wwPDB EM Validation Summary Report (i)

Sep 16, 2026 – 02:35 PM EDT

PDB ID	:	8G6X / pdb_00008g6x
EMDB ID	:	EMD-29787
Title	:	Structure of WT E.coli ribosome 50S subunit with complexed with mRNA, P-site fMet-NH-tRNAfMet and A-site meta-aminobenzoic acid charged NH-tRNAPhe
Authors	:	Majumdar, C.; Cate, J.H.D.
Deposited on	:	2023-02-16
Resolution	:	2.31 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

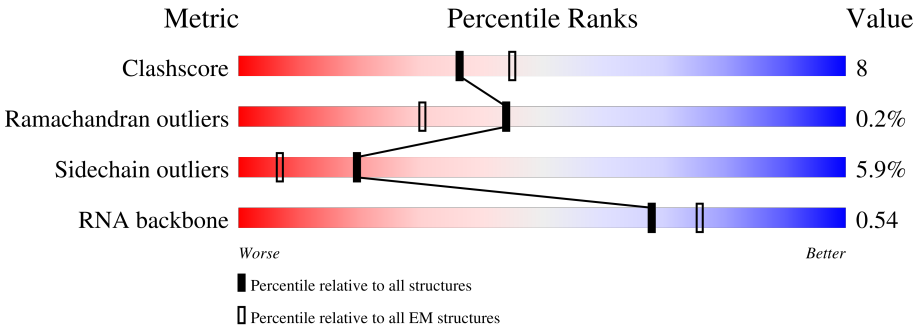
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

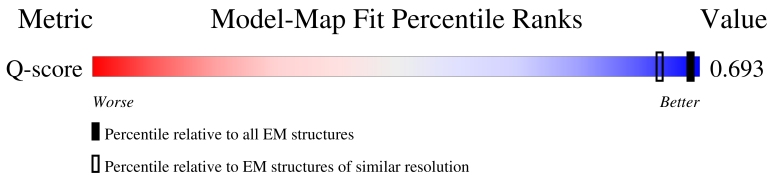
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 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.





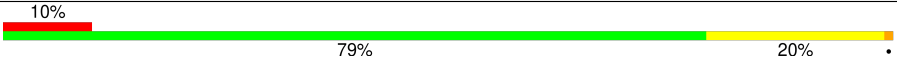
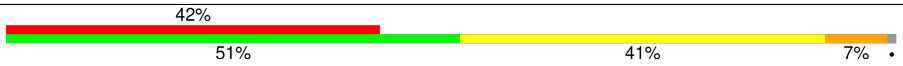
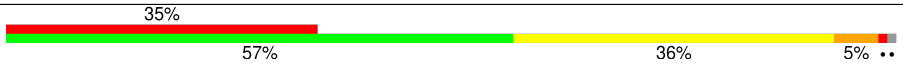
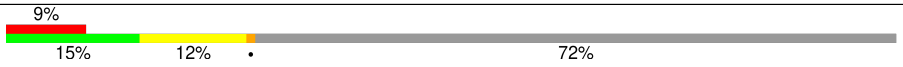
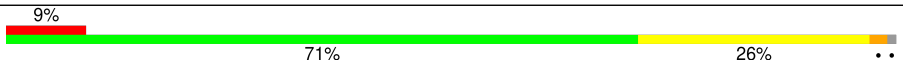
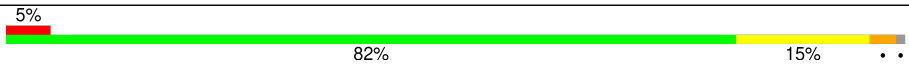
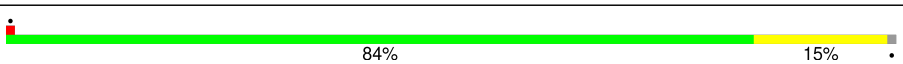
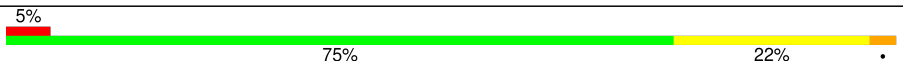
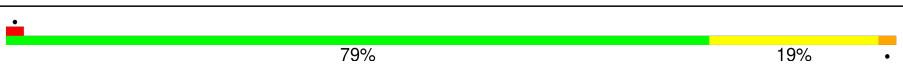
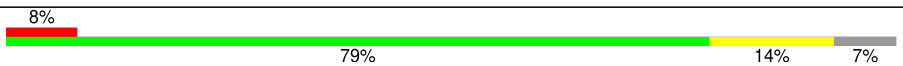
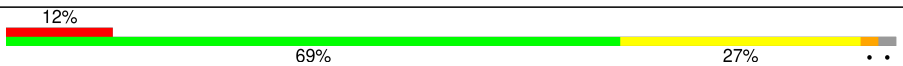
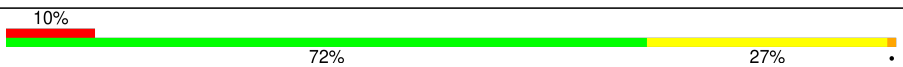
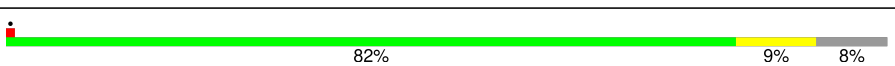
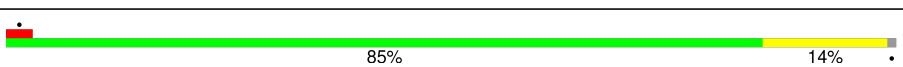
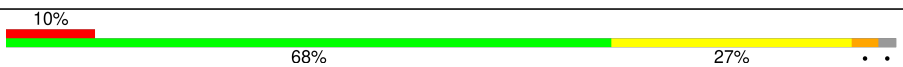
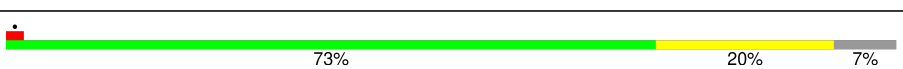
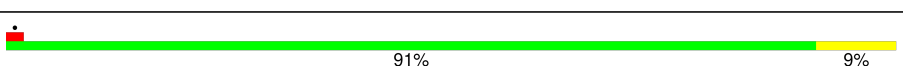
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4306 (1.81 - 2.81)

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	2904	5% 59% 31% 5% 5%
2	b	120	7% 62% 31% 6%
3	c	273	88% 11%

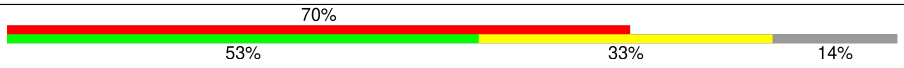
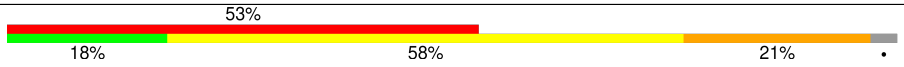
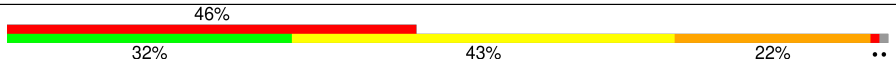
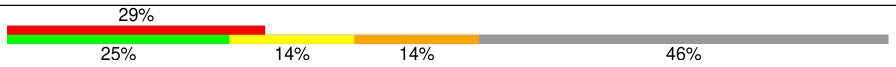
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	d	209	
5	e	201	
6	f	179	
7	g	177	
8	h	149	
9	i	142	
10	j	123	
11	k	144	
12	l	136	
13	m	127	
14	n	117	
15	o	115	
16	p	118	
17	q	103	
18	r	110	
19	s	100	
20	t	104	
21	u	94	
22	v	85	
23	w	78	
24	x	63	
25	y	59	
26	z	57	
27	0	55	
28	1	46	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	2	65	
30	3	38	
31	4	70	
32	Y	76	
33	Z	76	
34	X	28	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	SPD	a	6216	-	-	X	-

