Full wwPDB EM Validation Report ⓘ

Sep 27, 2026 – 04:03 AM JST

PDB ID	:	9XEC / pdb_00009xec
EMDB ID	:	EMD-66787
Title	:	Crimean-Congo hemorrhagic fever virus RNA polymerase containing a 9-bp RNA product
Authors	:	Xue, L.; Gui, J.; Pan, H.; Chang, T.; Xiong, X.
Deposited on	:	2025-10-27
Resolution	:	2.98 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:

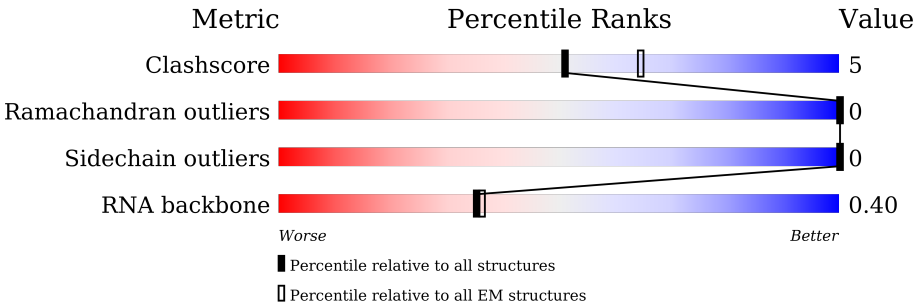
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

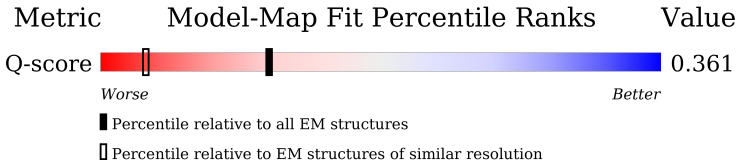
1 Overall quality at a glance

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

The reported resolution of this entry is 2.98 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	13236 (2.48 - 3.48)

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 <=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% 12% 20%
2	B	19	26% 21% 11% 42%
3	C	19	53% 11% 5% 32%

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Mol	Chain	Length	Quality of chain
3	E	19	16% 16% 11% 58%
4	D	9	67% 33%
5	F	3	33% 33% 33%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 26146 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	3148	Total	C	N	O	S	0	0
			25181	15984	4309	4724	164		

- 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(*GP*GP*GP*AP*UP*UP*GP*AP*UP*AP*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
			277	124	48	92	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(P*UP*CP*UP*CP*AP*AP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	9	Total	C	N	O	P	0	0
			192	86	35	62	9		

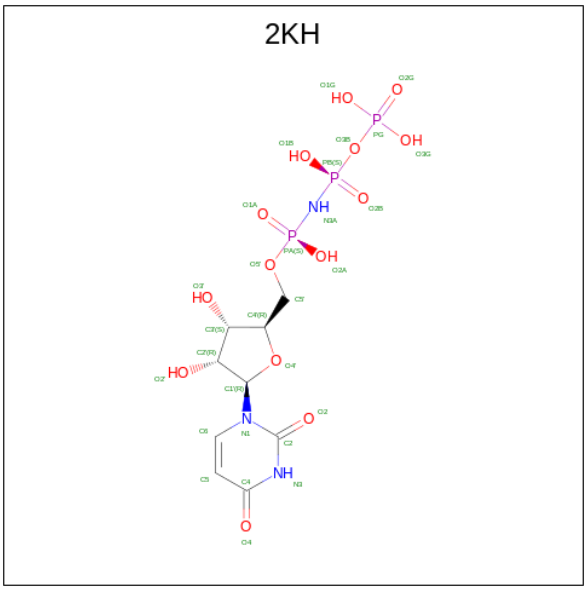
- Molecule 5 is a RNA chain called RNA (5'-R(P*UP*CP*U)-3').

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

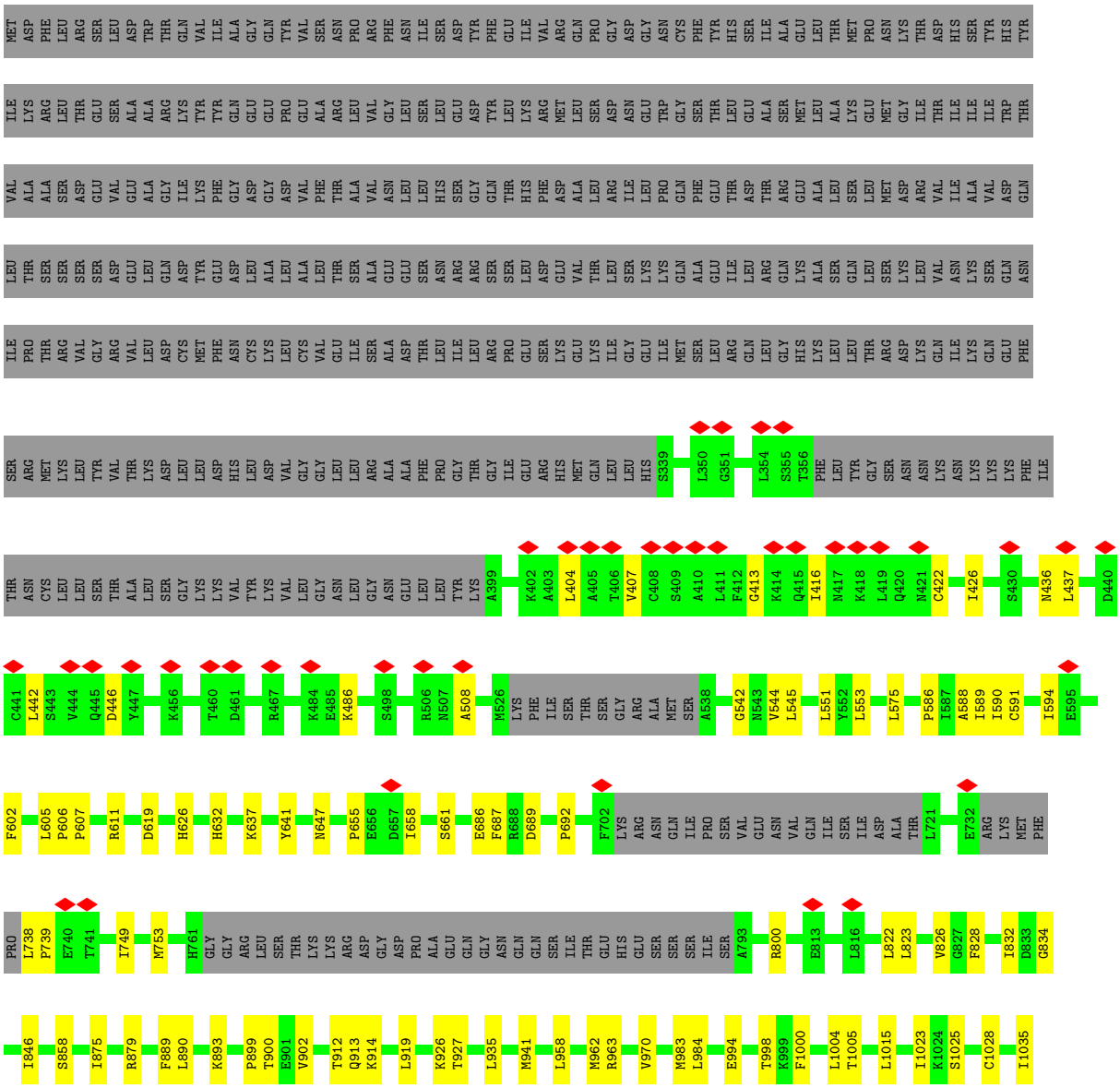
3 Residue-property plots (i)

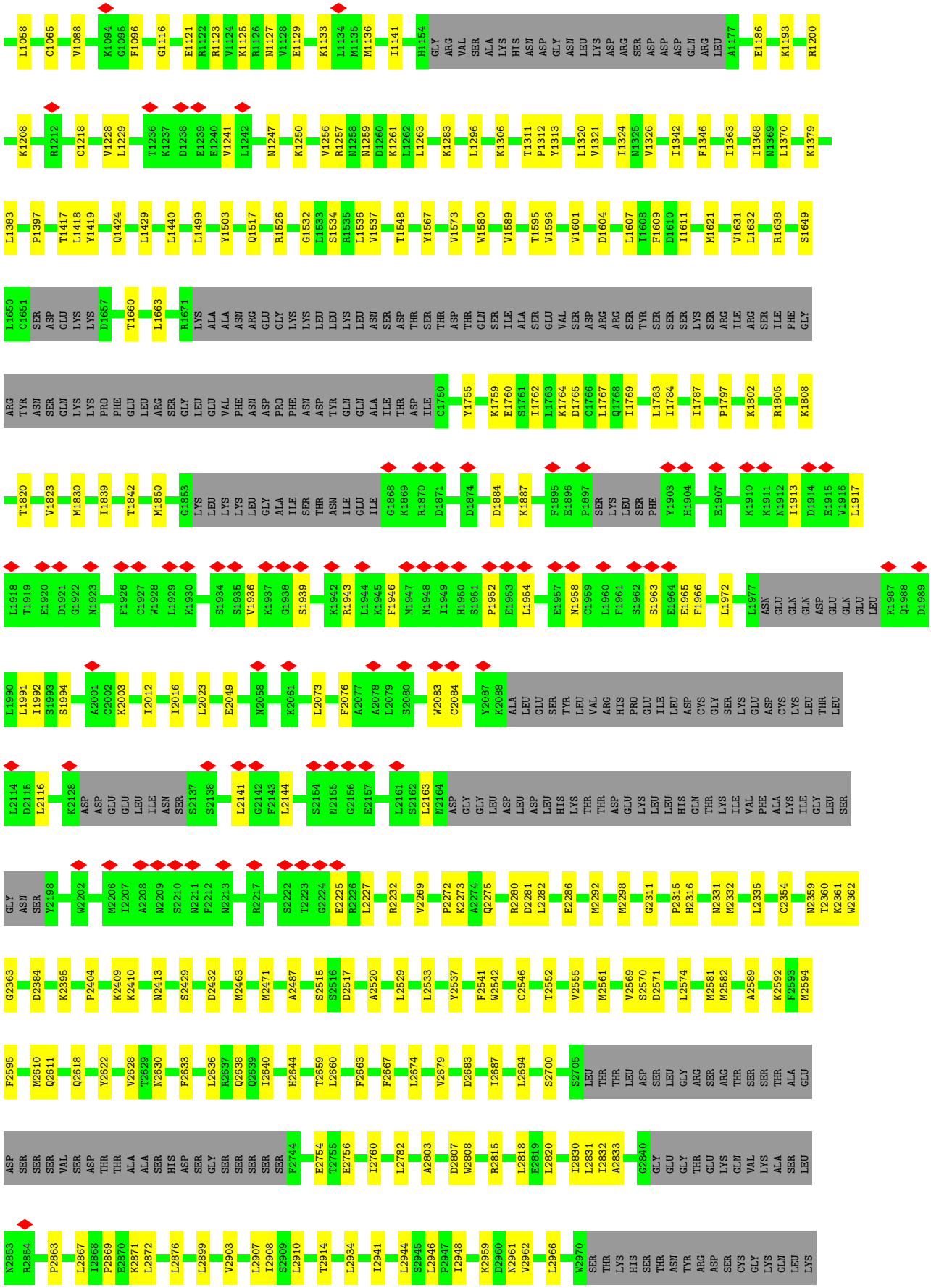
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

