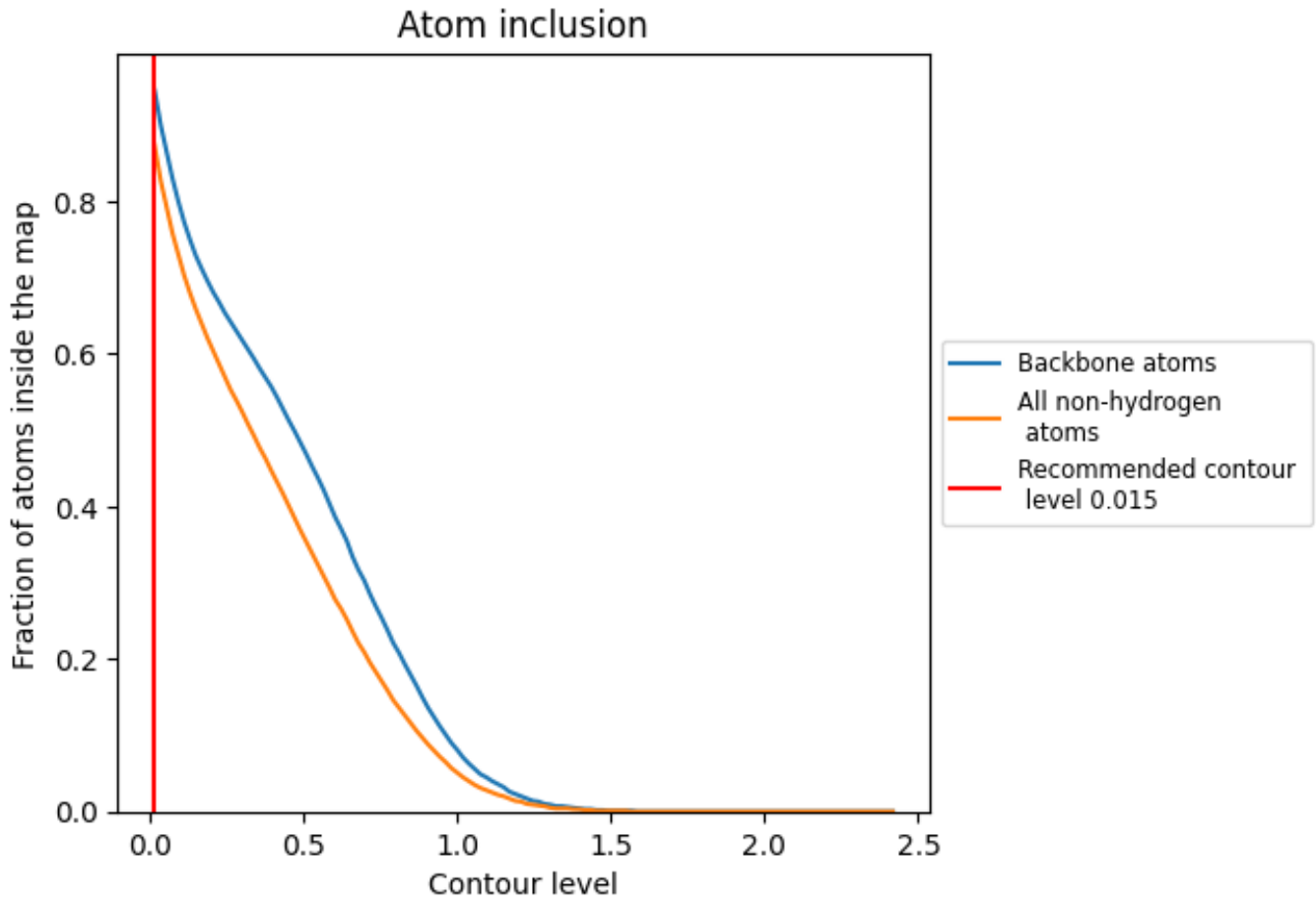
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.4410
A	0.8710	0.4390
B	0.9610	0.4840
C	0.9250	0.4650
D	0.9770	0.4940
E	0.9650	0.5140
F	1.0000	0.5510