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 93873 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	2753	59130	26384	10897	19096	2753	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	b	119	2549	1135	466	829	119	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	271	2082	1288	423	364	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	209	1566	980	288	294	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	201	1552	974	283	290	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	177	1410	899	249	256	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	n	116	Total 892	C 552	N 178	O 162	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	114	Total 917	C 574	N 179	O 163	S 1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	p	117	Total 947	C 604	N 192	O 151	0	0

- Molecule 17 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	103	Total 816	C 516	N 153	O 145	S 2	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	110	Total 857	C 532	N 166	O 156	S 3	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	93	Total 738	C 466	N 139	O 131	S 2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	t	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 32 is a RNA chain called A-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	74	Total	C	N	O	P	0	0
			1578	705	285	515	73		

- Molecule 33 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	75	Total	C	N	O	P	0	0
			1601	713	289	524	75		

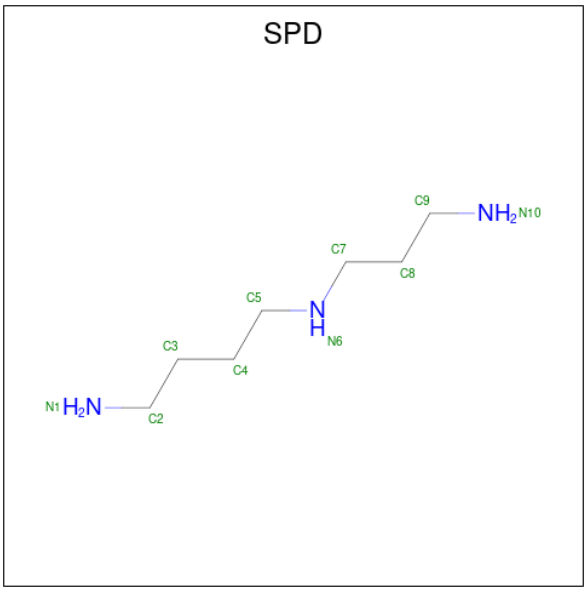
- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	X	15	Total	C	N	O	P	0	0
			317	143	56	103	15		

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
35	a	211	Total Mg 211 211	0
35	b	5	Total Mg 5 5	0
35	c	2	Total Mg 2 2	0
35	d	1	Total Mg 1 1	0
35	m	1	Total Mg 1 1	0
35	z	1	Total Mg 1 1	0
35	Y	1	Total Mg 1 1	0
35	Z	1	Total Mg 1 1	0

- Molecule 36 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



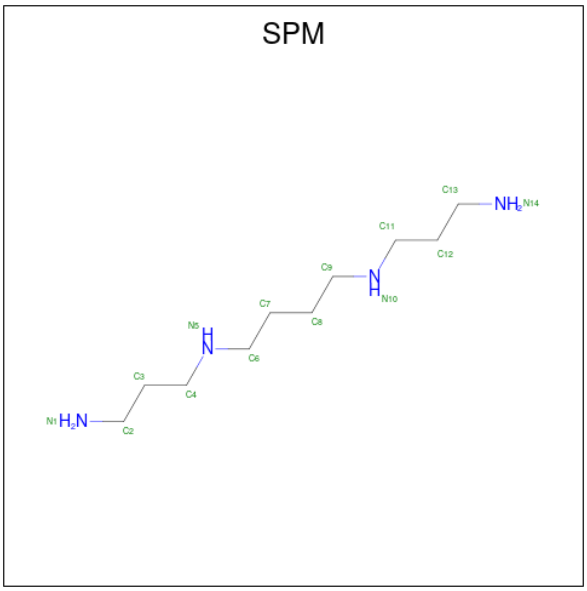
Mol	Chain	Residues	Atoms	AltConf
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0
36	a	1	Total C N 10 7 3	0

- Molecule 37 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).

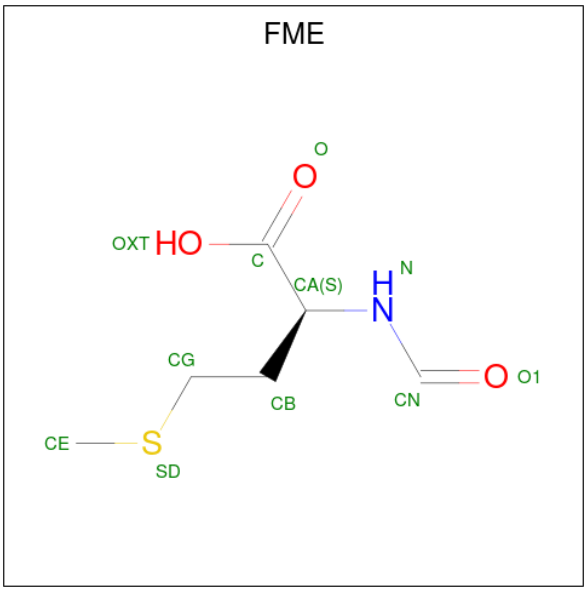


Mol	Chain	Residues	Atoms	AltConf
37	a	1	Total C N 14 10 4	0

- Molecule 38 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
38	a	5	Total K 5 5	0
38	c	1	Total K 1 1	0
38	e	1	Total K 1 1	0

- Molecule 39 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).

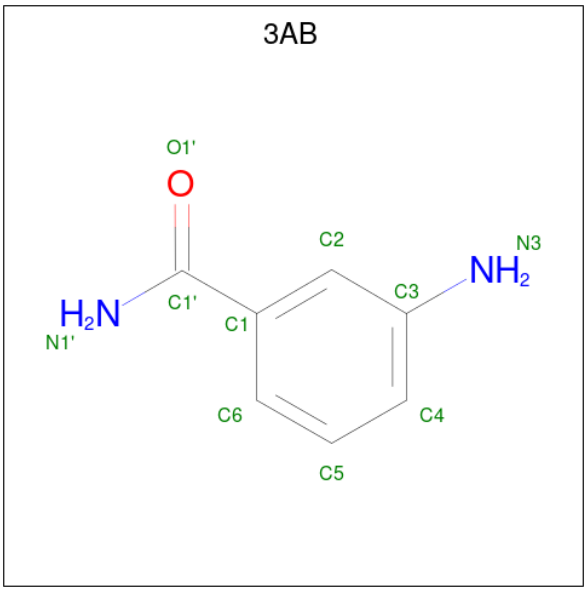


Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

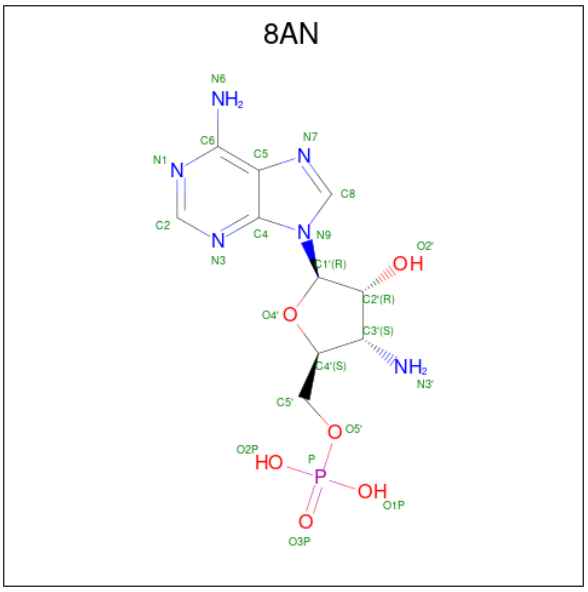
Mol	Chain	Residues	Atoms		AltConf
40	3	1	Total	Zn	0
			1	1	
40	4	1	Total	Zn	0
			1	1	

