wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 12:03 PM EST

PDB ID	:	7R78
EMDB ID	:	EMD-24295
Title	:	cryo-EM structure of DNMT5 quaternary complex with hemimethylated DNA, AMP-PNP and SAH
Authors	:	Wang, J.; Patel, D.J.
Deposited on	:	2021-06-24
Resolution	:	3.50 Å(reported)

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

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

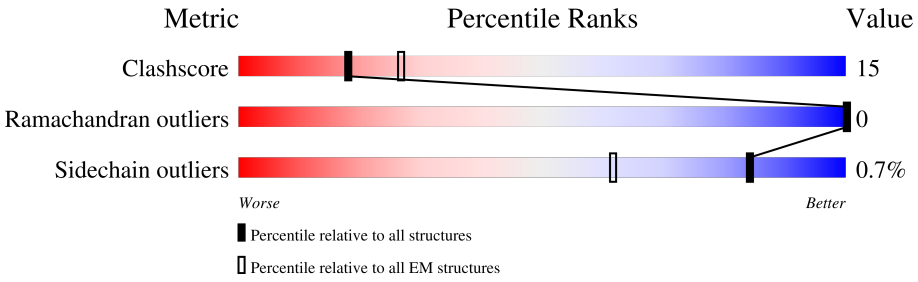
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



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

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	2348	55% 25% 20%
2	D	36	17% 78%
3	E	36	11% 17% 72%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15238 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA repair protein Rad8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1880	14810	9284	2675	2780	71	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP J9VI03
A	31	SER	-	expression tag	UNP J9VI03
A	32	TYR	-	expression tag	UNP J9VI03
A	33	TYR	-	expression tag	UNP J9VI03
A	34	HIS	-	expression tag	UNP J9VI03
A	35	HIS	-	expression tag	UNP J9VI03
A	36	HIS	-	expression tag	UNP J9VI03
A	37	HIS	-	expression tag	UNP J9VI03
A	38	HIS	-	expression tag	UNP J9VI03
A	39	HIS	-	expression tag	UNP J9VI03
A	40	ASP	-	expression tag	UNP J9VI03
A	41	TYR	-	expression tag	UNP J9VI03
A	42	ASP	-	expression tag	UNP J9VI03
A	43	ILE	-	expression tag	UNP J9VI03
A	44	PRO	-	expression tag	UNP J9VI03
A	45	THR	-	expression tag	UNP J9VI03
A	46	THR	-	expression tag	UNP J9VI03
A	47	GLU	-	expression tag	UNP J9VI03
A	48	ASN	-	expression tag	UNP J9VI03
A	49	LEU	-	expression tag	UNP J9VI03
A	50	TYR	-	expression tag	UNP J9VI03
A	51	PHE	-	expression tag	UNP J9VI03
A	52	GLN	-	expression tag	UNP J9VI03
A	53	GLY	-	expression tag	UNP J9VI03
A	54	ALA	-	expression tag	UNP J9VI03
A	55	MET	-	expression tag	UNP J9VI03
A	56	GLY	-	expression tag	UNP J9VI03
A	57	SER	-	expression tag	UNP J9VI03

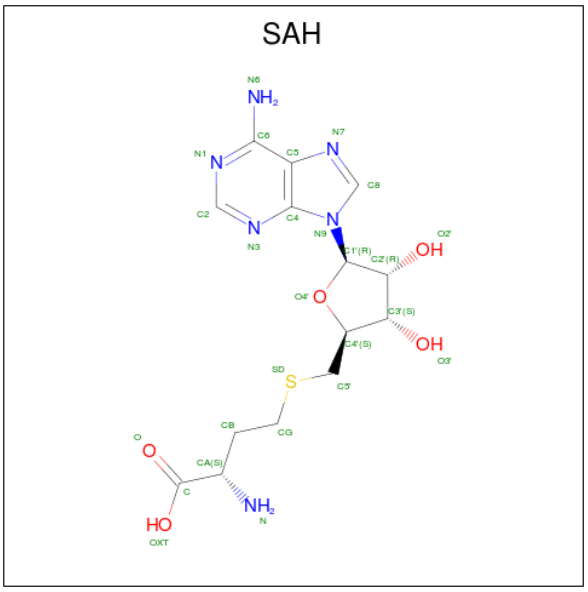
- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*AP*GP*(5CM)P*GP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	8	Total	C	N	O	P	0	0
			164	78	31	47	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	10	Total	C	N	O	P	0	0
			201	97	38	57	9		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



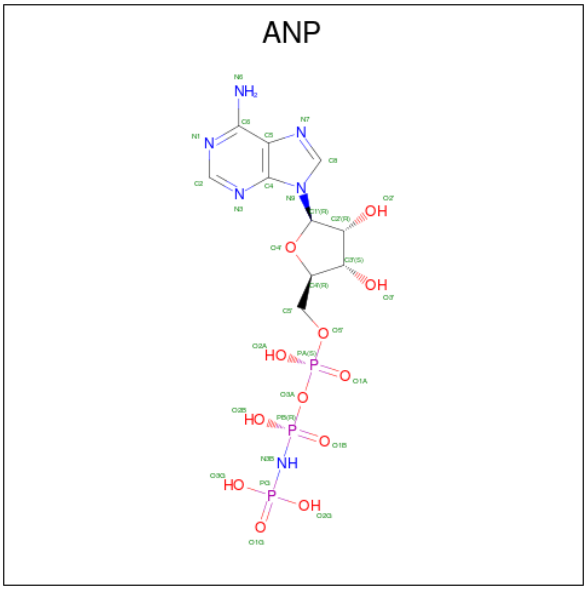
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	S	0
			26	14	6	5	1	