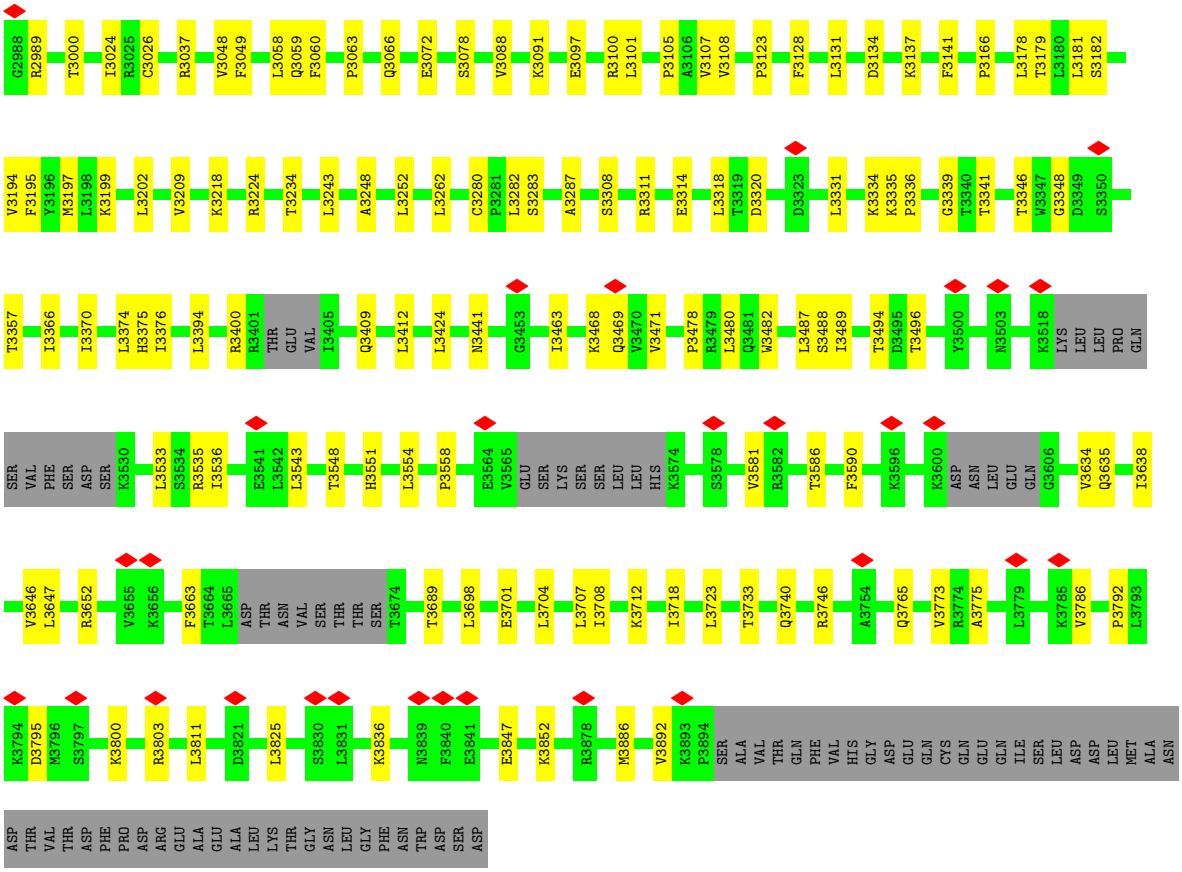
- Molecule 1: RNA-directed RNA polymerase L

Chain A:



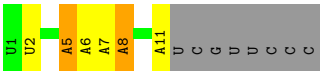



L1058 C1065 V1088 K1094 G1095 F1096 G1116 E1121 R1122 R1123 V1124 K1125 R1126 N1127 V1128 E1129 K1133 L1134 M1135 M1136 I1141 H1154 GLY ARG VAL SER ALA LYS HIS ASN ASP GLY ASN LEU LYS ASP ARG SER ASP ASP GLN ARG LEU A1177 E1186 K1193 R1200
K1208 R1212 C1218 V1228 L1229 T1236 K1237 D1238 E1239 E1240 V1241 L1242 N1247 K1250 V1256 R1257 N1258 N1259 D1260 K1261 L1262 L1263 K1283 L1296 K1306 T1311 P1312 Y1313 L1320 V1321 I1324 N1325 V1326 I1342 F1346 I1363 I1368 N1369 L1370 K1379
L1383 P1397 T1417 L1418 Y1419 Q1424 L1429 L1440 L1499 Y1503 Q1517 R1526 G1532 L1533 S1534 R1535 L1536 V1537 T1548 Y1567 V1573 W1580 V1589 T1595 V1596 V1601 D1604 L1607 I1608 F1609 D1610 I1611 M1621 V1631 L1632 R1638 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 K1759 E1760 S1761 I1762 L1763 K1764 D1765 C1766 L1767 Q1768 I1769 L1783 I1784 I1787 P1797 K1802 R1805 K1808
T1820 V1823 M1830 I1839 T1842 M1850 G1853 LYS LEU LYS LYS LEU GLY ALA ILE SER THR ASN ILE GLU ILE G1868 K1869 R1870 D1871 D1874 D1884 K1887 F1895 E1896 P1897 SER LYS LEU SER PHE Y1903 H1904 E1907 K1910 K1911 N1912 I1913 D1914 E1915 V1916 L1917
L1918 T1919 E1920 D1921 G1922 N1923 F1926 C1927 W1928 L1929 K1930 S1934 S1935 V1936 K1937 G1938 S1939 K1942 R1943 L1944 K1945 F1946 M1947 N1948 I1949 H1950 S1951 P1952 E1953 L1954 E1957 N1958 C1959 L1960 F1961 S1962 S1963 E1964 E1965 F1966 L1972 L1977 ASN GLU GLN GLN ASP GLU GLN GLU LEU K1987 Q1988 D1989
L1990 L1991 I1992 S1993 S1994 A2001 C2002 K2003 I2012 I2016 L2023 E2049 N2058 K2061 L2073 F2076 A2077 A2078 L2079 S2080 W2083 C2084 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 L2116 K2128 ASP ASP GLU GLU LEU ILE ASN SER S2137 S2138 L2141 G2142 F2143 L2144 S2154 N2155 G2156 E2157 L2161 S2162 L2163 N2164 ASP GLY GLY 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 W2202 M2206 I2207 A2208 N2209 S2210 N2211 F2212 N2213 R2217 S2222 T2223 G2224 E2225 R2226 L2227 R2232 V2269 P2272 K2273 K2274 Q2275 R2280 D2281 L2282 E2286 M2292 M2298 G2311 P2315 H2316 N2331 M2332 L2335 C2354 W2359 T2360 K2361 W2362
G2363 D2384 K2395 P2404 K2409 K2410 N2413 S2429 D2432 M2463 M2471 A2487 S2515 S2516 D2517 A2520 L2529 L2533 Y2537 F2541 W2542 C2546 T2552 V2555 M2561 V2569 S2570 D2571 L2574 M2581 M2582 A2589 K2592 F2593 M2594
F2595 M2610 Q2611 Q2618 Y2622 V2628 T2629 N2630 F2633 L2636 R2637 Q2638 Q2639 I2640 H2644 T2659 L2660 F2663 F2667 L2674 V2679 D2683 I2687 L2694 S2700 S2705 LEU THR THR LEU ASP SER LEU GLY ARG SER ARG THR 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 E2754 T2755 E2756 I2760 L2782 A2803 D2807 W2808 R2815 L2818 E2819 L2820 I2830 L2831 I2832 A2833 G2840 GLY GLU GLY THR GLU LYS GLN VAL LYS ALA SER LEU
N2853 R2854 P2863 L2867 I2868 P2869 E2870 K2871 L2872 L2876 L2899 V2903 L2907 I2908 S2909 L2910 T2914 L2934 I2941 L2944 S2945 L2946 P2947 I2948 K2959 D2960 N2961 V2962 L2966 W2970 SER THR LYS HIS SER THR ASN TYR ARG ASP SER CYS GLY LYS GLN LEU LYS



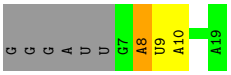
• Molecule 2: RNA (5'-R(*UP*UP*CP*CP*AP*AP*AP*AP*AP*AP*AP*UP*CP*GP*UP*UP *CP*CP*C)-3')

Chain B: 26% 21% 11% 42%



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

Chain C: 53% 11% 5% 32%



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

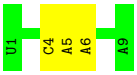
Chain E: 16% 16% 11% 58%



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

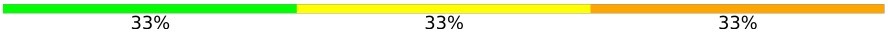
Chain D:





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

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53158	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	2.122	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	262.8, 262.8, 262.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.876, 0.876, 0.876	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN, 2KH

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	0.16	0/25606	0.35	0/34531
2	B	0.16	0/259	0.38	0/401
3	C	0.17	0/309	0.26	0/479
3	E	0.17	0/189	0.38	0/292
4	D	0.21	0/214	0.26	0/329
5	F	0.19	0/66	0.45	0/98
All	All	0.16	0/26643	0.35	0/36130

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	25181	0	25599	277	0
2	B	231	0	121	3	0
3	C	277	0	139	5	0
3	E	170	0	86	4	0
4	D	192	0	97	4	0
5	F	61	0	32	1	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	2	0
8	A	1	0	0	0	0
All	All	26146	0	26087	286	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 5.