- Molecule 41 is 3-aminobenzamide (CCD ID: 3AB) (formula: $C_7H_8N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
41	Y	1	20	14	4	2	1

- Molecule 42 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (CCD ID: 8AN) (formula: $C_{10}H_{15}N_6O_6P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
42	Z	1	22	10	6	5	1	0

- Molecule 43 is water.

Mol	Chain	Residues	Atoms	AltConf
43	a	3013	Total O 3013 3013	0
43	b	40	Total O 40 40	0
43	c	86	Total O 86 86	0
43	d	33	Total O 33 33	0
43	e	27	Total O 27 27	0
43	h	1	Total O 1 1	0
43	i	12	Total O 12 12	0
43	j	12	Total O 12 12	0
43	k	32	Total O 32 32	0
43	l	20	Total O 20 20	0
43	m	20	Total O 20 20	0
43	o	10	Total O 10 10	0
43	p	19	Total O 19 19	0
43	q	14	Total O 14 14	0
43	r	24	Total O 24 24	0
43	s	5	Total O 5 5	0
43	t	1	Total O 1 1	0
43	u	3	Total O 3 3	0
43	v	12	Total O 12 12	0
43	w	9	Total O 9 9	0
43	x	1	Total O 1 1	0
43	y	1	Total O 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
43	z	21	Total O 21 21	0
43	1	17	Total O 17 17	0
43	2	24	Total O 24 24	0
43	3	3	Total O 3 3	0
43	Z	2	Total O 2 2	0

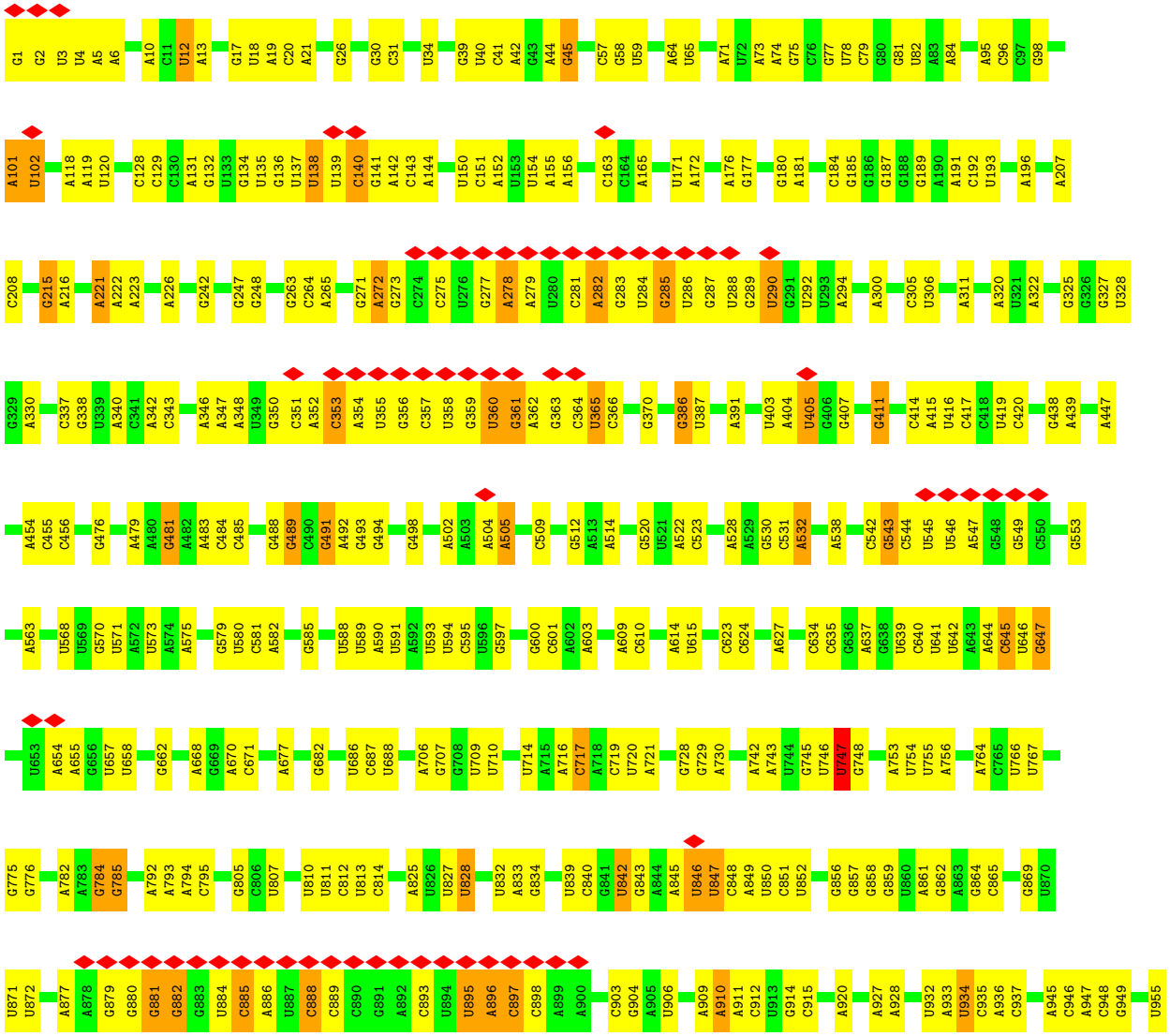
3 Residue-property plots (i)