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

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

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

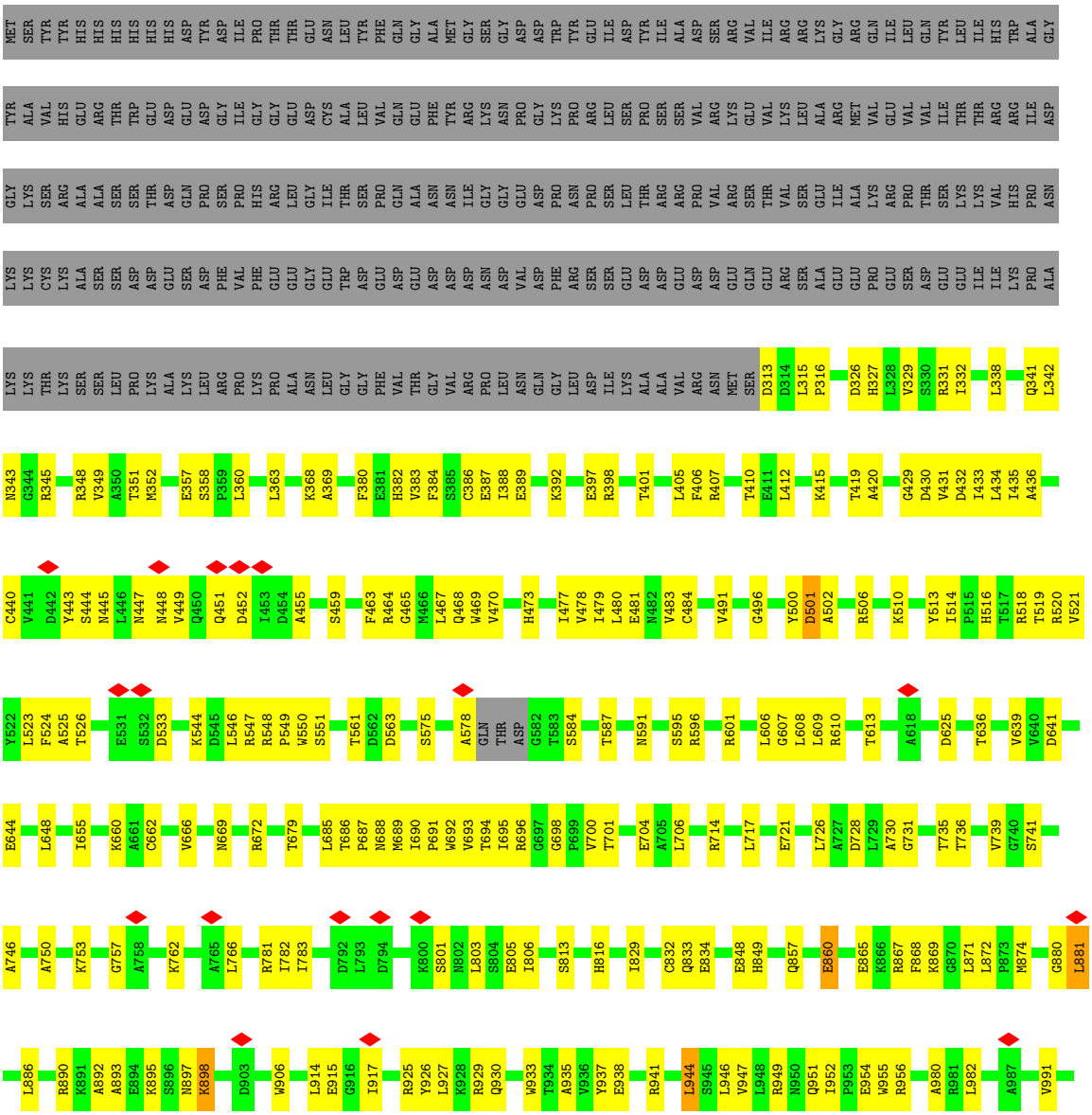
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	

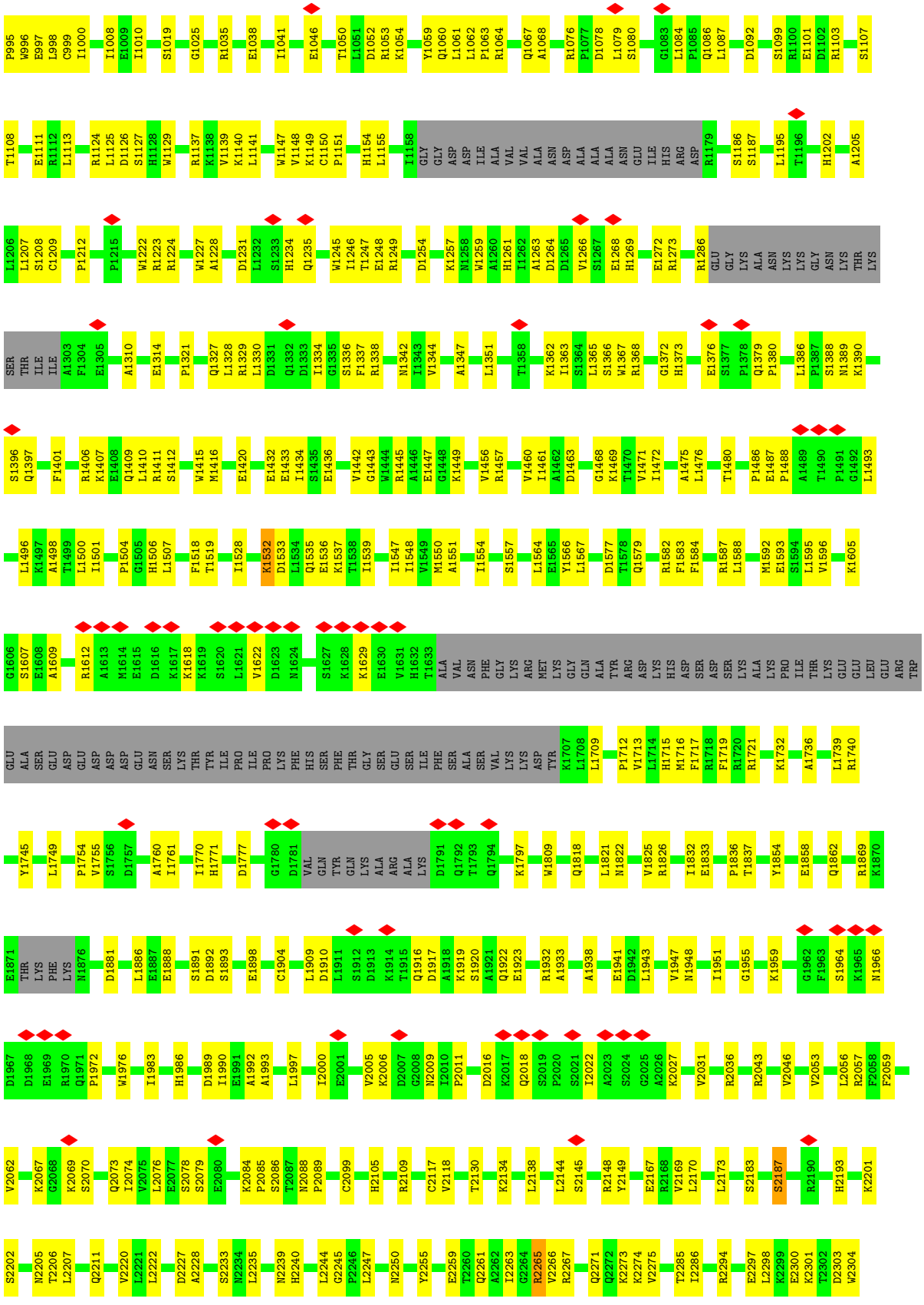
3 Residue-property plots (i)

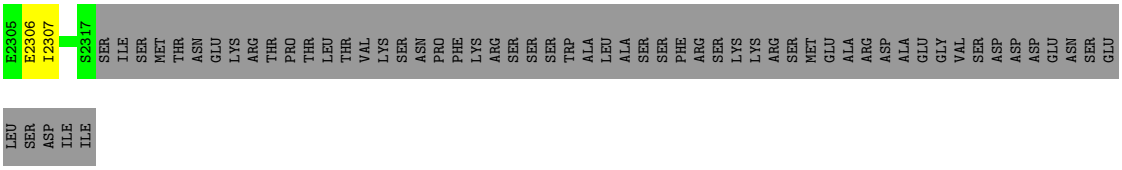
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA repair protein Rad8

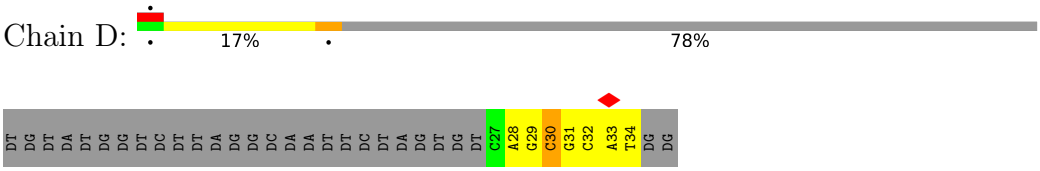
Chain A:



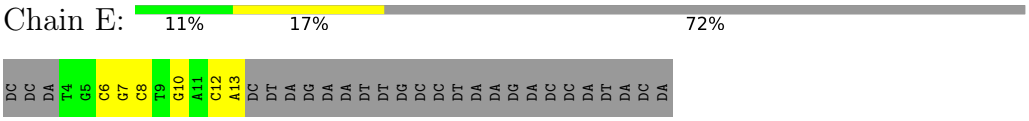

P995 W996 E997 L998 C999 I1000
I1008 E1009 I1010
S1019
G1025
R1035
E1038
I1041
E1046
T1050 L1051 D1052 R1053 K1054
Y1059 Q1060 L1061 L1062 P1063 R1064
Q1067 A1068
R1076 P1077 D1078 L1079 S1080
G1083 L1084 P1085 Q1086 L1087
D1092
S1099 R1100 E1101 D1102 R1103
S1107
T1108
E1111 R1112 L1113
R1124 L1125 D1126 S1127 H1128 W1129
R1137 K1138 V1139 K1140 L1141
W1147 V1148 K1149 C1150 P1151
H1154 L1155
I1158 GLY GLY ASP ASP ILE ALA VAL VAL ALA ASN ASP ALA ALA ALA ASN GLU ILE HIS ARG ASP R1179
S1186 S1187
L1195 T1196
H1202
A1205
L1206 L1207 S1208 C1209
P1212
P1215
W1222 R1223 R1224
W1227 A1228
D1231 L1232 S1233 H1234 Q1235
W1245 I1246 T1247 E1248 R1249
D1254
K1257 N1258 W1259 A1260 H1261 I1262 A1263 D1264 D1265 V1266 S1267 E1268 H1269
E1272 R1273
R1286 GLU GLY LYS ALA ASN LYS LYS GLY ASN LYS THR LYS
SER THR ILE ILE A1303 F1304 E1305
A1310
E1314
P1321
Q1327 L1328 R1329 L1330
D1331 Q1332 D1333 I1334 G1335 S1336 F1337 R1338
N1342 I1343 V1344
A1347
L1351
T1358
K1362 I1363 S1364 L1365 S1366 W1367 R1368
G1372 H1373
E1376 S1377 P1378 Q1379 P1380
L1386 P1387 S1388 N1389 K1390
S1396 Q1397
F1401
R1406 K1407 E1408 Q1409 L1410 R1411 S1412
W1415 M1416
E1420
E1432 E1433 I1434 S1435 E1436
V1442 G1443 W1444 R1445 A1446 E1447 G1448 K1449
V1456 R1457
V1460 I1461 A1462 D1463
G1468 K1469 T1470 V1471 I1472
A1475 L1476
T1480
P1486 E1487 P1488 A1489 T1490 P1491 G1492 L1493
L1496 K1497 A1498 T1499 L1500 I1501
P1504 G1505 H1506 L1507
F1518 T1519
I1528
K1532 D1533 L1534 Q1535 E1536 K1537 T1538 I1539
I1547 I1548 V1549 M1550 A1551
I1554
S1557
L1564 E1565 Y1566 L1567
D1577 T1578 Q1579
R1582 F1583 F1584
R1587 L1588
M1592 E1593 S1594 L1595 V1596
K1605
G1606 S1607 E1608 A1609
R1612 A1613 M1614 E1615 D1616 K1617 K1618 K1619 S1620 L1621 V1622 D1623 N1624
S1627 K1628 K1629 E1630 V1631 H1632 T1633
ALA VAL ASN PHE GLY LYS ARG MET LYS GLY GLN ALA TYR ARG ASP LYS HIS ASP SER ASP SER LYS ALA LYS PRO ILE THR LYS GLU GLU LEU GLU ARG TRP
GLU ALA SER GLU ASP GLU ASP ASP ASP GLU ASN SER LYS THR TYR ILE PRO ILE PRO LYS PHE HIS SER PHE THR GLY SER GLU SER ILE PHE SER ALA SER VAL LYS LYS ASP TYR K1707 L1708 L1709
P1712 V1713 L1714 H1715 M1716 F1717 R1718 F1719 R1720 R1721
K1732
A1736
L1739 R1740
Y1745
L1749
P1754 V1755 S1756 D1757
A1760 I1761
I1770 H1771
D1777
G1780 D1781 VAL GLN TYR GLN LYS ALA ARG ALA LYS D1791 Q1792 T1793 Q1794
K1797
W1809
Q1818
L1821 N1822
V1825 R1826
I1832 E1833
P1836 T1837
Y1854
E1858
Q1862
R1869
K1870
E1871 THR LYS PHE LYS N1876
D1881
L1886 E1887 E1888
S1891 D1892 S1893
E1898
C1904
L1909 D1910 L1911 S1912 D1913 K1914 T1915 Q1916 D1917 A1918 K1919 S1920 A1921 Q1922 E1923
R1932 A1933
A1938
E1941 D1942 L1943
V1947 N1948
I1951
G1955
K1959
G1962 F1963 S1964 K1965 N1966
D1967 D1968 E1969 R1970 Q1971 P1972
W1976
I1983
H1986
D1989 I1990 E1991 A1992 A1993
L1997
I2000 E2001
V2005 K2006 D2007 G2008 N2009 I2010 P2011
D2016 K2017 Q2018 S2019 P2020 S2021 I2022 A2023 S2024 G2025 A2026 K2027
V2031
R2036
R2043
V2046
V2053
L2056 R2057 F2058 F2059
V2062
K2067 G2068 K2069 S2070
Q2073 I2074 V2075 L2076 E2077 S2078 S2079 E2080
K2084 P2085 S2086 T2087 N2088 P2089
C2099
H2105
R2109
C2117 V2118
T2130
K2134
L2138
L2144 S2145
R2148 Y2149
E2167 R2168 V2169 L2170
L2173
S2183
S2187
R2190
H2193
K2201
S2202
N2205 T2206 L2207
Q2211
V2220 L2221 L2222
D2227 A2228
S2233 N2234 L2235
N2239 H2240
L2244 G2245 P2246 L2247
N2250
Y2255
E2259 T2260 Q2261 A2262 I2263 G2264 R2265 V2266 R2267
Q2271 Q2272 K2273 K2274 V2275
T2285 I2286
R2294
E2297 L2298 K2299 E2300 K2301 T2302 D2303 W2304



• Molecule 2: DNA (5'-D(P*CP*AP*GP*(5CM)P*GP*CP*AP*T)-3')



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



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23621	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	47262	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	272.384, 272.384, 272.384	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 5CM, ANP, SAH

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	0.38	0/15111	0.50	0/20456
2	D	0.55	0/160	0.85	0/242
3	E	0.64	0/225	0.87	0/346
All	All	0.39	0/15496	0.52	0/21044

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	14810	0	14758	434	0
2	D	164	0	92	12	0
3	E	201	0	111	7	0
4	A	26	0	19	5	0
5	A	5	0	0	0	0
6	A	31	0	13	2	0
7	A	1	0	0	0	0
All	All	15238	0	14993	446	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 15.