All (286) 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:1127:ASN:HD21	1:A:1186:GLU:HB3	1.37	0.89
1:A:3336:PRO:HB3	1:A:3341:THR:HG21	1.69	0.73
1:A:3134:ASP:HA	1:A:3137:LYS:HB2	1.70	0.73
1:A:2831:LEU:HD11	1:A:2962:VAL:HG21	1.72	0.71
1:A:2537:TYR:O	1:A:2541:PHE:HB2	1.91	0.70
1:A:899:PRO:HG2	1:A:3334:LYS:HE3	1.74	0.70
3:E:12:C:H5'	3:E:13:U:H3'	1.76	0.68
1:A:1638:ARG:HH21	1:A:2361:LYS:HG3	1.59	0.66
1:A:2899:LEU:HB3	1:A:3166:PRO:HB3	1.78	0.66
1:A:1802:LYS:HE2	1:A:3400:ARG:HE	1.61	0.66
1:A:436:ASN:HD22	1:A:3558:PRO:HB3	1.61	0.66
1:A:542:GLY:HA3	1:A:900:THR:HG21	1.76	0.66
1:A:998:THR:HG23	1:A:1000:PHE:H	1.62	0.64
1:A:3469:GLN:HB2	1:A:3496:THR:HG22	1.80	0.64
1:A:2232:ARG:HE	1:A:2269:VAL:HG11	1.63	0.64
1:A:2311:GLY:H	1:A:2515:SER:HB2	1.63	0.64
1:A:3331:LEU:HD23	1:A:3478:PRO:HG3	1.79	0.63
1:A:2610:MET:HG3	1:A:2667:PHE:HB2	1.81	0.62
1:A:2622:TYR:HA	1:A:3195:PHE:HB2	1.80	0.62
1:A:1536:LEU:HB2	1:A:2569:VAL:HB	1.82	0.62
1:A:2863:PRO:HA	1:A:2959:LYS:HE2	1.83	0.61
1:A:983:MET:HE1	1:A:1762:ILE:HB	1.82	0.60
1:A:1797:PRO:HD2	1:A:3412:LEU:HD22	1.84	0.60
1:A:3548:THR:HA	1:A:3551:HIS:CE1	2.36	0.60
1:A:2754:GLU:HB2	1:A:3287:ALA:HB1	1.83	0.60
1:A:1663:LEU:HD22	1:A:1769:ILE:HD11	1.83	0.59
1:A:927:THR:HB	1:A:2384:ASP:HB2	1.84	0.59
1:A:2429:SER:H	1:A:2432:ASP:HB2	1.66	0.59
1:A:3733:THR:HG23	1:A:3775:ALA:HB2	1.83	0.59
1:A:3243:LEU:HD21	1:A:3318:LEU:HD21	1.84	0.59
1:A:3586:THR:O	1:A:3590:PHE:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3551:HIS:HB3	1:A:3698:LEU:HG	1.85	0.58
1:A:3100:ARG:HH21	1:A:3308:SER:HB2	1.68	0.57
1:A:2360:THR:HG22	1:A:2361:LYS:HG2	1.85	0.57
1:A:1228:VAL:HG13	1:A:1229:LEU:HD12	1.86	0.57
1:A:1839:ILE:HG13	1:A:2227:LEU:HD21	1.85	0.57
1:A:1972:LEU:HD22	1:A:1991:LEU:HD11	1.87	0.57
1:A:2638:GLN:HE22	1:A:2667:PHE:HB3	1.70	0.57
1:A:1058:LEU:HD21	1:A:1263:LEU:HD22	1.87	0.57
1:A:2694:LEU:HD12	1:A:2830:ILE:HD12	1.87	0.56
1:A:404:LEU:HA	1:A:407:VAL:HG12	1.87	0.56
1:A:1383:LEU:HD11	1:A:1397:PRO:HB2	1.87	0.56
1:A:3718:ILE:HG12	1:A:3723:LEU:HD12	1.88	0.56
1:A:1503:TYR:HE2	1:A:1595:THR:HG23	1.70	0.56
1:A:1632:LEU:HD22	1:A:2404:PRO:HD2	1.87	0.56
1:A:3740:GLN:HG3	1:A:3852:LYS:HE3	1.87	0.56
1:A:2908:ILE:HG22	1:A:3107:VAL:HA	1.89	0.55
1:A:1517:GLN:HG3	1:A:1548:THR:HB	1.87	0.55
1:A:1992:ILE:HA	1:A:2116:LEU:HD11	1.88	0.55
1:A:2700:SER:HB3	1:A:2807:ASP:HB3	1.86	0.55
1:A:3707:LEU:HD23	1:A:3886:MET:HE2	1.89	0.55
1:A:1193:LYS:HA	1:A:1200:ARG:HH21	1.72	0.55
1:A:3088:VAL:HG21	1:A:3202:LEU:HA	1.87	0.55
1:A:1808:LYS:HB3	1:A:2298:MET:HE2	1.87	0.55
1:A:2049:GLU:HG2	1:A:2163:LEU:HD13	1.89	0.54
1:A:2659:THR:HG22	1:A:2660:LEU:H	1.71	0.54
1:A:3394:LEU:HD13	1:A:3409:GLN:HB3	1.89	0.54
1:A:1663:LEU:HD21	1:A:1765:ASP:HB3	1.90	0.54
1:A:1943:ARG:HA	1:A:1958:ASN:HB3	1.89	0.54
1:A:941:MET:HE2	1:A:2395:LYS:HG2	1.90	0.54
1:A:2083:TRP:CD1	1:A:2084:CYS:HG	2.26	0.54
1:A:3366:ILE:HG12	1:A:3463:ILE:HD12	1.91	0.53
1:A:1604:ASP:HB2	1:A:2582:MET:HB2	1.89	0.53
1:A:692:PRO:HG3	1:A:823:LEU:HD22	1.91	0.53
1:A:553:LEU:HD22	1:A:3097:GLU:HB3	1.91	0.53
1:A:1936:VAL:HG11	1:A:2076:PHE:HE1	1.74	0.53
1:A:2914:THR:HG22	1:A:3123:PRO:HA	1.90	0.53
1:A:588:ALA:HA	1:A:591:CYS:HB2	1.90	0.53
1:A:3311:ARG:HB3	1:A:3314:GLU:HB2	1.91	0.53
1:A:1913:ILE:HG12	1:A:1917:LEU:HD13	1.91	0.53
1:A:2700:SER:HB2	1:A:2808:TRP:HB2	1.91	0.52
1:A:602:PHE:HD1	1:A:605:LEU:HD12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:HD11	1:A:1783:LEU:HD11	1.91	0.52
1:A:2756:GLU:HB3	1:A:3058:LEU:HD11	1.90	0.52
1:A:1580:TRP:HE3	1:A:1589:VAL:HG11	1.75	0.52
1:A:2273:LYS:HB2	1:A:2282:LEU:HD11	1.92	0.52
4:D:5:A:H2'	4:D:6:A:H8	1.75	0.52
1:A:2275:GLN:HE22	1:A:2280:ARG:HH21	1.57	0.51
4:D:5:A:H2'	4:D:6:A:C8	2.45	0.51
1:A:413:GLY:HA2	1:A:416:ILE:HG22	1.93	0.51
1:A:586:PRO:HD2	1:A:589:ILE:HD13	1.93	0.51
1:A:1532:GLY:HA2	1:A:1573:VAL:HG12	1.93	0.51
1:A:3811:LEU:HD21	1:A:3825:LEU:HD21	1.91	0.51
1:A:3091:LYS:HG2	1:A:3194:VAL:HG22	1.92	0.51
1:A:1429:LEU:HB3	1:A:3218:LYS:HE3	1.93	0.51
1:A:594:ILE:HG13	1:A:890:LEU:HD13	1.93	0.51
1:A:1025:SER:HB2	1:A:1261:LYS:HB3	1.92	0.51
1:A:1321:VAL:HB	1:A:2782:LEU:HD13	1.92	0.51
1:A:1004:LEU:HD21	1:A:2542:TRP:HB3	1.92	0.51
1:A:3469:GLN:HE21	1:A:3494:THR:HG23	1.75	0.51
1:A:2331:ASN:O	1:A:2335:LEU:HB2	2.11	0.50
1:A:2363:GLY:HA2	1:A:2471:MET:HE2	1.92	0.50
1:A:594:ILE:HG21	1:A:890:LEU:HD22	1.92	0.50
1:A:1306:LYS:HD2	1:A:2818:LEU:HD11	1.94	0.50
1:A:1088:VAL:HG22	1:A:1368:ILE:HD11	1.94	0.50
1:A:3635:GLN:HE22	1:A:3647:LEU:HD23	1.77	0.50
1:A:1342:ILE:HG12	1:A:1363:ILE:HD13	1.94	0.50
1:A:1820:THR:HB	3:C:10:A:H5"	1.94	0.50
1:A:2589:ALA:HB3	1:A:2592:LYS:HD3	1.94	0.49
1:A:551:LEU:HD22	1:A:3141:PHE:HE1	1.76	0.49
1:A:1312:PRO:HD2	1:A:3072:GLU:HA	1.94	0.49
1:A:2876:LEU:HD13	1:A:2934:LEU:HD21	1.94	0.49
1:A:3197:MET:HE2	1:A:3199:LYS:HB3	1.93	0.49
1:A:3339:GLY:HA2	1:A:3468:LYS:HD2	1.95	0.49
1:A:3374:LEU:HG	1:A:3376:ILE:HG12	1.93	0.49
1:A:3489:ILE:HB	1:A:3533:LEU:HB2	1.94	0.49
1:A:1418:LEU:HB3	1:A:2595:PHE:HZ	1.78	0.49
1:A:1218:CYS:HB3	3:E:17:A:N7	2.28	0.49
1:A:1311:THR:HG22	1:A:1313:TYR:H	1.76	0.49
1:A:912:THR:HG21	1:A:3128:PHE:HB3	1.95	0.49
1:A:1256:VAL:HG13	1:A:1257:ARG:H	1.77	0.49
1:A:3370:ILE:HG13	1:A:3375:HIS:HD2	1.77	0.49
1:A:611:ARG:HH22	1:A:3441:ASN:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:VAL:HG13	1:A:1440:LEU:HD21	1.94	0.48
1:A:3708:ILE:HG22	1:A:3712:LYS:HE3	1.95	0.48
1:A:2910:LEU:HD12	1:A:3179:THR:HG21	1.96	0.48
1:A:889:PHE:O	1:A:893:LYS:HB2	2.13	0.48
1:A:2618:GLN:HG3	1:A:2674:LEU:HD22	1.94	0.48
1:A:2630:ASN:HA	1:A:2633:PHE:CE2	2.48	0.48
1:A:1023:ILE:HD11	1:A:1035:ILE:HD13	1.96	0.48
1:A:2687:ILE:HD12	1:A:2833:ALA:HB3	1.94	0.48
1:A:3424:LEU:HD11	1:A:3652:ARG:HD2	1.94	0.48
1:A:2867:LEU:HD22	1:A:2948:ILE:HG12	1.96	0.48
1:A:1830:MET:HG2	1:A:2463:MET:HB3	1.94	0.48
1:A:3773:VAL:HG12	1:A:3786:VAL:HG22	1.94	0.48
1:A:2760:ILE:HD11	1:A:3058:LEU:HD22	1.96	0.48
1:A:3331:LEU:HD21	1:A:3489:ILE:HG21	1.96	0.48
1:A:2966:LEU:HD22	1:A:3000:THR:HG21	1.95	0.48
1:A:3059:GLN:HG3	1:A:3060:PHE:HD1	1.79	0.47
1:A:2961:ASN:HB2	1:A:2989:ARG:HH21	1.79	0.47
1:A:590:ILE:HD13	1:A:893:LYS:HG3	1.96	0.47
1:A:2966:LEU:HD23	1:A:3037:ARG:HH12	1.79	0.47
1:A:3101:LEU:HD22	1:A:3134:ASP:HB2	1.96	0.47
1:A:1129:GLU:O	1:A:1133:LYS:HG2	2.14	0.47
1:A:3280:CYS:HB3	1:A:3283:SER:HB2	1.97	0.47
1:A:3282:LEU:HD23	1:A:3701:GLU:HG2	1.97	0.47
1:A:3836:LYS:HG3	1:A:3847:GLU:HB2	1.96	0.47
1:A:1649:SER:HB2	1:A:1660:THR:HB	1.96	0.47
1:A:1952:PRO:HG2	1:A:1954:LEU:HD21	1.97	0.47
1:A:1631:VAL:HG22	1:A:2281:ASP:HA	1.97	0.47
1:A:1346:PHE:HB2	1:A:1370:LEU:HD21	1.97	0.47
1:A:1607:LEU:HD23	1:A:2582:MET:HE2	1.97	0.47
1:A:3765:GLN:HB2	1:A:3773:VAL:HG23	1.96	0.47
4:D:4:C:H2'	4:D:5:A:C8	2.50	0.47
1:A:1884:ASP:HA	1:A:1887:LYS:HE2	1.98	0.46
1:A:3800:LYS:HA	1:A:3803:ARG:HE	1.80	0.46
1:A:544:VAL:HG12	1:A:575:LEU:HD11	1.96	0.46
1:A:800:ARG:HG2	1:A:832:ILE:HG21	1.96	0.46
1:A:2409:LYS:O	1:A:2413:ASN:HB2	2.15	0.46
1:A:1259:ASN:HA	2:B:5:A:H62	1.79	0.46