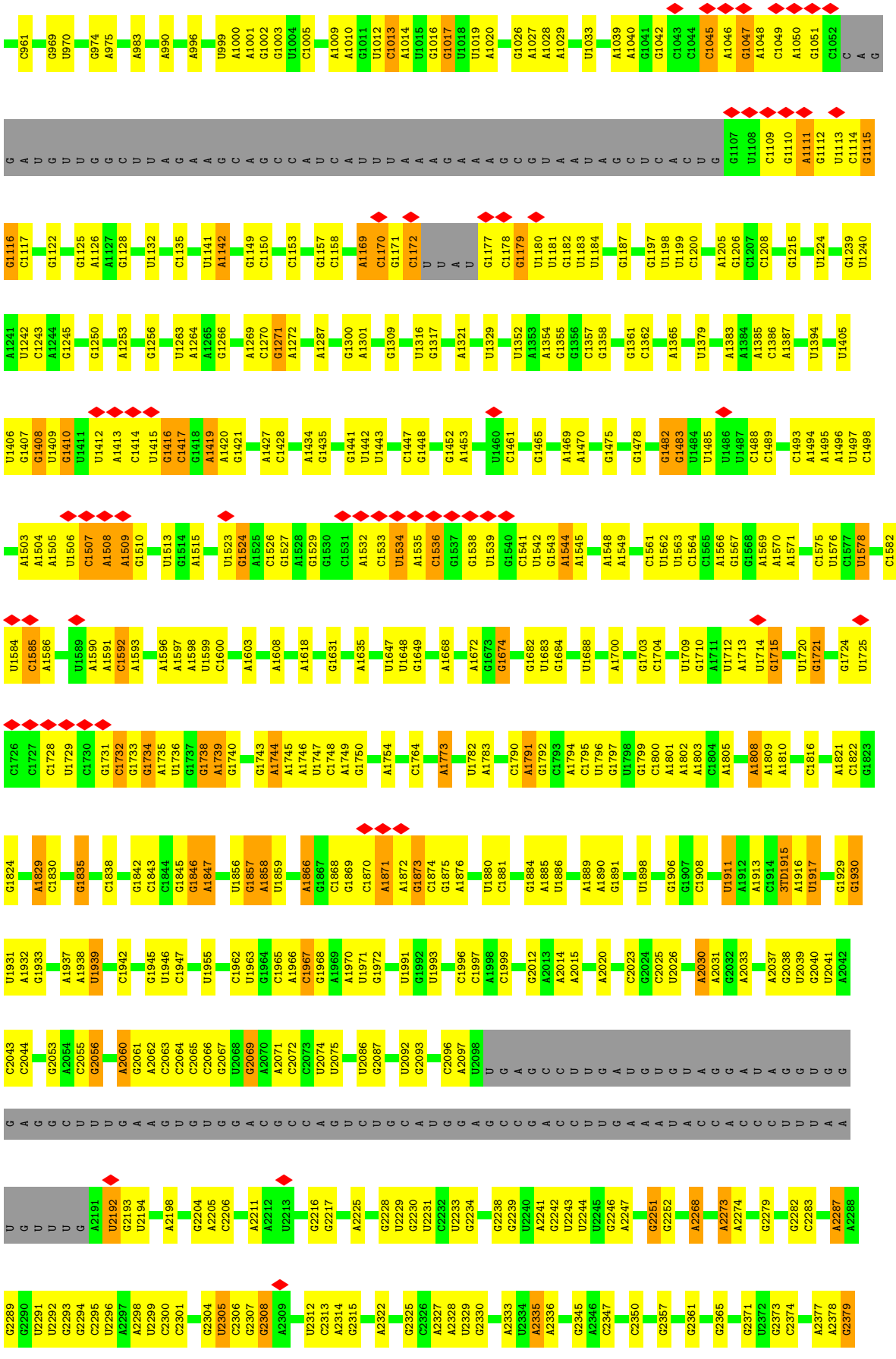
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

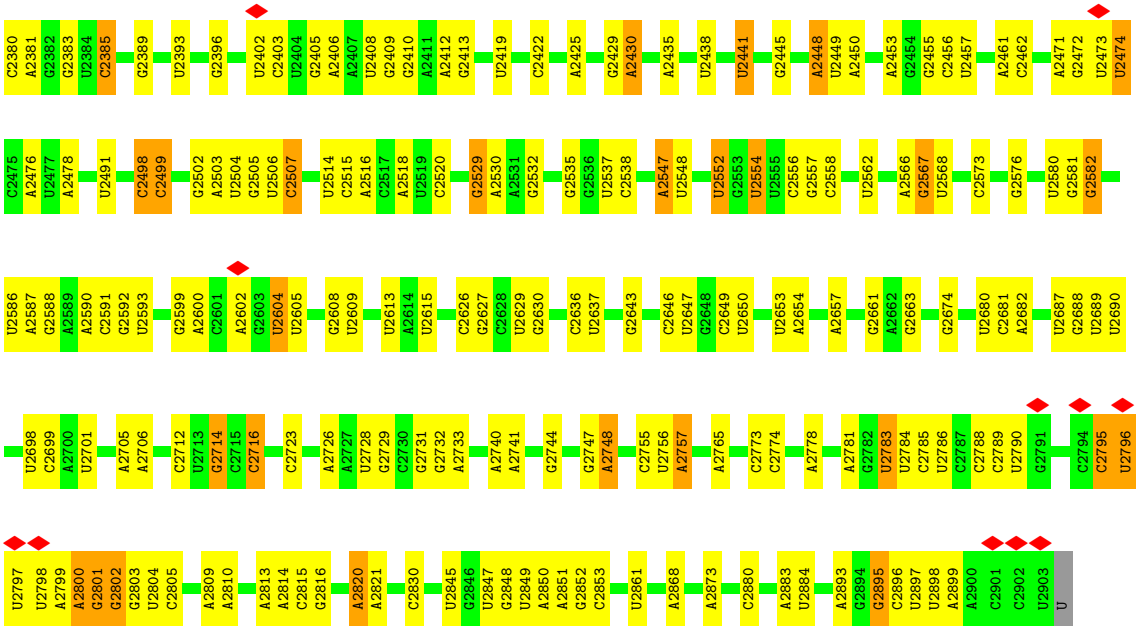
- Molecule 1: 23S rRNA

Chain a:





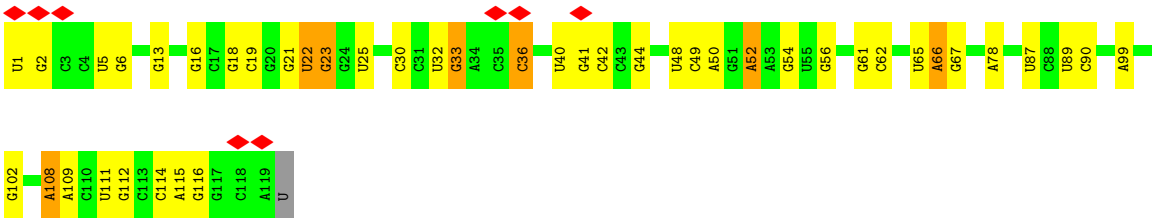

C961 G969 U970 G974 A975 A983 A990 A996 U999 A1000 A1001 G1002 G1003 U1004 C1005 A1009 A1010 G1011 U1012 C1013 A1014 U1015 G1016 G1017 U1018 U1019 A1020 G1026 A1027 A1028 A1029 U1033 A1039 A1040 G1041 G1042 C1043 C1044 C1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C A G
G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115
G1116 C1117 G1122 G1125 A1126 A1127 G1128 U1132 C1135 U1141 A1142 C1149 C1150 C1153 G1157 C1158 A1169 C1170 G1171 C1172 U U A U G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1187 G1197 U1198 U1199 C1200 A1205 G1206 C1207 C1208 G1215 U1224 G1239 U1240
A1241 U1242 C1243 A1244 G1245 G1250 A1253 G1256 U1263 A1264 A1265 G1266 A1269 C1270 G1271 A1272 A1287 G1300 A1301 G1309 U1316 G1317 A1321 U1329 U1352 A1353 A1354 G1355 G1356 C1357 C1358 G1361 C1362 A1365 U1379 A1383 A1384 A1385 C1386 A1387 U1394 U1405
U1406 G1407 G1408 U1409 G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 G1421 A1427 C1428 A1434 G1435 G1441 U1442 U1443 C1447 G1448 G1452 A1453 U1460 C1461 G1465 A1469 A1470 G1475 G1478 G1482 G1483 U1484 U1485 U1486 U1487 C1488 C1489 C1493 A1494 A1495 A1496 U1497 C1498
A1503 A1504 A1505 U1506 C1507 A1508 A1509 G1510 U1513 G1514 A1515 U1523 G1524 A1525 C1526 G1527 A1528 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1544 A1545 A1548 A1549 C1561 U1562 U1563 C1564 C1565 A1566 G1567 G1568 A1569 A1570 A1571 C1575 U1576 C1577 U1578 C1582 A1583
U1584 C1585 A1586 U1589 A1590 A1591 C1592 A1593 A1596 A1597 A1598 U1599 C1600 A1603 A1608 A1618 G1631 A1635 U1647 U1648 G1649 A1668 A1672 G1673 G1674 G1682 U1683 C1684 A1688 A1700 G1703 C1704 U1709 G1710 A1711 U1712 A1713 U1714 G1715 U1720 G1721 G1724 U1725
C1726 C1727 C1728 U1729 C1730 G1731 C1732 G1733 G1734 A1735 U1736 G1737 G1738 A1739 G1740 G1743 A1744 A1745 A1746 U1747 C1748 A1749 G1750 A1754 C1764 A1773 U1782 A1783 C1790 A1791 G1792 C1793 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 C1804 A1805 A1808 A1809 A1810 C1816 A1821 C1822 G1823
G1824 A1829 C1830 G1835 C1838 G1842 C1843 C1844 G1845 G1846 A1847 U1856 G1857 A1858 U1859 A1866 G1867 C1868 G1869 C1870 A1871 A1872 G1873 C1874 G1875 A1876 U1880 C1881 G1884 A1885 U1886 A1889 A1890 G1891 U1898 G1906 G1907 C1908 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 G1929 G1930
U1931 A1932 G1933 A1937 A1938 U1939 C1942 G1945 U1946 C1947 U1955 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 U1971 G1972 U1991 G1992 U1993 C1996 C1997 A1998 C1999 G2012 A2013 A2014 A2015 A2020 C2023 G2024 C2025 U2026 A2030 A2031 G2032 A2033 A2037 G2038 U2039 G2040 U2041 A2042
C2043 C2044 G2053 A2054 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 A2070 A2071 C2072 C2073 U2074 U2075 U2086 G2087 U2092 G2093 C2096 A2097 U2098 U G A G C A C C U U G A U G G U G U A A C A C G A A C C A U G G G U U G A
G A A G G C U U U G A A A G U G C A A G U C U C C A C C C A G U C C U G G A A C C A G G G C C U G G G A A A
U G G U U U U G A2191 U2192 G2193 U2194 A2198 G2204 A2205 C2206 A2211 A2212 U2213 G2216 G2217 A2225 G2228 U2229 G2230 U2231 C2232 U2233 G2234 G2238 G2239 U2240 A2241 G2242 U2243 U2244 U2245 G2246 A2247 G2251 G2252 A2268 A2273 A2274 G2279 G2282 C2283 A2287 A2288
G2289 G2290 U2291 U2292 G2293 G2294 C2295 U2296 A2297 A2298 U2299 C2300 C2301 G2304 U2305 C2306 G2307 G2308 A2309 U2312 C2313 A2314 G2315 A2322 G2325 C2326 A2327 A2328 U2329 G2330 A2333 U2334 A2335 A2336 G2345 A2346 C2347 C2350 G2357 G2361 G2365 G2371 U2372 G2373 C2374 A2377 A2378 G2379



• Molecule 2: 5S rRNA

Chain b:

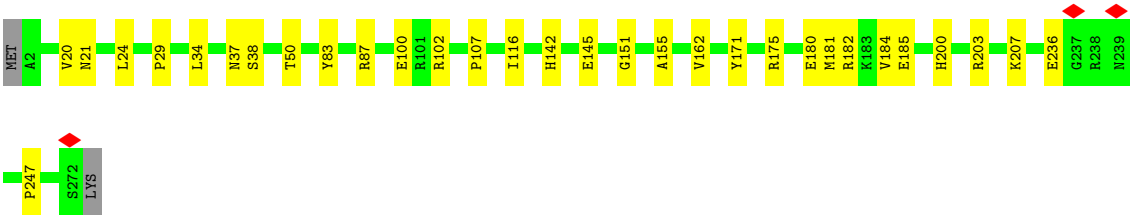




• Molecule 3: 50S ribosomal protein L2

Chain c:



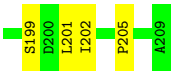


• Molecule 4: 50S ribosomal protein L3

Chain d:



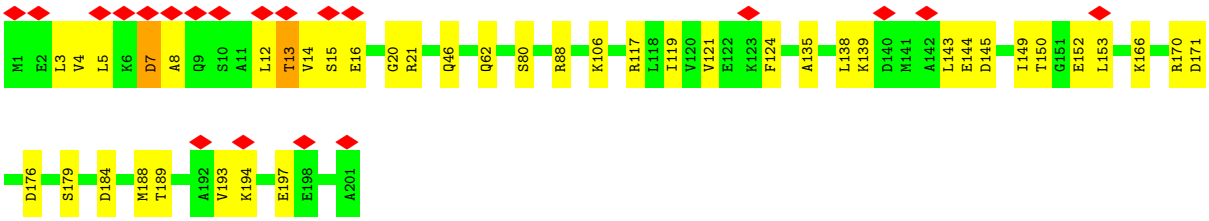




• Molecule 5: 50S ribosomal protein L4

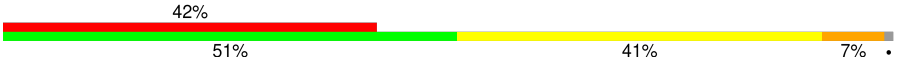
Chain e:

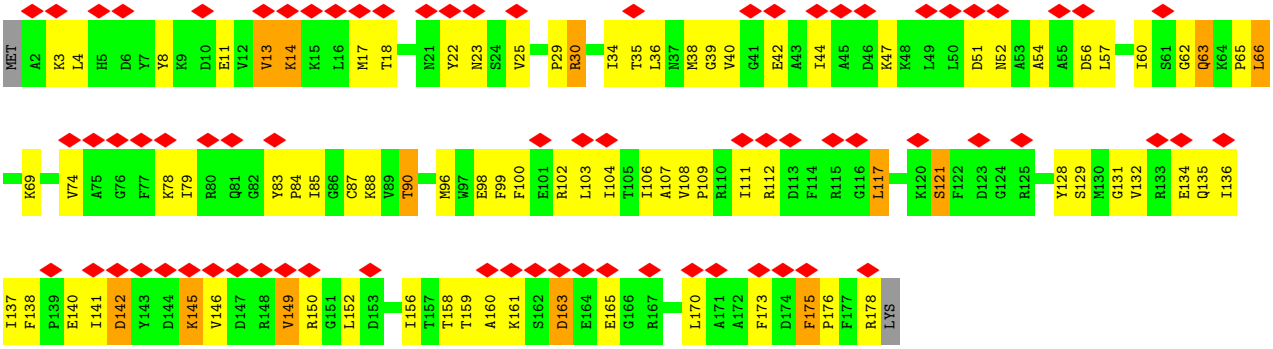




• Molecule 6: 50S ribosomal protein L5

Chain f:

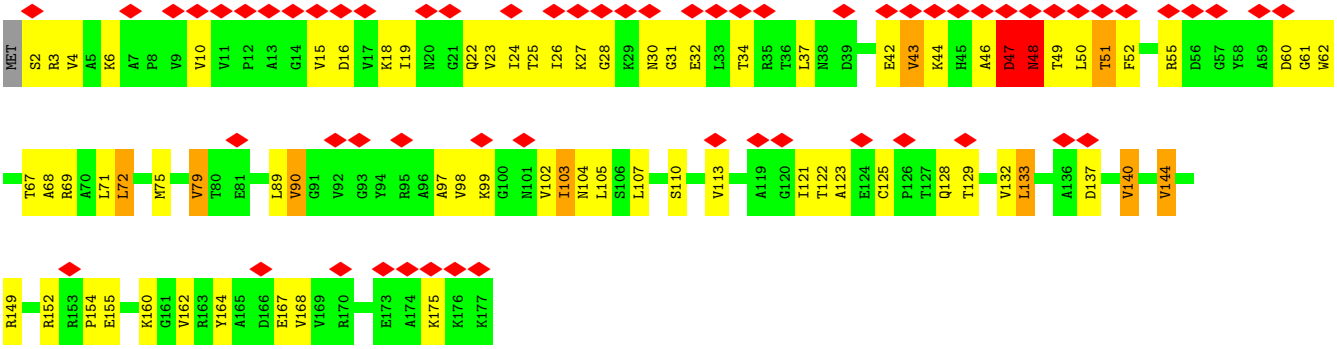




• Molecule 7: 50S ribosomal protein L6

Chain g:

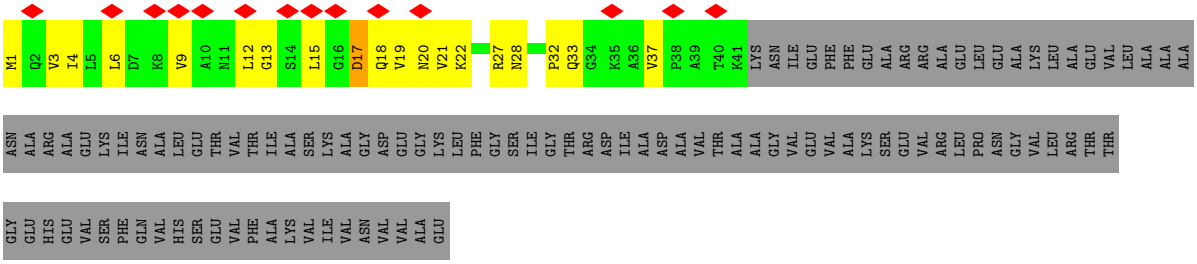




• Molecule 8: 50S ribosomal protein L9

Chain h:

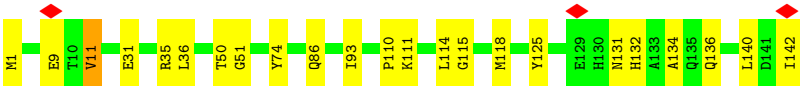




• Molecule 9: 50S ribosomal protein L13

Chain i:

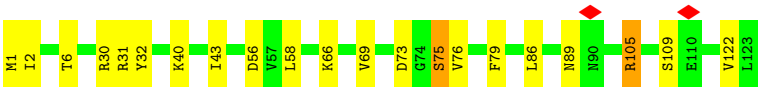




• Molecule 10: 50S ribosomal protein L14

Chain j:

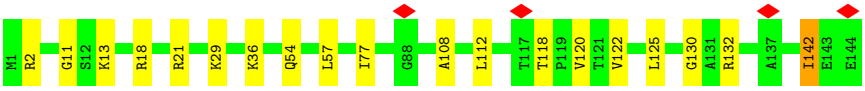




• Molecule 11: 50S ribosomal protein L15

Chain k:

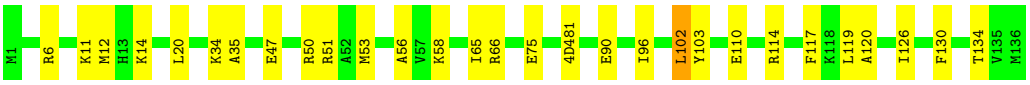




• Molecule 12: 50S ribosomal protein L16

Chain l:





• Molecule 13: 50S ribosomal protein L17

Chain m:

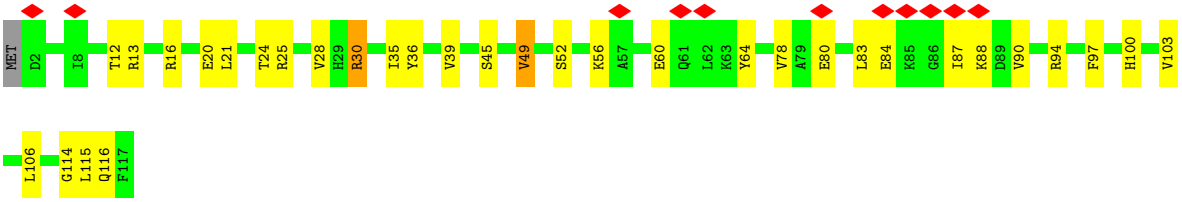




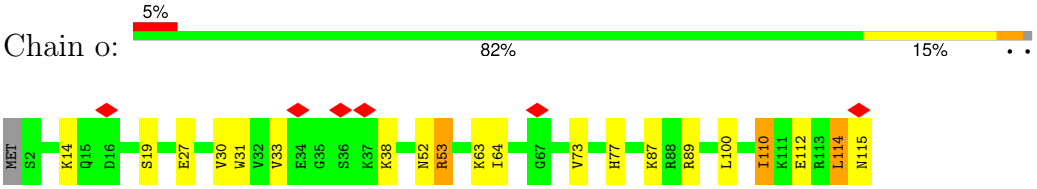
• Molecule 14: 50S ribosomal protein L18

Chain n:

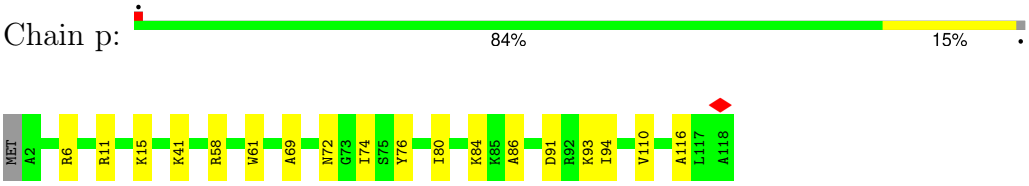




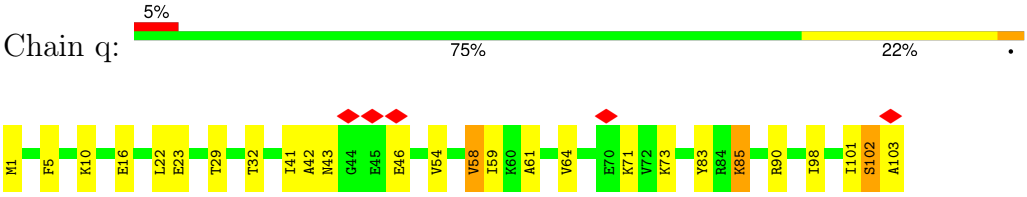
• Molecule 15: 50S ribosomal protein L19