The worst 5 of 446 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:1379:GLN:HG3	1:A:1380:PRO:HD3	1.54	0.87
1:A:2265:ARG:HG2	1:A:2265:ARG:HH21	1.40	0.84
1:A:636:THR:HG21	2:D:28:DA:H5'	1.61	0.83
1:A:2265:ARG:HG2	1:A:2265:ARG:NH2	1.98	0.79
1:A:880:GLY:HA3	1:A:917:ILE:HD11	1.64	0.78

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	1866/2348 (80%)	1622 (87%)	244 (13%)	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	1607/2015 (80%)	1596 (99%)	11 (1%)	84	93

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1532	LYS
1	A	1797	LYS
1	A	2265	ARG
1	A	2187	SER
1	A	930	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1879	GLN
1	A	2101	HIS
1	A	2038	GLN
1	A	2211	GLN
1	A	1342	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5CM	D	30	2,3	17,21,22	1.01	2 (11%)	24,30,33	1.33	2 (8%)

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
2	5CM	D	30	2,3	-	2/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	30	5CM	C6-C5	2.84	1.39	1.34
2	D	30	5CM	C6-N1	-2.20	1.34	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	30	5CM	C5-C6-N1	-3.58	119.66	123.34
2	D	30	5CM	C5-C4-N3	-2.50	118.98	121.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	30	5CM	C3'-C4'-C5'-O5'
2	D	30	5CM	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	30	5CM	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SAH	A	2401	-	24,28,28	0.66	0	25,40,40	0.66	0
6	ANP	A	2407	7	29,33,33	1.20	5 (17%)	31,52,52	1.07	4 (12%)

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
4	SAH	A	2401	-	-	8/11/31/31	0/3/3/3
6	ANP	A	2407	7	-	6/14/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2407	ANP	PG-O1G	3.20	1.51	1.46
6	A	2407	ANP	PB-O1B	2.97	1.50	1.46
6	A	2407	ANP	PB-O2B	-2.21	1.50	1.56
6	A	2407	ANP	PG-O3G	-2.04	1.51	1.56
6	A	2407	ANP	PG-O2G	-2.03	1.51	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2407	ANP	O2B-PB-O1B	4.08	118.48	109.92
6	A	2407	ANP	C5-C6-N6	2.07	123.49	120.35
6	A	2407	ANP	O3G-PG-O1G	-2.02	108.37	113.45
6	A	2407	ANP	O2G-PG-O1G	-2.01	108.41	113.45

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2401	SAH	N-CA-CB-CG
4	A	2401	SAH	C-CA-CB-CG
4	A	2401	SAH	O4'-C4'-C5'-SD
4	A	2401	SAH	C3'-C4'-C5'-SD
6	A	2407	ANP	C5'-O5'-PA-O2A

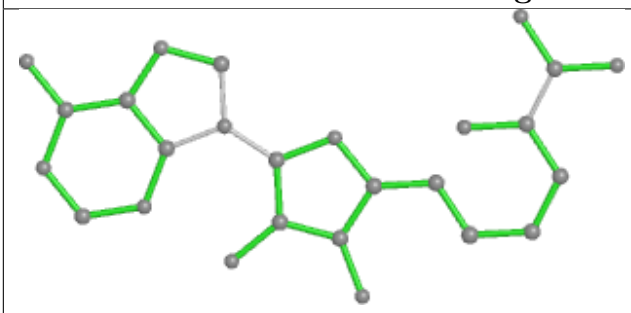
There are no ring outliers.

2 monomers are involved in 7 short contacts:

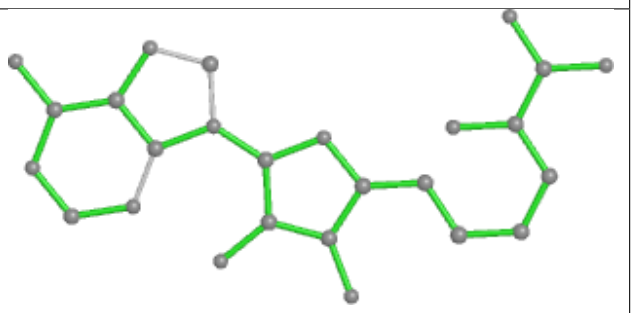
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2401	SAH	5	0
6	A	2407	ANP	2	0

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.