1:A:2362:TRP:CZ3	1:A:2561:MET:HG2	2.51	0.46
1:A:3357:THR:HG22	1:A:3366:ILE:HG22	1.97	0.46
1:A:1296:LEU:HD13	1:A:2636:LEU:HD23	1.97	0.46
1:A:2012:ILE:HG13	1:A:2073:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3638:ILE:HG21	1:A:3646:VAL:HB	1.97	0.46
1:A:486:LYS:HG2	1:A:508:ALA:HB1	1.97	0.46
1:A:637:LYS:HD3	1:A:828:PHE:HD2	1.80	0.46
1:A:994:GLU:HG3	1:A:1767:LEU:HD22	1.98	0.46
1:A:2611:GLN:HG2	1:A:2679:VAL:HG21	1.97	0.46
1:A:3635:GLN:H	1:A:3638:ILE:HG12	1.80	0.46
1:A:822:LEU:HD13	1:A:858:SER:HB2	1.98	0.46
4:D:4:C:H2'	4:D:5:A:H8	1.80	0.46
1:A:3137:LYS:HA	1:A:3141:PHE:CD2	2.51	0.45
1:A:437:LEU:HD21	1:A:3581:VAL:HG13	1.97	0.45
1:A:935:LEU:HD11	1:A:963:ARG:HH21	1.80	0.45
1:A:2756:GLU:O	1:A:2760:ILE:HG12	2.16	0.45
1:A:3488:SER:HA	1:A:3535:ARG:HG2	1.98	0.45
1:A:626:HIS:HB3	1:A:902:VAL:HG11	1.99	0.45
1:A:875:ILE:HD12	1:A:879:ARG:HB3	1.98	0.45
1:A:1015:LEU:HD11	1:A:1567:TYR:HB2	1.98	0.45
2:B:7:A:H5"	2:B:8:A:C8	2.52	0.45
1:A:687:PHE:HB3	1:A:846:ILE:HD11	1.98	0.45
1:A:1424:GLN:HE22	1:A:2628:VAL:HB	1.80	0.45
1:A:647:ASN:HB3	1:A:879:ARG:HH21	1.82	0.45
1:A:1499:LEU:HG	1:A:1596:VAL:HG22	1.98	0.45
1:A:1823:VAL:HB	1:A:2286:GLU:HA	1.99	0.45
1:A:3024:ILE:HD13	1:A:3048:VAL:HG11	1.98	0.45
1:A:749:ILE:HD13	1:A:822:LEU:HB2	1.98	0.45
1:A:1784:ILE:HA	1:A:1787:ILE:HG22	1.98	0.45
1:A:2903:VAL:O	1:A:2907:LEU:HB2	2.17	0.45
7:A:4005:2KH:H15	3:C:10:A:H61	1.63	0.45
1:A:641:TYR:HE2	1:A:826:VAL:HB	1.82	0.44
1:A:1028:CYS:HB3	1:A:1065:CYS:HA	1.99	0.44
1:A:1963:SER:HA	1:A:1966:PHE:CE2	2.51	0.44
1:A:1023:ILE:HD13	1:A:1035:ILE:HG21	1.98	0.44
1:A:1241:VAL:HG13	1:A:1850:MET:HE2	2.00	0.44
1:A:1939:SER:HB3	1:A:2003:LYS:HE3	2.00	0.44
1:A:3543:LEU:HA	1:A:3689:THR:HG22	1.98	0.44
1:A:1534:SER:HA	1:A:2570:SER:HB3	2.00	0.44
1:A:1621:MET:HE1	1:A:2272:PRO:HG2	2.00	0.44
1:A:2871:LYS:HB2	1:A:2871:LYS:HE3	1.88	0.44
1:A:2636:LEU:O	1:A:2640:ILE:HG13	2.18	0.44
1:A:3792:PRO:HG2	1:A:3795:ASP:HB2	1.99	0.44
1:A:1913:ILE:HG23	1:A:1917:LEU:HD22	1.99	0.44
1:A:2869:PRO:HG3	1:A:2944:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:4005:2KH:O5'	7:A:4005:2KH:H14	2.18	0.44
1:A:686:GLU:HA	1:A:926:LYS:HD2	2.00	0.44
1:A:422:CYS:O	1:A:426:ILE:HG13	2.18	0.43
1:A:1417:THR:HB	1:A:2595:PHE:HE1	1.82	0.43
1:A:958:LEU:O	1:A:962:MET:HG3	2.18	0.43
1:A:2581:MET:HE3	1:A:2581:MET:HB3	1.91	0.43
1:A:3178:LEU:HD23	1:A:3181:LEU:HD12	2.00	0.43
1:A:970:VAL:HB	1:A:1755:TYR:HE1	1.83	0.43
1:A:3339:GLY:HA2	1:A:3468:LYS:HB3	1.99	0.43
1:A:2660:LEU:HG	1:A:2832:ILE:HD11	1.99	0.43
1:A:3746:ARG:HB3	1:A:3892:VAL:HG22	2.00	0.43
1:A:3248:ALA:O	1:A:3252:LEU:HG	2.19	0.43
1:A:1247:ASN:HA	1:A:1250:LYS:HE2	2.00	0.43
1:A:1283:LYS:HG3	1:A:1440:LEU:HB3	2.00	0.43
1:A:2660:LEU:HD22	1:A:2683:ASP:HA	2.01	0.43
1:A:3335:LYS:HA	1:A:3533:LEU:HD21	2.00	0.43
1:A:749:ILE:HG23	1:A:822:LEU:HD22	2.01	0.43
1:A:914:LYS:HE2	1:A:914:LYS:HB3	1.89	0.43
1:A:2869:PRO:HD2	1:A:2872:LEU:HD12	2.00	0.43
1:A:3105:PRO:HA	1:A:3108:VAL:HG22	2.01	0.43
1:A:619:ASP:HB3	1:A:632:HIS:CE1	2.54	0.42
1:A:661:SER:HB2	1:A:689:ASP:HA	2.00	0.42
1:A:1116:GLY:HA2	1:A:1121:GLU:HB3	2.01	0.42
1:A:2529:LEU:HD22	1:A:2533:LEU:HD23	2.00	0.42
1:A:834:GLY:HA2	1:A:914:LYS:HD2	2.01	0.42
1:A:1123:ARG:O	1:A:1127:ASN:HB2	2.18	0.42
1:A:2663:PHE:CZ	1:A:2863:PRO:HG2	2.54	0.42
1:A:3137:LYS:HA	1:A:3141:PHE:HD2	1.82	0.42
1:A:3209:VAL:HG13	1:A:3234:THR:HG22	1.99	0.42
1:A:655:PRO:HD2	1:A:658:ILE:HD11	2.01	0.42
1:A:1363:ILE:HD12	1:A:1368:ILE:HB	2.01	0.42
1:A:919:LEU:HD11	1:A:3128:PHE:CE2	2.53	0.42
1:A:1760:GLU:HG2	1:A:1764:LYS:HE2	2.01	0.42
1:A:1965:GLU:HG3	1:A:1994:SER:HB2	2.01	0.42
1:A:1136:MET:HG3	1:A:1141:ILE:HB	2.02	0.42
1:A:749:ILE:O	1:A:753:MET:HG2	2.20	0.42
1:A:2315:PRO:HG2	1:A:2316:HIS:CE1	2.55	0.42
1:A:3078:SER:H	1:A:3224:ARG:HB2	1.84	0.42
1:A:542:GLY:O	1:A:545:LEU:HG	2.20	0.42
1:A:3487:LEU:HD21	1:A:3536:ILE:HD12	2.02	0.42
1:A:919:LEU:HD11	1:A:3128:PHE:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:THR:HG22	1:A:1537:VAL:HG12	2.02	0.42
1:A:2292:MET:HE2	1:A:2292:MET:HB3	1.95	0.42
1:A:983:MET:HE2	1:A:1759:LYS:HA	2.02	0.41
1:A:1125:LYS:HE2	1:A:1125:LYS:HB3	1.89	0.41
1:A:2023:LEU:HD22	1:A:2144:LEU:HD13	2.01	0.41
1:A:2552:THR:HA	1:A:2555:VAL:HG12	2.01	0.41
1:A:2815:ARG:HE	1:A:2815:ARG:HB2	1.75	0.41
1:A:442:LEU:HB3	1:A:446:ASP:HB2	2.01	0.41
1:A:1536:LEU:HD21	1:A:2546:CYS:HB2	2.02	0.41
1:A:1609:PHE:HE2	1:A:2594:MET:HE1	1.85	0.41
1:A:1379:LYS:NZ	3:C:8:A:H61	2.19	0.41
1:A:1419:TYR:CE1	1:A:1499:LEU:HB3	2.56	0.41
1:A:2941:ILE:HG23	1:A:2941:ILE:HD12	1.82	0.41
1:A:3320:ASP:HB3	1:A:3489:ILE:HG13	2.02	0.41
1:A:1946:PHE:HE1	1:A:1954:LEU:H	1.68	0.41
1:A:2282:LEU:HD13	3:C:10:A:N7	2.36	0.41
1:A:2354:CYS:HB3	1:A:2574:LEU:HD13	2.03	0.41
1:A:2016:ILE:HD11	1:A:2141:LEU:HD13	2.02	0.41
1:A:2803:ALA:HB1	1:A:2820:LEU:HD21	2.02	0.41
1:A:3480:LEU:HB3	1:A:3482:TRP:CZ3	2.55	0.41
1:A:3698:LEU:HA	1:A:3704:LEU:HD22	2.02	0.41
1:A:1805:ARG:HE	1:A:1805:ARG:HB2	1.56	0.41
1:A:3063:PRO:HA	1:A:3066:GLN:HG2	2.03	0.41
1:A:3105:PRO:HB2	1:A:3182:SER:HB2	2.02	0.41
1:A:3108:VAL:HG12	1:A:3131:LEU:HD23	2.03	0.41
1:A:1320:LEU:O	1:A:1324:ILE:HG13	2.21	0.41
1:A:1601:VAL:HG11	1:A:1607:LEU:HB2	2.03	0.41
1:A:2232:ARG:HD2	3:C:8:A:H4'	2.02	0.41
1:A:2463:MET:HE3	1:A:2463:MET:HB2	1.89	0.41
1:A:2644:HIS:NE2	1:A:2946:LEU:HD23	2.36	0.41
1:A:2871:LYS:HD3	1:A:2944:LEU:HD11	2.03	0.41
1:A:3346:THR:HG22	1:A:3348:GLY:H	1.85	0.41
1:A:913:GLN:HB2	5:F:2:C:N4	2.36	0.41
1:A:1787:ILE:HD11	1:A:2487:ALA:HA	2.03	0.40
1:A:2410:LYS:HG2	2:B:8:A:OP1	2.22	0.40
1:A:3026:CYS:HB2	1:A:3049:PHE:CE2	2.56	0.40
1:A:2332:MET:HE1	1:A:2571:ASP:HB2	2.04	0.40
1:A:2359:ASN:HB2	1:A:2517:ASP:HB2	2.02	0.40
1:A:3262:LEU:HD11	1:A:3554:LEU:HD21	2.02	0.40
3:E:16:G:C2	3:E:17:A:H2'	2.56	0.40
1:A:1096:PHE:HB2	3:E:16:G:O6	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:LYS:HE3	1:A:1208:LYS:HB2	1.92	0.40
1:A:2520:ALA:HB1	1:A:2574:LEU:HD11	2.02	0.40
1:A:738:LEU:HA	1:A:739:PRO:HD3	1.94	0.40
1:A:1526:ARG:HA	1:A:1611:ILE:HB	2.03	0.40
1:A:1842:THR:HG22	1:A:2225:GLU:HB3	2.03	0.40
1:A:3394:LEU:HD23	1:A:3394:LEU:HA	1.93	0.40
1:A:606:PRO:HA	1:A:607:PRO:HD3	1.98	0.40
1:A:3469:GLN:HG3	1:A:3471:VAL:H	1.86	0.40
1:A:3634:VAL:HG11	1:A:3663:PHE:HE2	1.85	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	3102/3945 (79%)	2939 (95%)	163 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	2891/3601 (80%)	2891 (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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	ASN
1	A	550	ASN
1	A	987	ASN
1	A	1074	ASN
1	A	1127	ASN
1	A	1244	ASN
1	A	1768	GLN
1	A	1885	GLN
1	A	2252	GLN
1	A	2348	ASN
1	A	2600	ASN
1	A	2630	ASN
1	A	2853	ASN
1	A	3043	GLN
1	A	3098	GLN
1	A	3177	HIS
1	A	3296	GLN
1	A	3377	HIS
1	A	3481	GLN
1	A	3595	ASN
1	A	3653	ASN
1	A	3765	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	10/19 (52%)	5 (50%)	0
3	C	12/19 (63%)	2 (16%)	0
3	E	7/19 (36%)	3 (42%)	0
4	D	8/9 (88%)	0	0
5	F	2/3 (66%)	2 (100%)	0
All	All	39/69 (56%)	12 (30%)	0

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	5	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	6	A
2	B	8	A
2	B	11	A
3	C	8	A
3	C	9	U
3	E	13	U
3	E	14	U
3	E	17	A
5	F	2	C
5	F	3	U

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	3.90	21 (72%)	42,47,47	1.63	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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'	-8.70	1.29	1.53
7	A	4005	2KH	C2-N3	6.92	1.50	1.38
7	A	4005	2KH	C2-N1	6.19	1.48	1.38
7	A	4005	2KH	C6-C5	5.99	1.49	1.35
7	A	4005	2KH	PB-O3B	5.85	1.66	1.59
7	A	4005	2KH	O4'-C4'	-5.79	1.32	1.45
7	A	4005	2KH	O4'-C1'	5.00	1.53	1.42
7	A	4005	2KH	C1'-N1	-4.90	1.33	1.47
7	A	4005	2KH	C3'-C4'	4.23	1.63	1.53
7	A	4005	2KH	PB-O2B	3.84	1.52	1.46
7	A	4005	2KH	PB-N3A	3.49	1.72	1.63
7	A	4005	2KH	O4-C4	-3.49	1.17	1.24
7	A	4005	2KH	PA-O1A	3.41	1.51	1.46
7	A	4005	2KH	O3'-C3'	3.18	1.50	1.43
7	A	4005	2KH	PG-O2G	2.59	1.58	1.50
7	A	4005	2KH	C5-C4	2.58	1.49	1.43
7	A	4005	2KH	C4-N3	2.51	1.43	1.38
7	A	4005	2KH	C6-N1	2.45	1.43	1.38
7	A	4005	2KH	PA-N3A	2.38	1.69	1.63
7	A	4005	2KH	O2'-C2'	2.26	1.48	1.43
7	A	4005	2KH	PG-O3G	-2.03	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	4005	2KH	C4-N3-C2	-4.98	120.01	126.58
7	A	4005	2KH	N3-C2-N1	3.78	119.91	114.89
7	A	4005	2KH	C5-C4-N3	3.65	120.31	114.84
7	A	4005	2KH	PB-O3B-PG	-3.06	121.84	132.62
7	A	4005	2KH	O4-C4-C5	-2.80	120.24	125.16
7	A	4005	2KH	C3'-C2'-C1'	2.46	106.09	101.43
7	A	4005	2KH	C2'-C3'-C4'	2.33	107.16	102.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

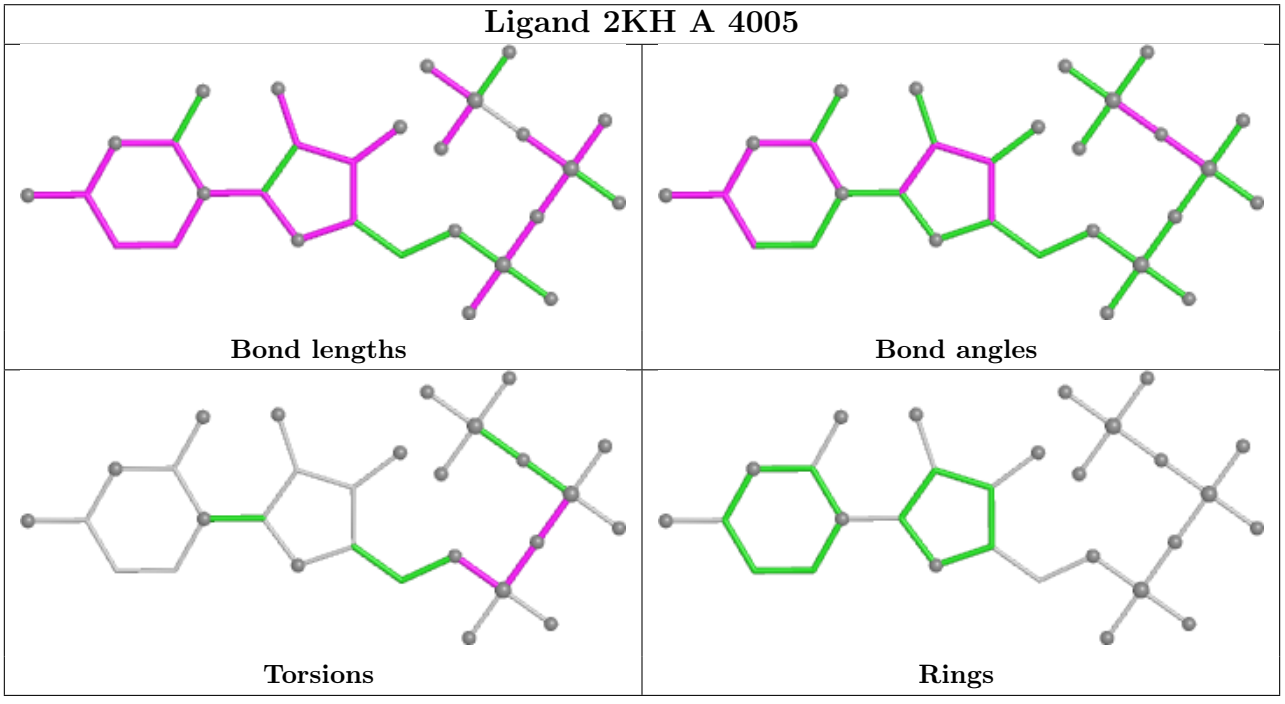
Mol	Chain	Res	Type	Atoms
7	A	4005	2KH	PB-N3A-PA-O1A
7	A	4005	2KH	C5'-O5'-PA-O2A
7	A	4005	2KH	PA-N3A-PB-O2B
7	A	4005	2KH	PA-N3A-PB-O3B
7	A	4005	2KH	C5'-O5'-PA-O1A
7	A	4005	2KH	C5'-O5'-PA-N3A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	4005	2KH	2	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 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.



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.

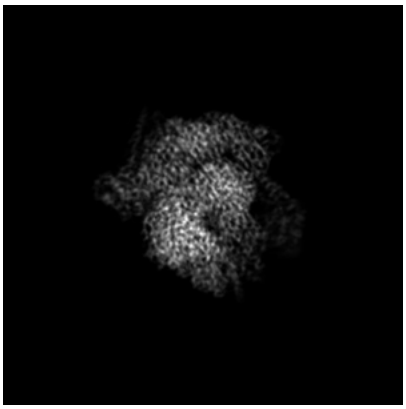
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66787. These allow visual inspection of the internal detail of the map and identification of artifacts.

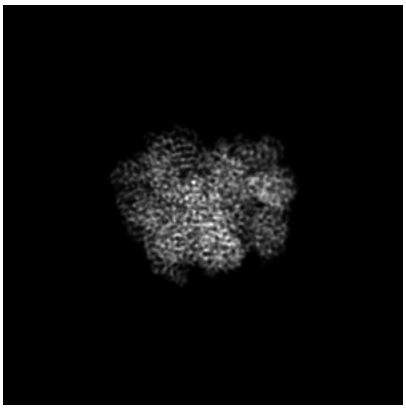
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