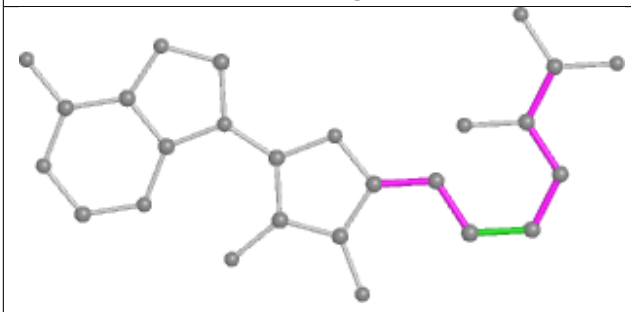
Ligand SAH A 2401



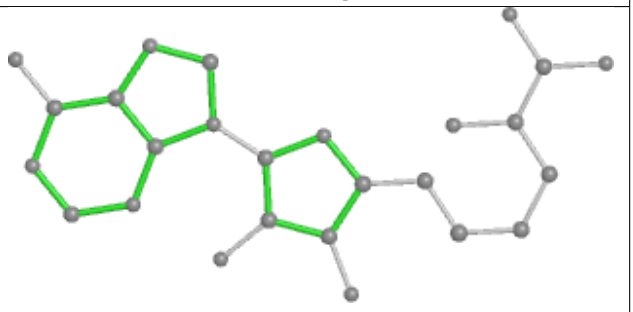
Bond lengths



Bond angles

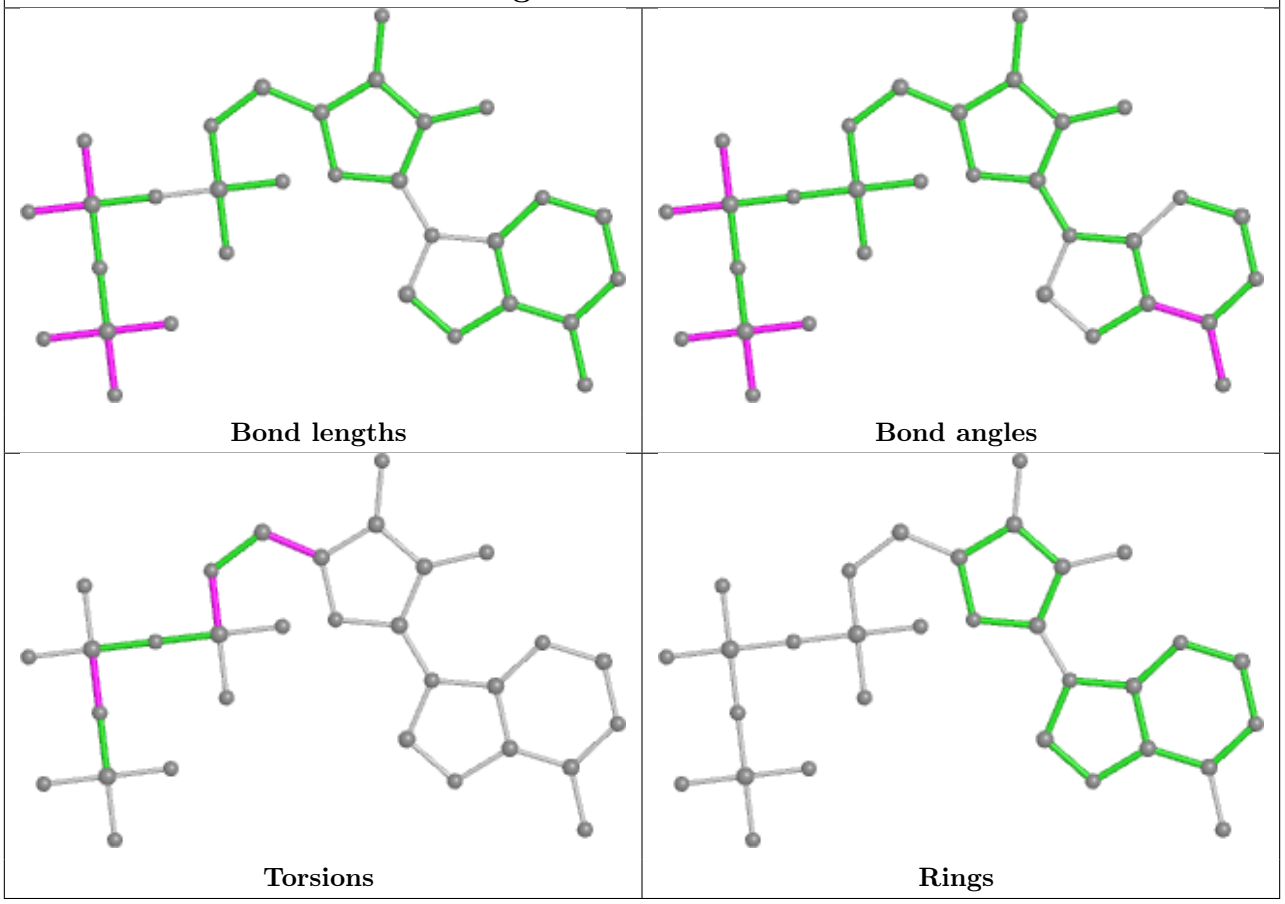


Torsions



Rings

Ligand ANP A 2407



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.

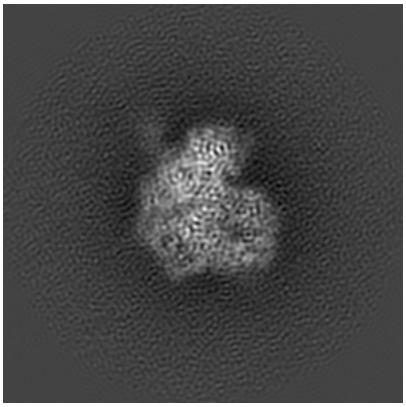
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24295. These allow visual inspection of the internal detail of the map and identification of artifacts.

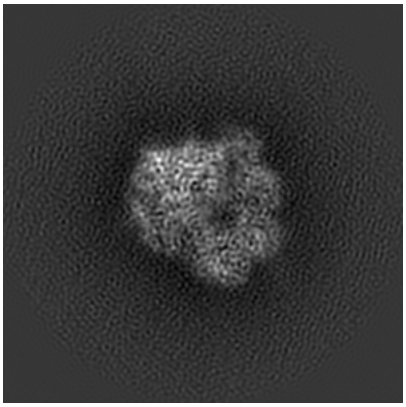
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

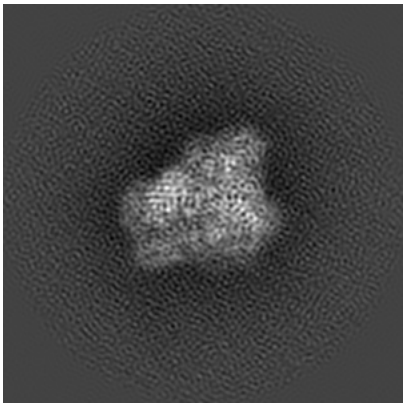
6.1.1 Primary map



X



Y

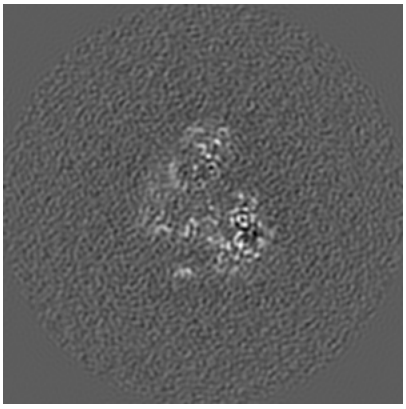


Z

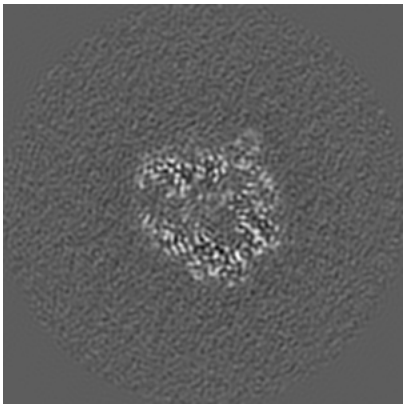
The images above show the map projected in three orthogonal directions.

6.2 Central slices

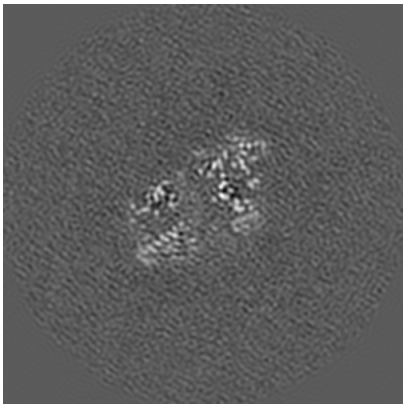
6.2.1 Primary map



X Index: 128



Y Index: 128

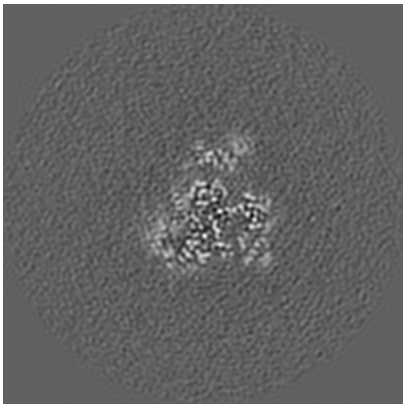


Z Index: 128

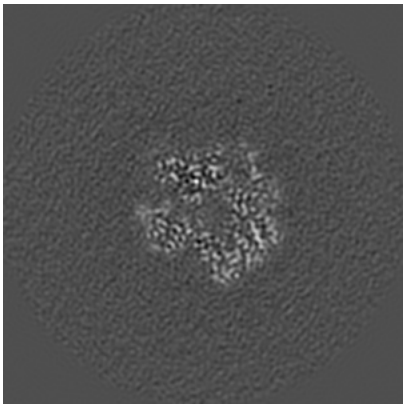
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