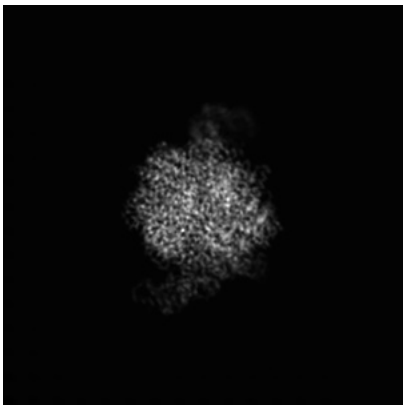
6.1.1 Primary map



X

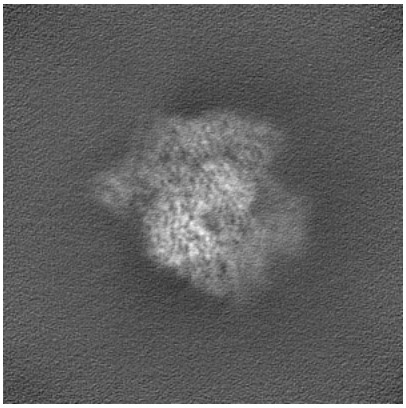


Y

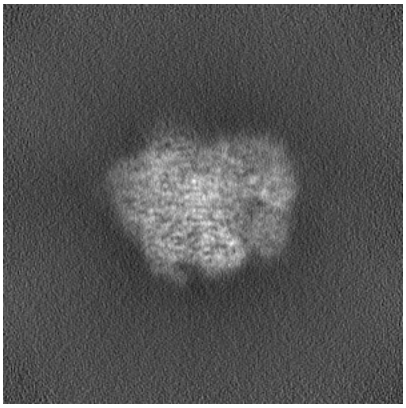


Z

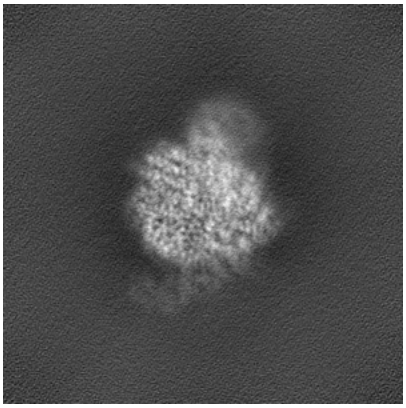
6.1.2 Raw map



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

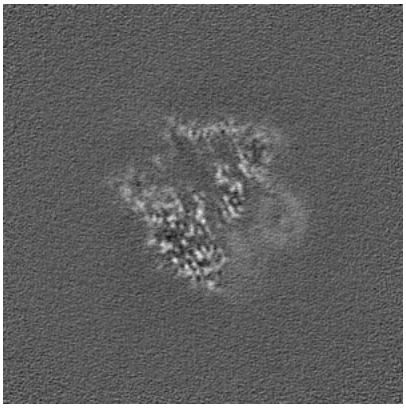


Y Index: 150

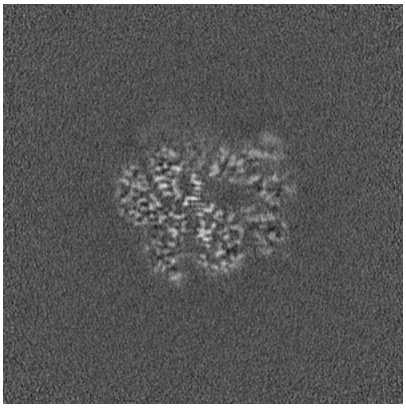


Z Index: 150

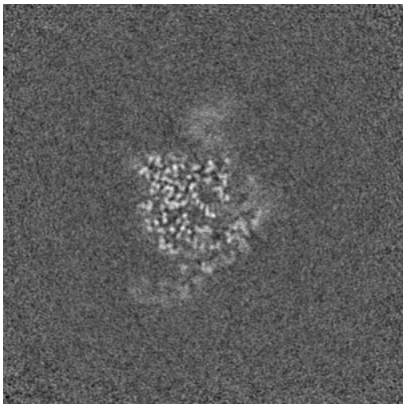
6.2.2 Raw map



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: 135

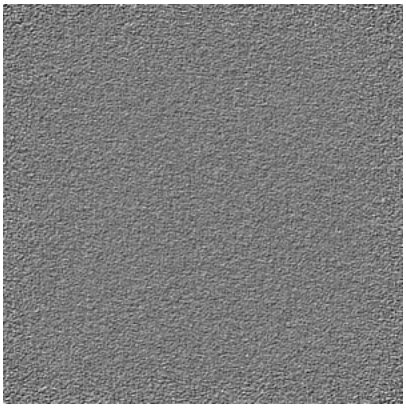


Y Index: 153

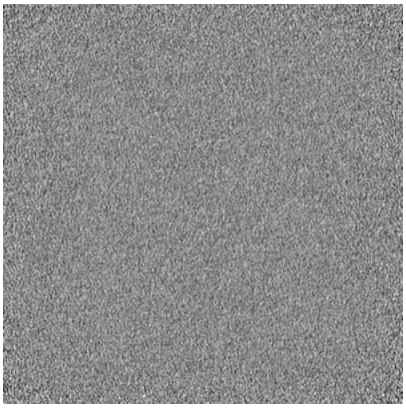


Z Index: 162

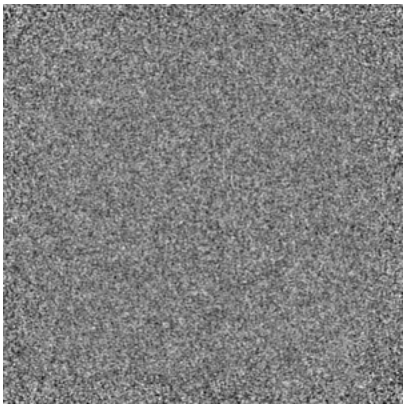
6.3.2 Raw map



X Index: 0



Y Index: 0

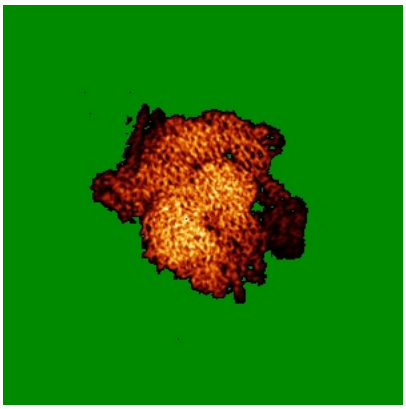


Z Index: 299

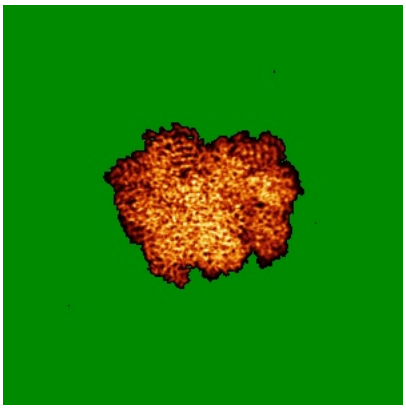
The images above show the largest variance slices of the map in three orthogonal directions.

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

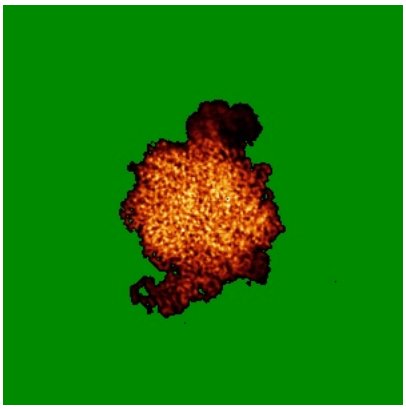
6.4.1 Primary map



X

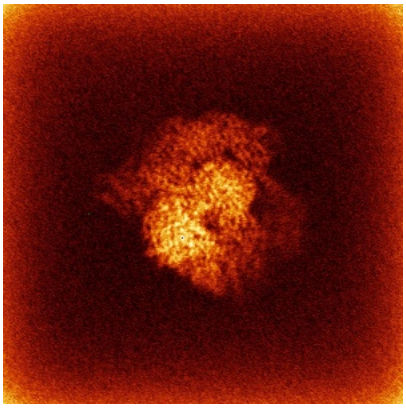


Y

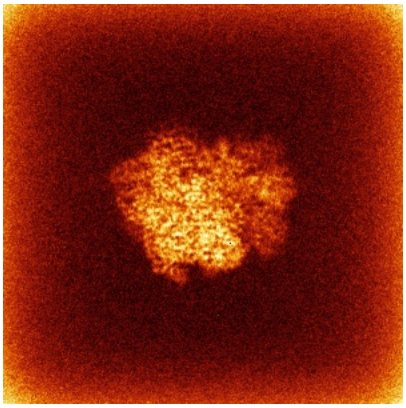


Z

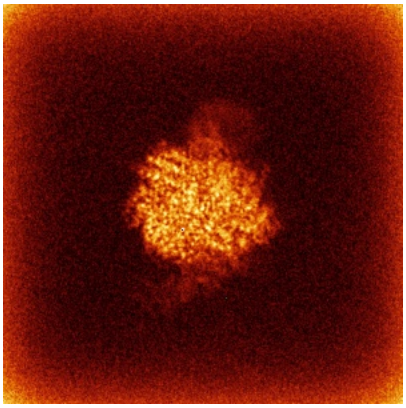
6.4.2 Raw map



X



Y

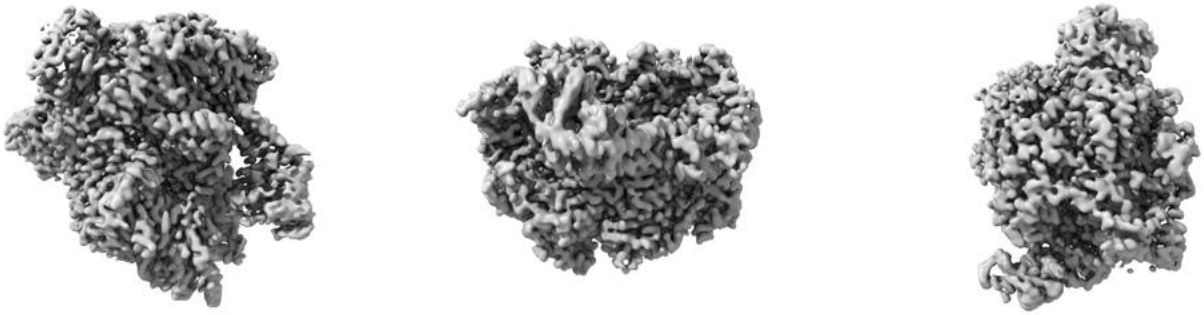


Z

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)

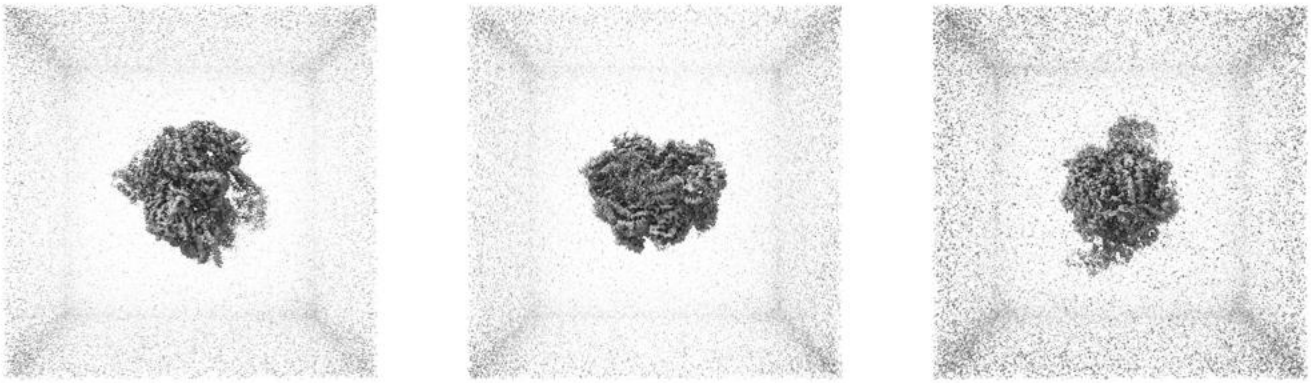
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

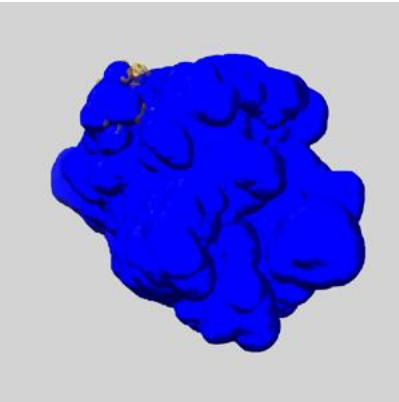
6.6 Mask visualisation (i)

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

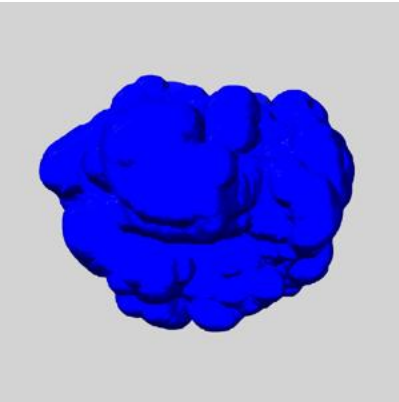
A mask typically either:

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

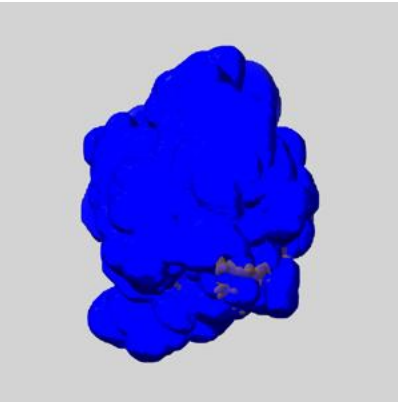
6.6.1 emd_66787_msk_1.map (i)