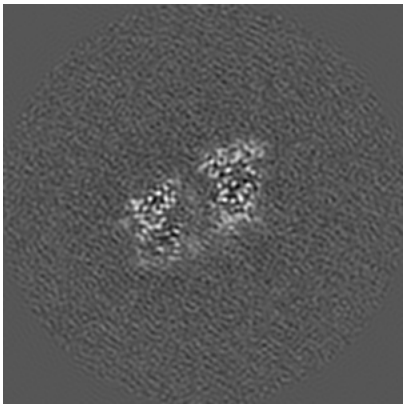
6.3.1 Primary map



X Index: 149



Y Index: 133

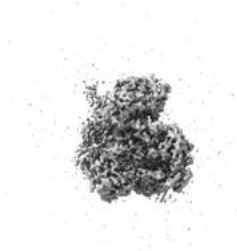


Z Index: 132

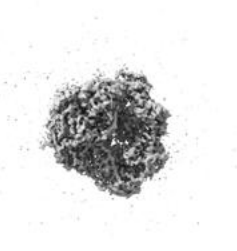
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

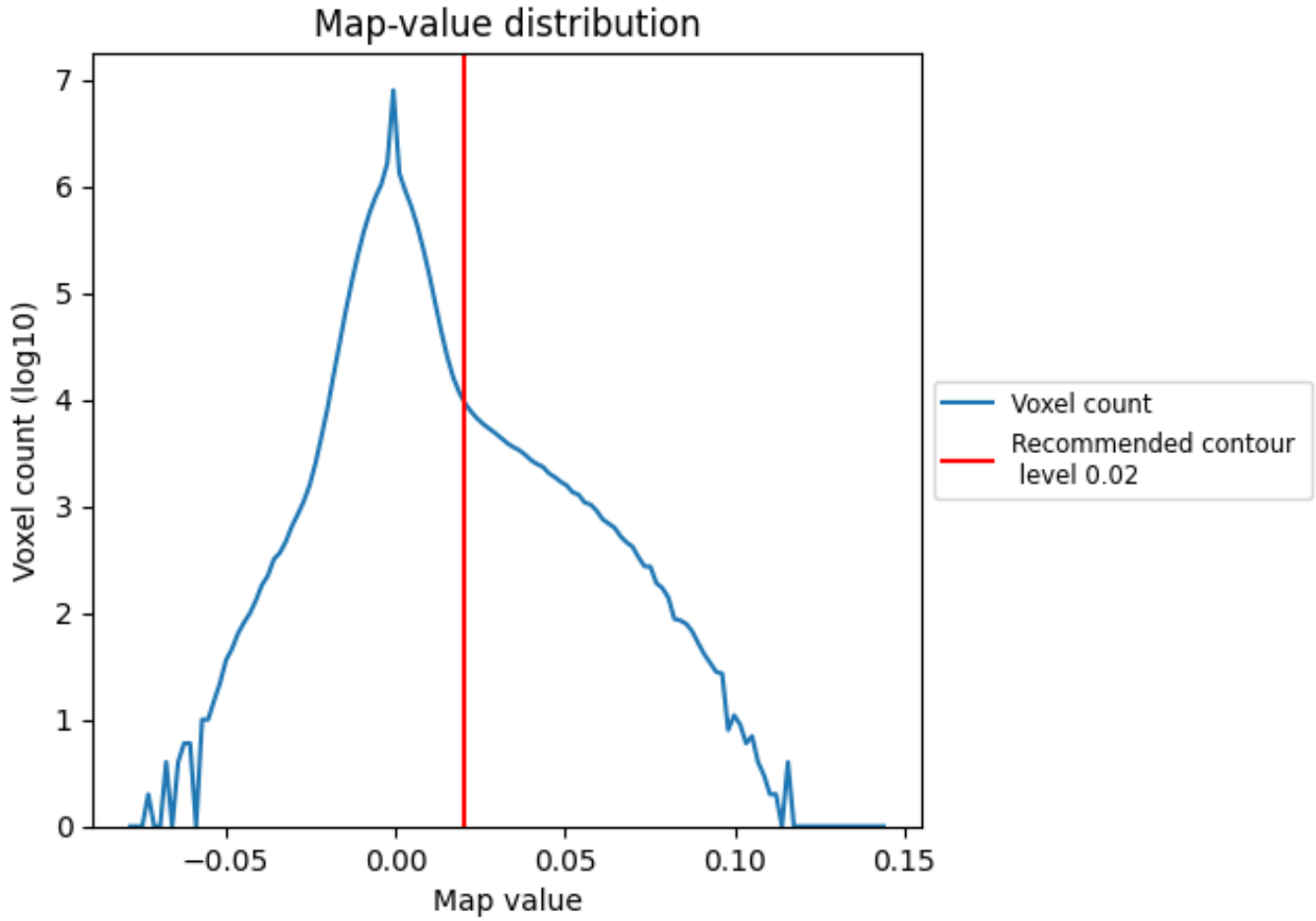
6.5 Mask visualisation (i)

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

7 Map analysis

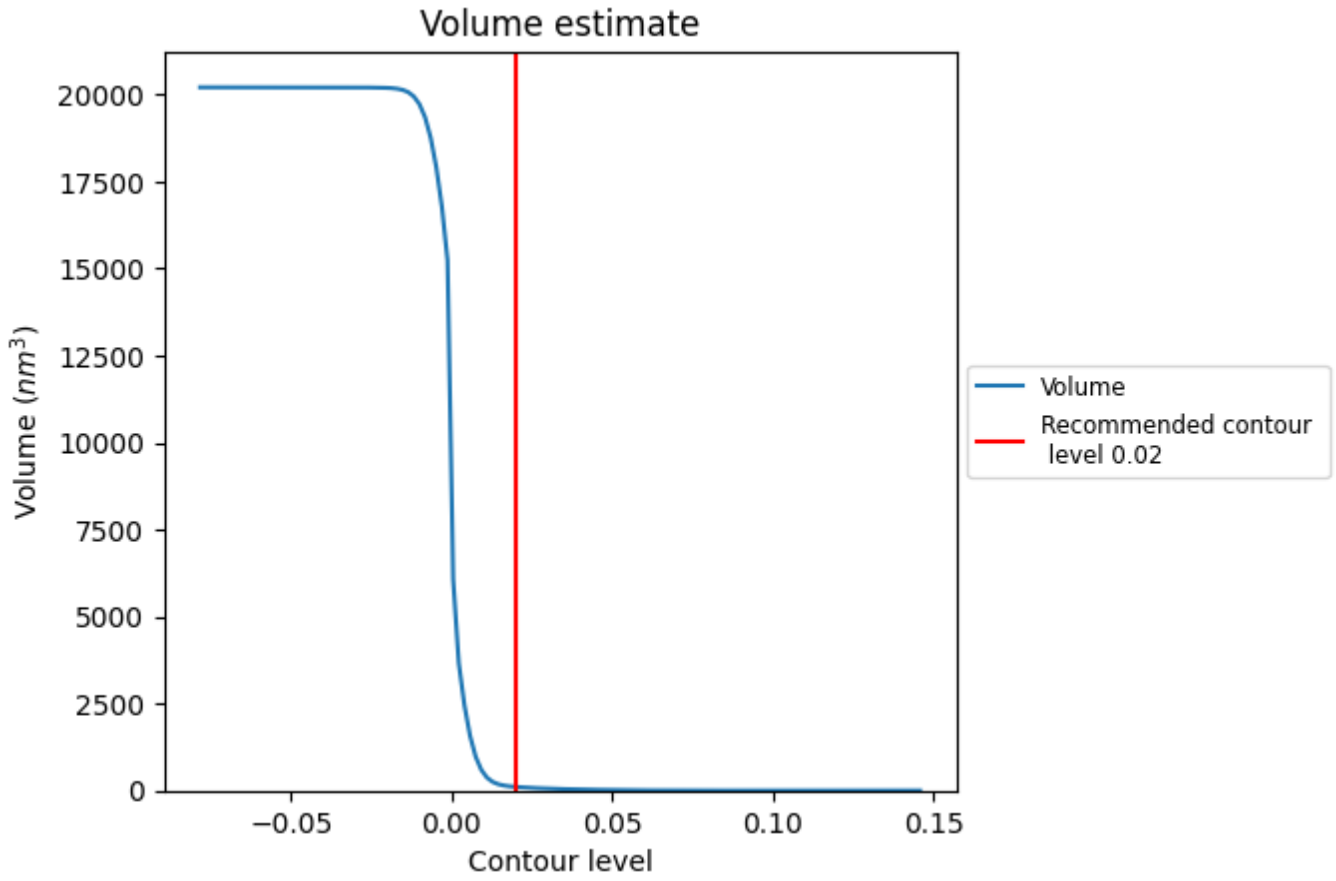
This section contains the results of statistical analysis of the map.