X



Y

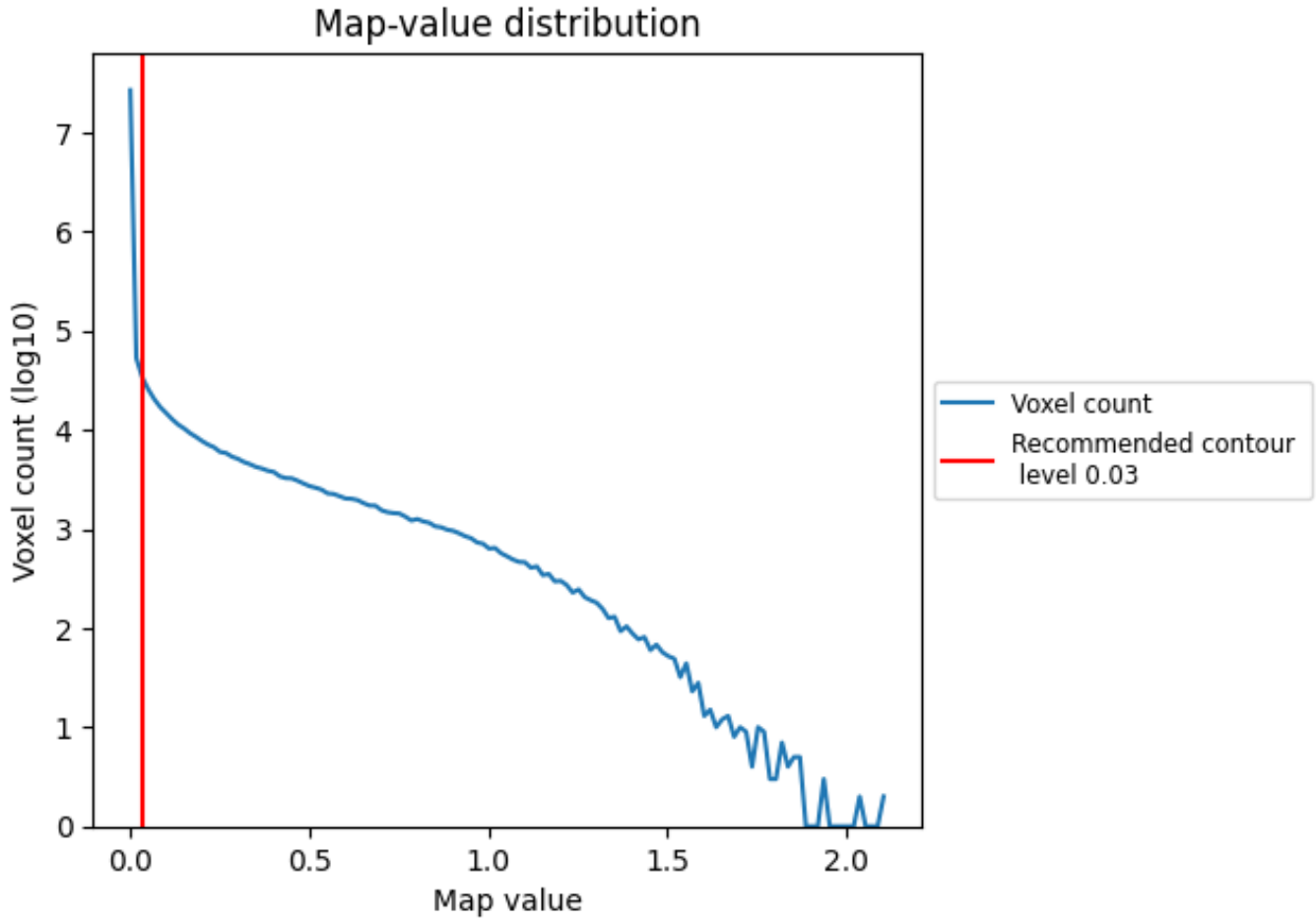


Z

7 Map analysis

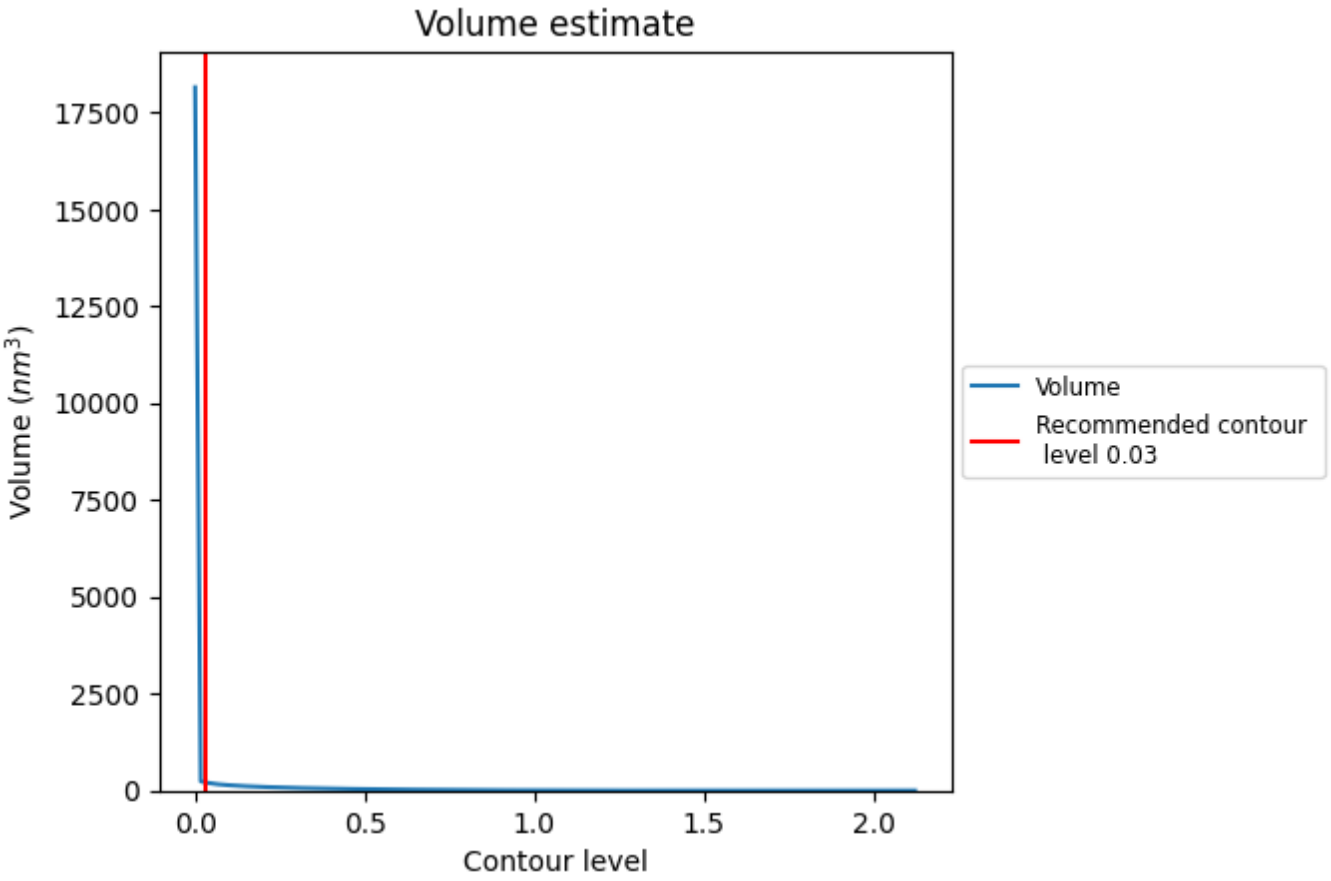
This section contains the results of statistical analysis of the map.

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.

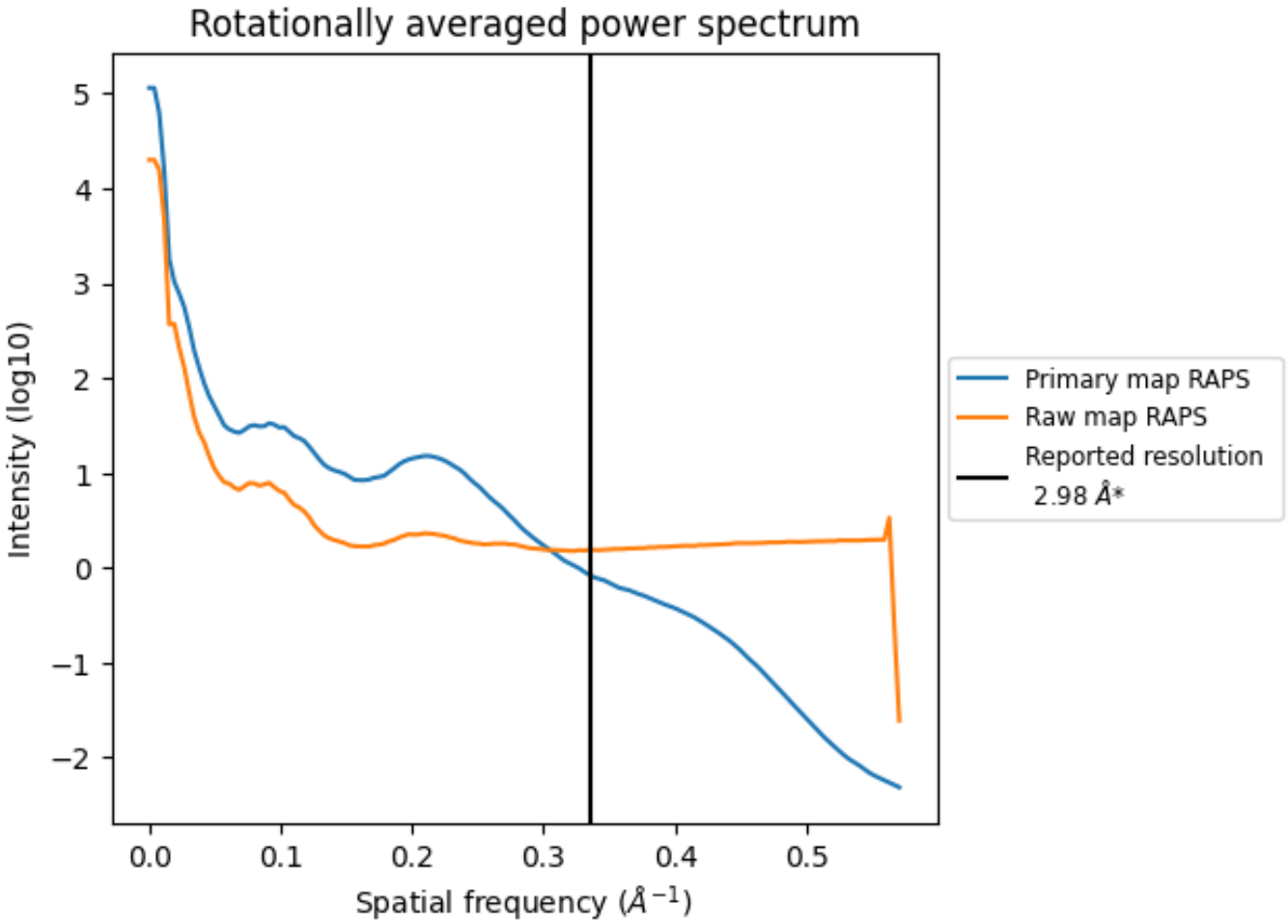
7.2 Volume estimate



The volume at the recommended contour level is 207 nm^3; this corresponds to an approximate mass of 187 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)

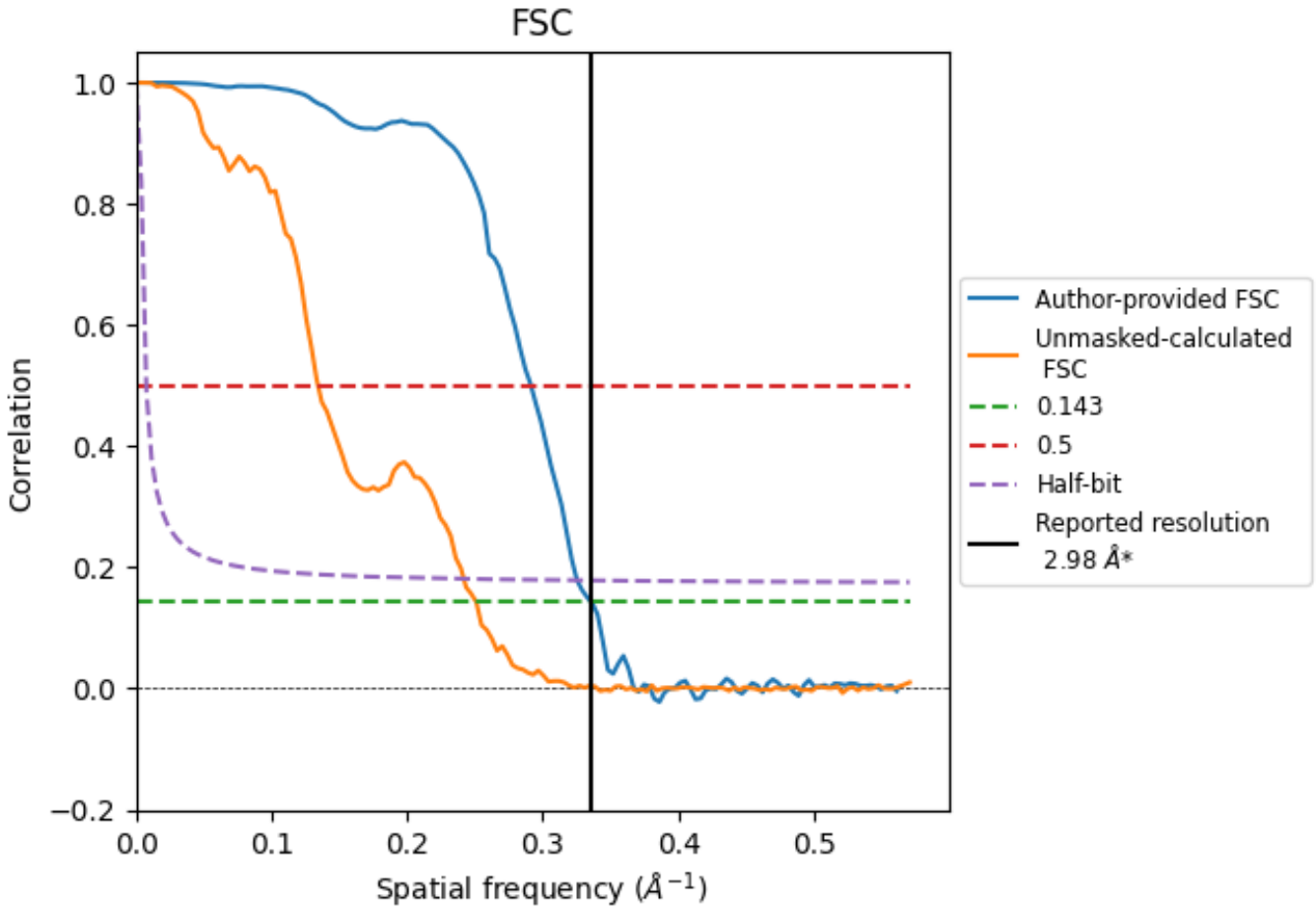


*Reported resolution corresponds to spatial frequency of 0.336 Å^{-1}

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 0.336 Å^{-1}

8.2 Resolution estimates (i)

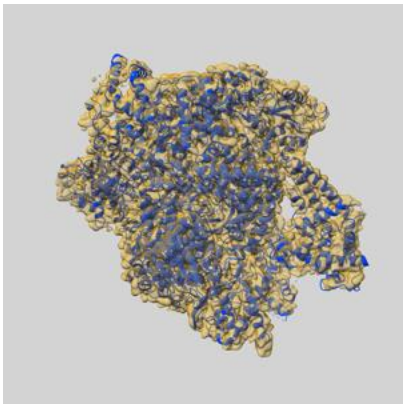
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.43	3.07
Unmasked-calculated*	3.98	7.45	4.13

*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 3.98 differs from the reported value 2.98 by more than 10 %

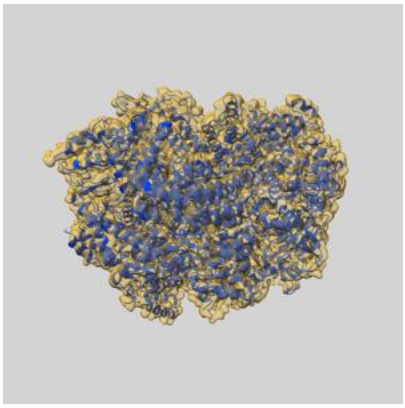
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66787 and PDB model 9XEC. Per-residue inclusion information can be found in section 3 on page 6.

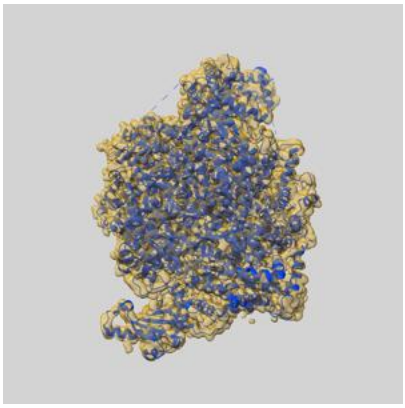
9.1 Map-model overlay



X



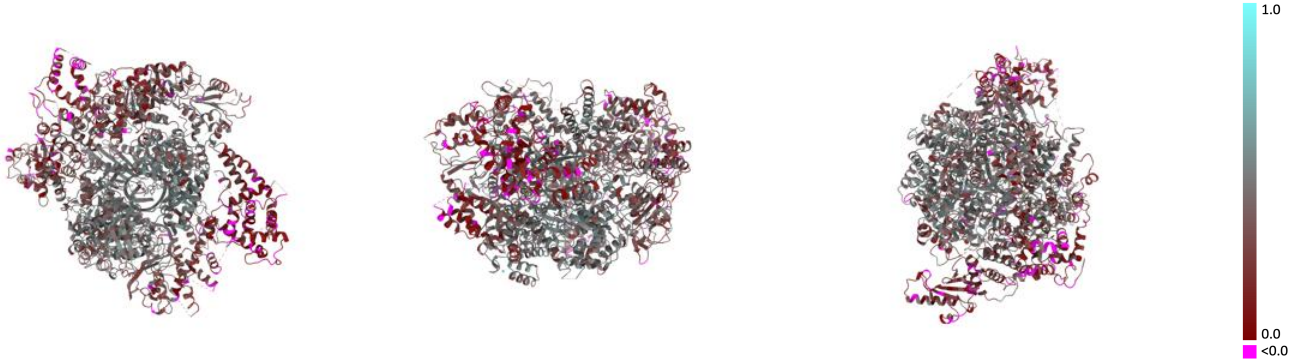
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

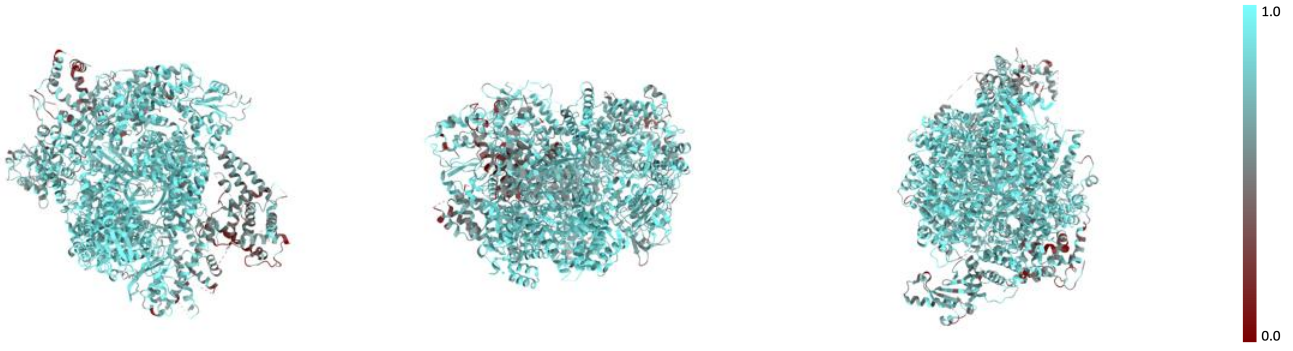
9.2 Q-score mapped to coordinate model



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.

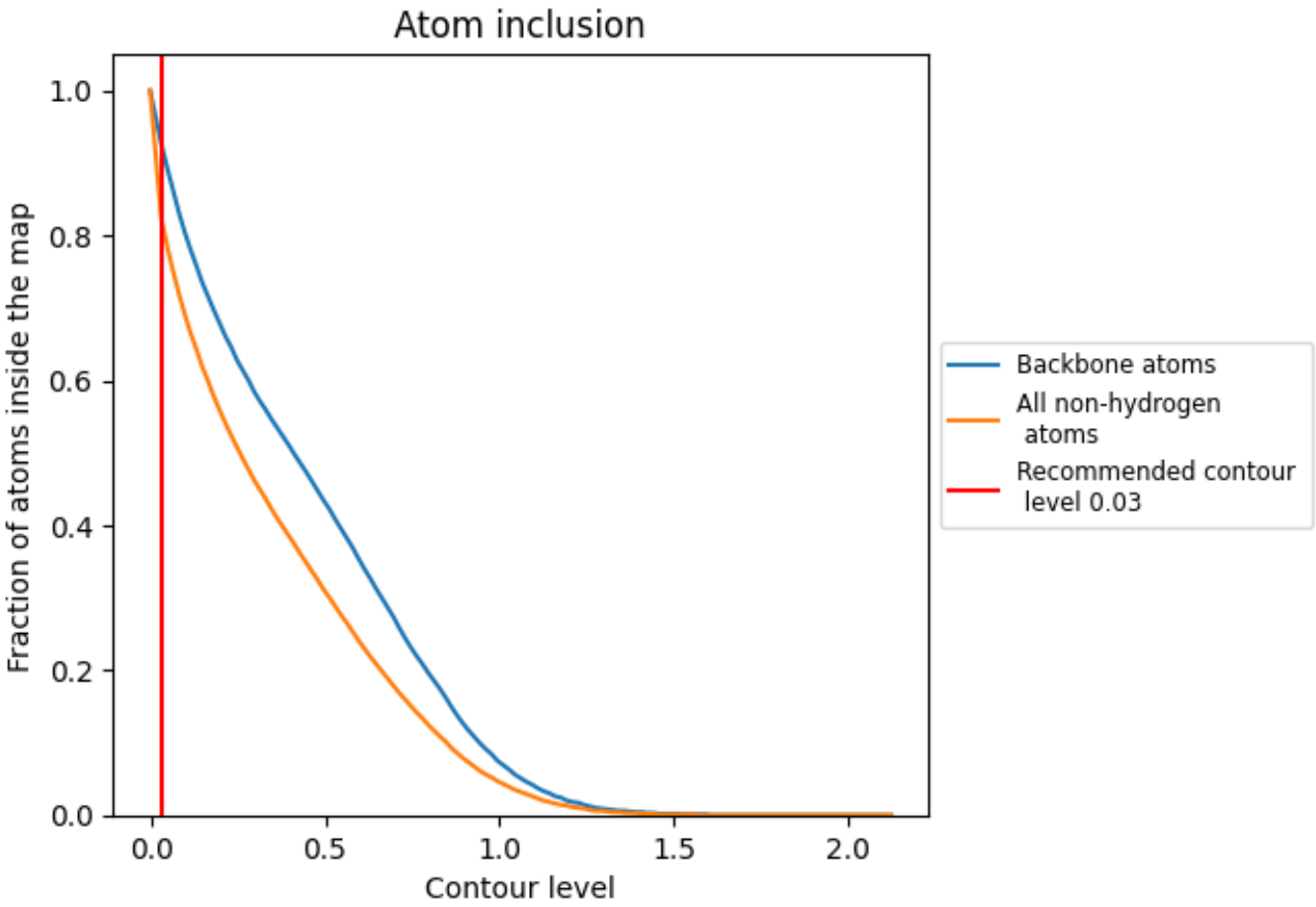
9.3 Atom inclusion mapped to coordinate model



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.3610
A	0.8210	0.3590
B	0.8660	0.3920
C	0.9280	0.4350
D	0.9840	0.5150
E	0.8240	0.3190
F	0.9510	0.4550