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.

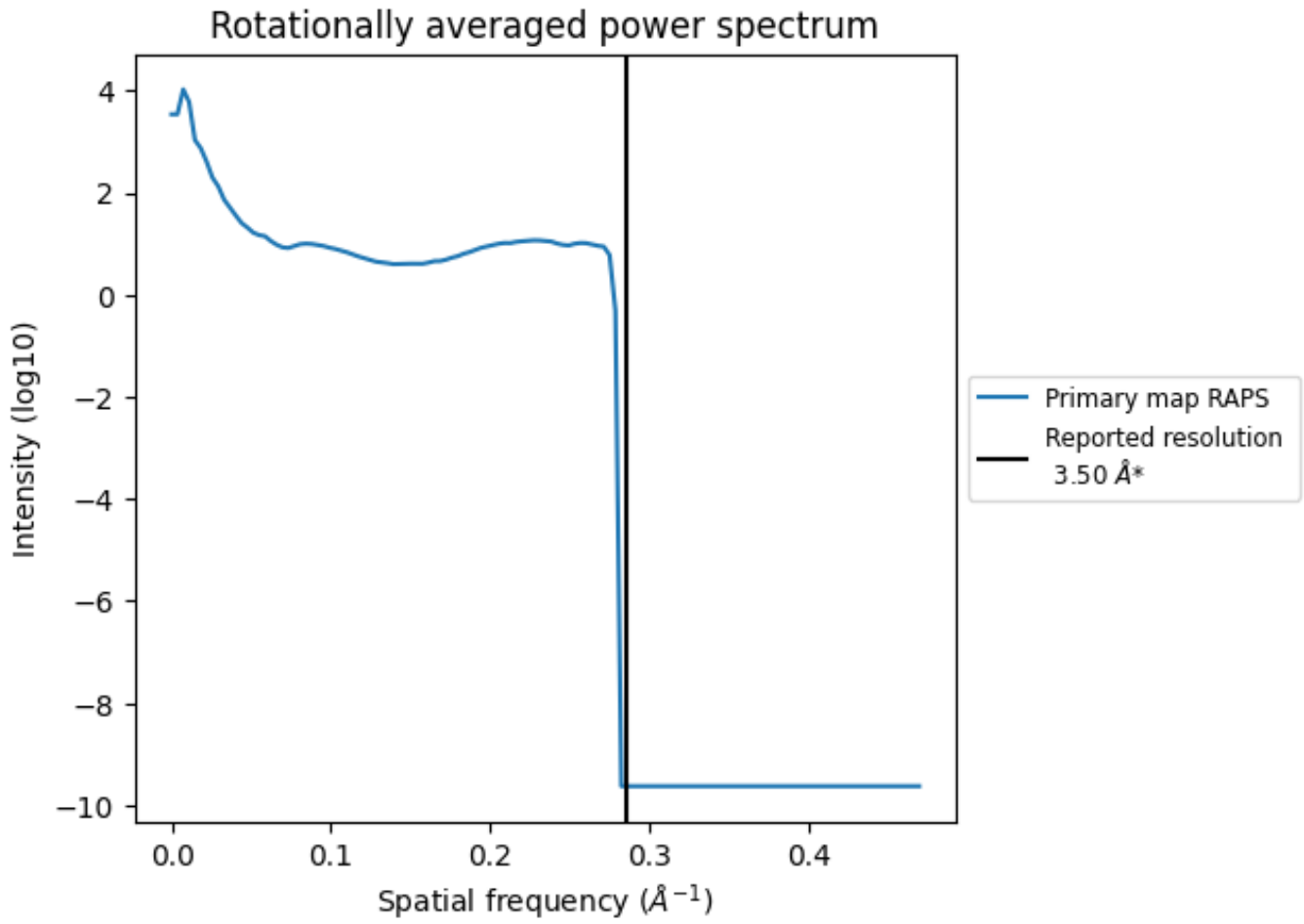
7.2 Volume estimate (i)



The volume at the recommended contour level is 105 nm^3; this corresponds to an approximate mass of 95 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 0.286 Å^{-1}

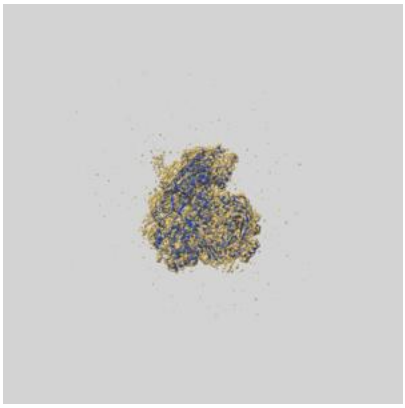
8 Fourier-Shell correlation

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

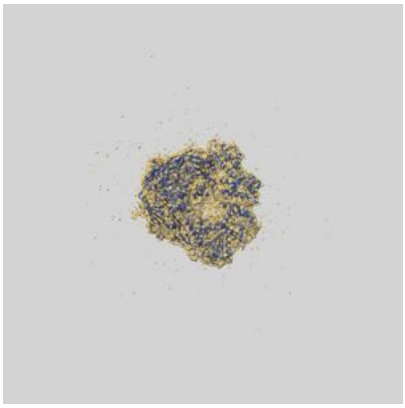
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24295 and PDB model 7R78. Per-residue inclusion information can be found in section 3 on page 6.

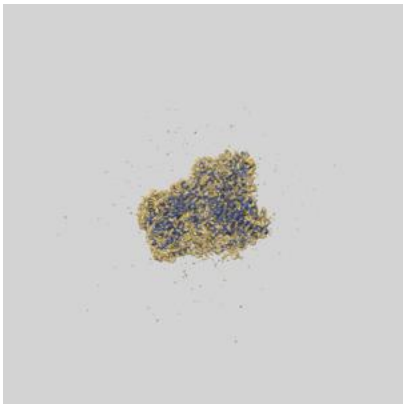
9.1 Map-model overlay



X



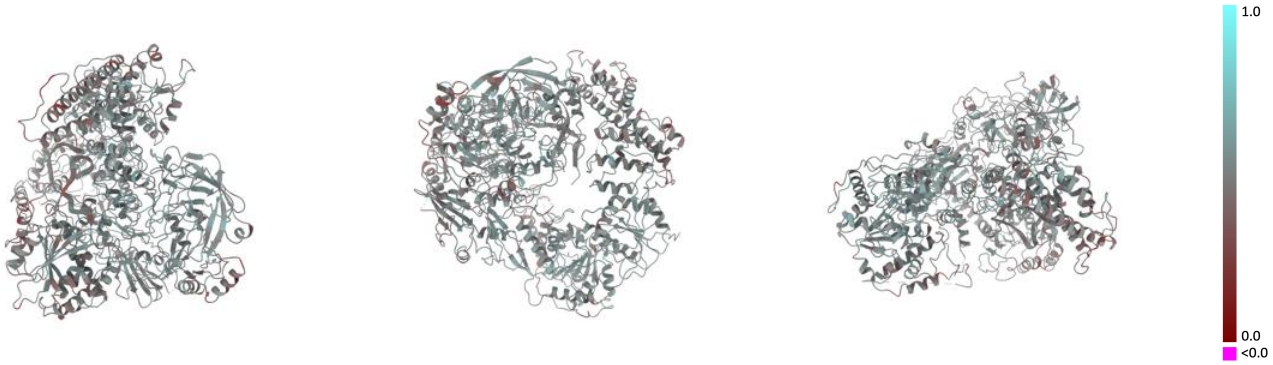
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

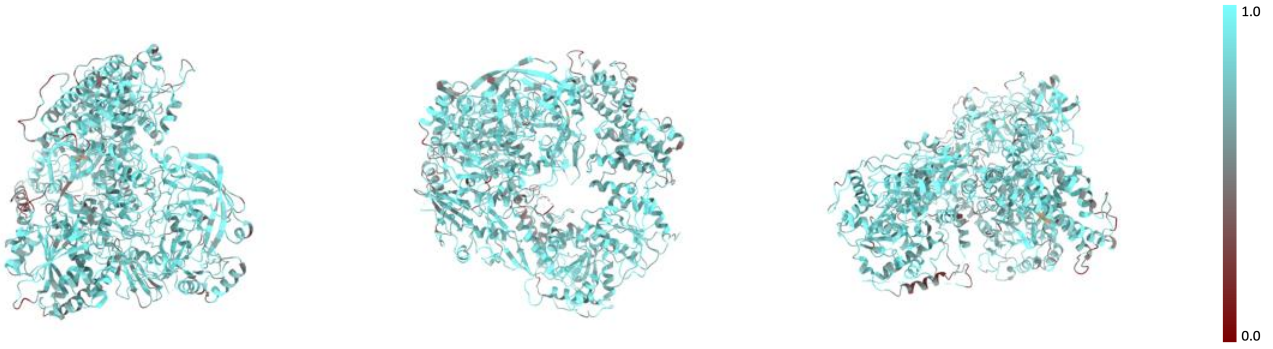
9.2 Q-score mapped to coordinate model (i)



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.

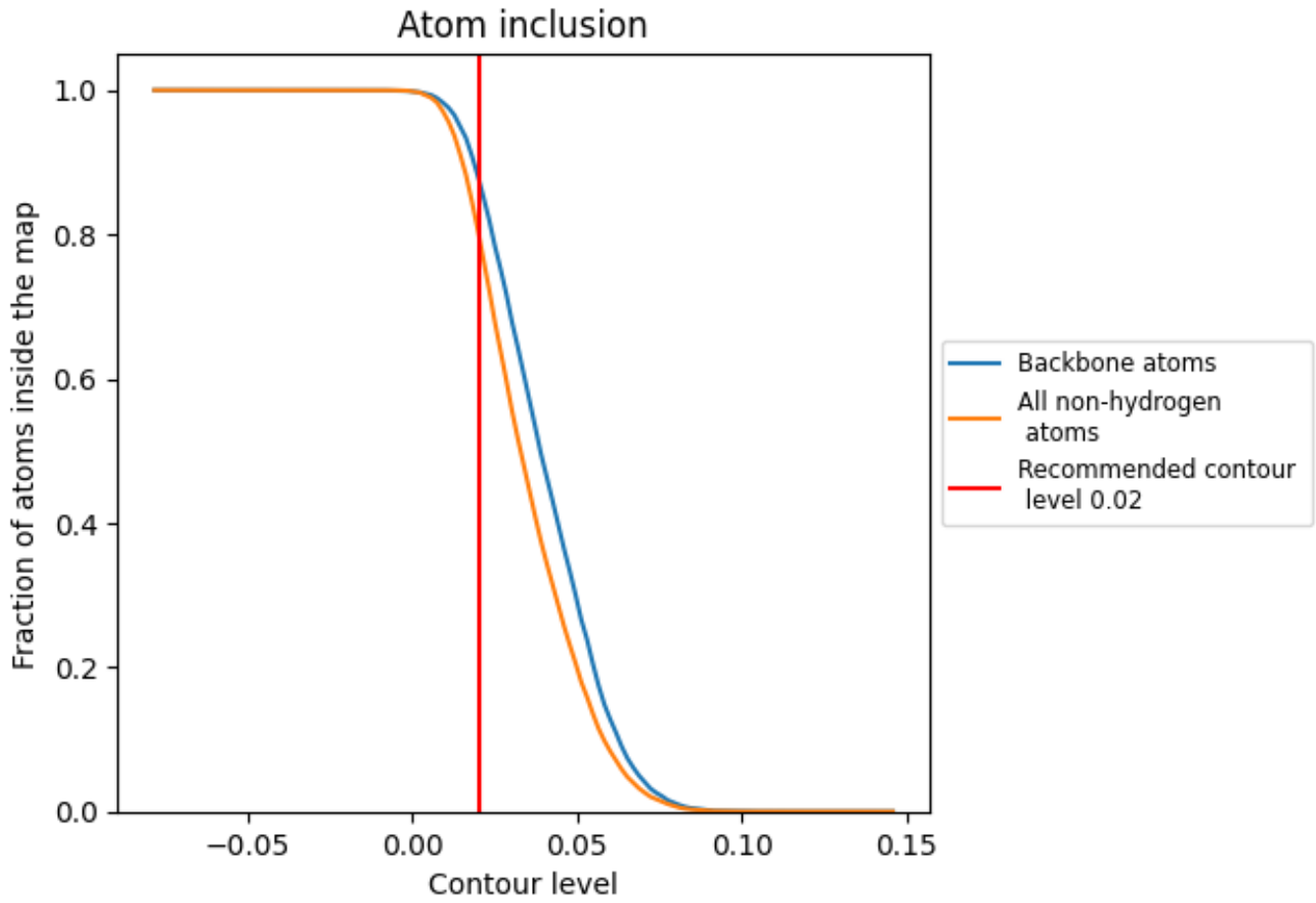
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8032	0.4980
A	0.8029	0.4990
D	0.7866	0.4410
E	0.8358	0.4690