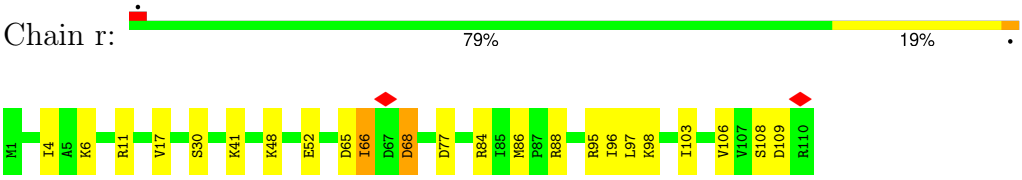
• Molecule 16: 50S ribosomal protein L20



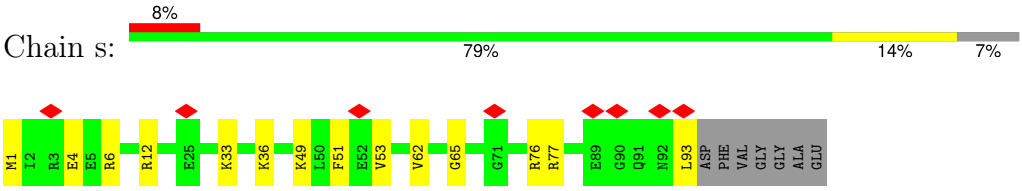
• Molecule 17: Ribosomal protein L21



• Molecule 18: 50S ribosomal protein L22

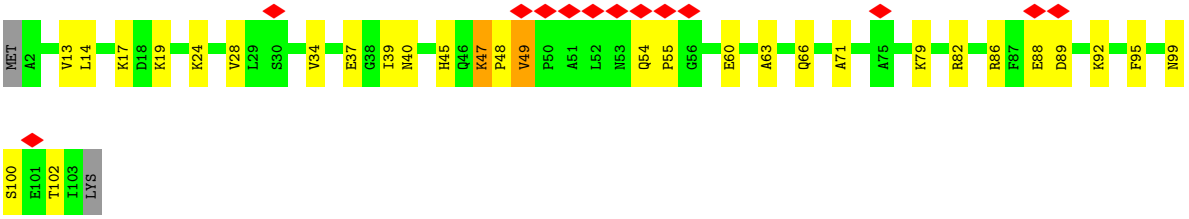


• Molecule 19: 50S ribosomal protein L23

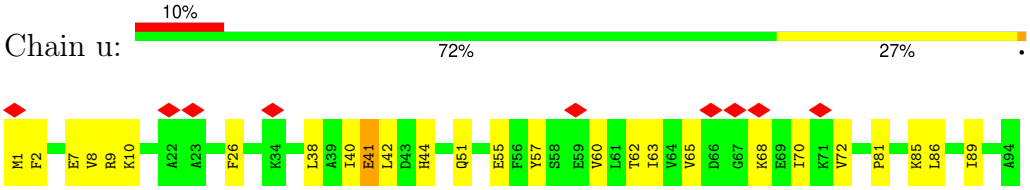


• Molecule 20: 50S ribosomal protein L24

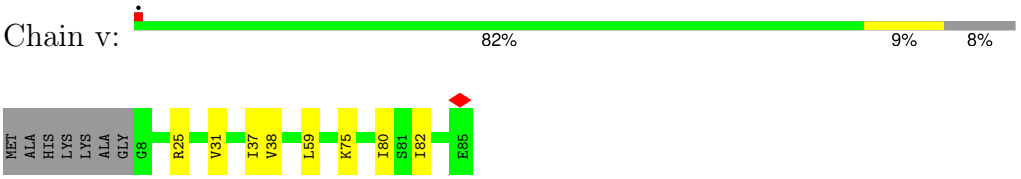




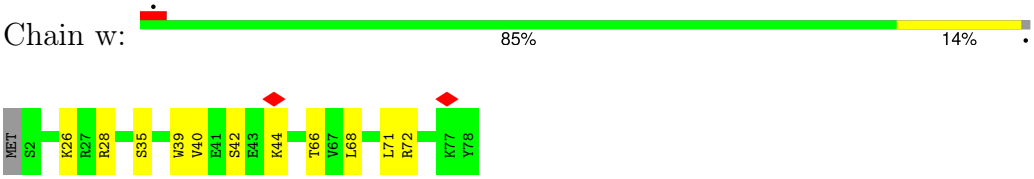
• Molecule 21: 50S ribosomal protein L25



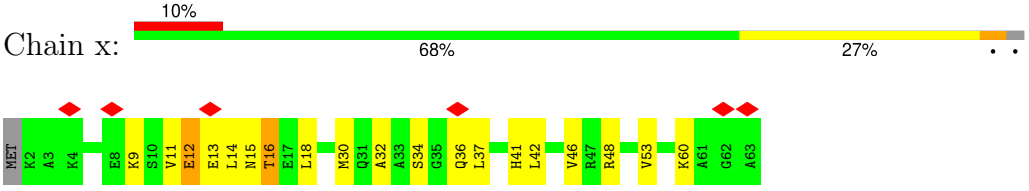
• Molecule 22: 50S ribosomal protein L27



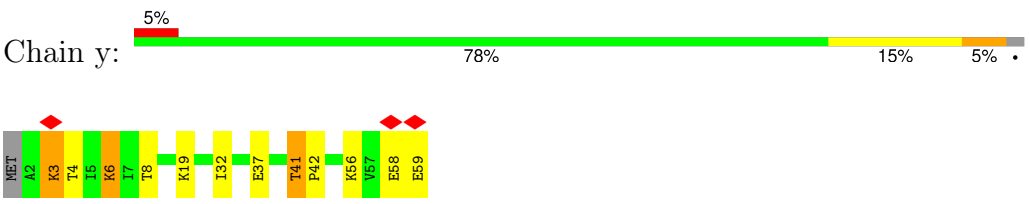
• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29

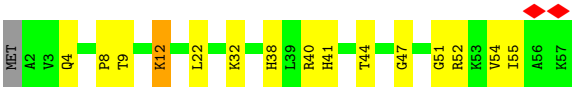


• Molecule 25: 50S ribosomal protein L30



• Molecule 26: 50S ribosomal protein L32

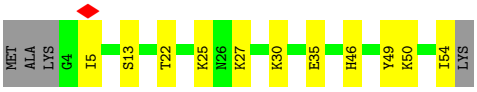




• Molecule 27: 50S ribosomal protein L33

Chain 0:

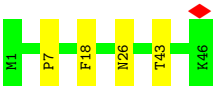




• Molecule 28: 50S ribosomal protein L34

Chain 1:

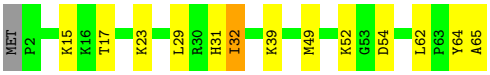




• Molecule 29: 50S ribosomal protein L35

Chain 2:

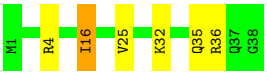




• Molecule 30: 50S ribosomal protein L36

Chain 3:

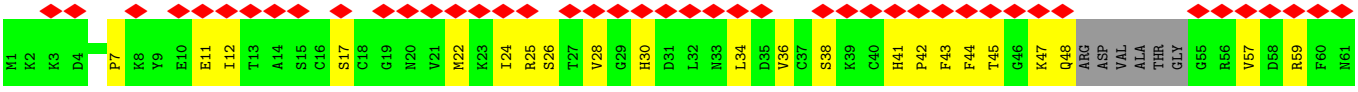


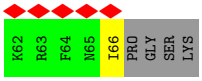


• Molecule 31: 50S ribosomal protein L31

Chain 4:

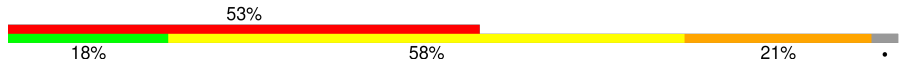


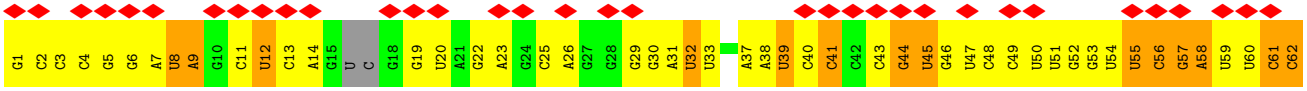


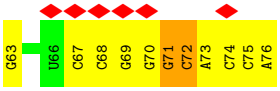


• Molecule 32: A-site tRNA Phe

Chain Y:

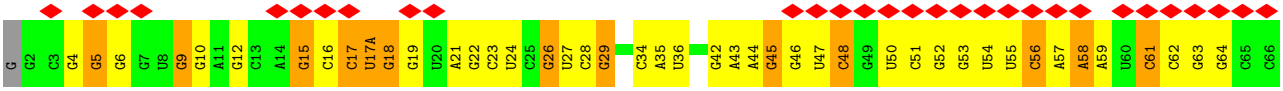


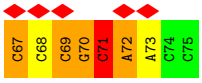




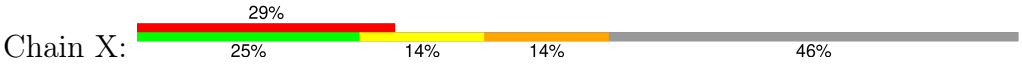
• Molecule 33: P-site tRNA fMet

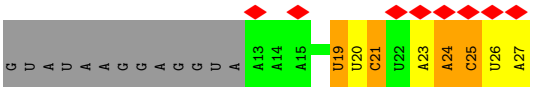






• Molecule 34: mRNA





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144049	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.238	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0246	Depositor
Map size (Å)	353.4, 353.4, 353.4	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7125, 0.7125, 0.7125	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SPM, 6MZ, ZN, 2MG, OMC, 3AB, 3TD, 1MG, H2U, 8AN, MEQ, MG, MS6, 5MC, PSU, 4D4, K, G7M, OMU, 5MU, FME, OMG, SPD, 2MA

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	0.34	1/65651 (0.0%)	0.45	13/102413 (0.0%)
2	b	0.28	0/2850	0.39	0/4444
3	c	0.29	0/2121	0.53	0/2852
4	d	0.29	0/1576	0.49	0/2119
5	e	0.28	0/1571	0.54	0/2113
6	f	0.27	0/1434	0.62	0/1926
7	g	0.28	0/1343	0.67	0/1816
8	h	0.28	0/306	0.78	1/413 (0.2%)
9	i	0.28	0/1152	0.49	0/1551
10	j	0.33	0/955	0.52	0/1279
11	k	0.31	0/1062	0.60	0/1413
12	l	0.29	0/1073	0.53	0/1433
13	m	0.31	0/958	0.55	0/1281
14	n	0.27	0/902	0.56	0/1209
15	o	0.29	0/929	0.50	0/1242
16	p	0.31	0/960	0.54	0/1278
17	q	0.31	0/829	0.56	0/1107
18	r	0.30	0/864	0.53	0/1156
19	s	0.29	0/744	0.51	0/994
20	t	0.29	0/787	0.65	0/1051
21	u	0.28	0/766	0.56	0/1025
22	v	0.31	0/593	0.50	0/785
23	w	0.34	0/635	0.51	0/848
24	x	0.28	0/502	0.55	0/667
25	y	0.30	0/453	0.55	0/605
26	z	0.28	0/450	0.50	0/599
27	0	0.28	0/424	0.53	0/565
28	1	0.29	0/380	0.53	0/498
29	2	0.30	0/513	0.56	0/676
30	3	0.33	0/303	0.58	0/397
31	4	0.26	0/488	0.72	0/649

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Y	3.57	3/1763 (0.2%)	0.91	4/2745 (0.1%)
33	Z	0.27	0/1788	0.54	2/2786 (0.1%)
34	X	0.50	2/354 (0.6%)	0.53	0/548
All	All	0.58	6/97479 (0.0%)	0.49	20/146483 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	g	0	2
29	2	0	1
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y	39	U	C1'-N1	147.45	3.69	1.48
32	Y	8	U	C4-O4	17.96	1.59	1.23
1	a	2605	PSU	O3'-P	-11.99	1.43	1.61
34	X	21	C	C1'-N1	5.66	1.56	1.48
34	X	19	U	C1'-N1	5.65	1.56	1.48

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Y	39	U	C6-N1-C1'	-33.93	19.41	121.20
1	a	2453	A	O3'-P-O5'	-18.86	75.72	104.00
32	Y	39	U	O4'-C1'-N1	-12.50	89.75	108.50
1	a	2453	A	P-O3'-C3'	12.41	138.81	120.20
32	Y	72	C	P-O3'-C3'	-8.18	107.92	120.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	2	31	HIS	Peptide
7	g	46	ALA	Peptide
7	g	47	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	59130	0	29767	645	0
2	b	2549	0	1291	29	0
3	c	2082	0	2154	21	0
4	d	1566	0	1618	23	0
5	e	1552	0	1619	24	0
6	f	1410	0	1444	74	0
7	g	1323	0	1371	50	0
8	h	303	0	327	7	0
9	i	1129	0	1162	12	0
10	j	946	0	1023	14	0
11	k	1053	0	1129	16	0
12	l	1075	0	1146	20	0
13	m	945	0	989	12	0
14	n	892	0	923	19	0
15	o	917	0	962	11	0
16	p	947	0	1019	12	0
17	q	816	0	839	14	0
18	r	857	0	922	16	0
19	s	738	0	807	9	0
20	t	779	0	831	19	0
21	u	753	0	780	17	0
22	v	586	0	596	5	0
23	w	625	0	652	4	0
24	x	501	0	531	11	0
25	y	449	0	488	12	0
26	z	444	0	458	14	0
27	0	417	0	451	6	0
28	1	377	0	418	3	0
29	2	504	0	572	7	0
30	3	302	0	340	4	0
31	4	480	0	478	24	0
32	Y	1578	0	800	42	0
33	Z	1601	0	813	32	0
34	X	317	0	161	5	0
35	Y	1	0	0	0	0
35	Z	1	0	0	0	0
35	a	211	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	b	5	0	0	0	0
35	c	2	0	0	0	0
35	d	1	0	0	0	0
35	m	1	0	0	0	0
35	z	1	0	0	0	0
36	a	170	0	322	41	0
37	a	14	0	26	0	0
38	a	5	0	0	0	0
38	c	1	0	0	0	0
38	e	1	0	0	0	0
39	a	10	0	10	0	0
40	3	1	0	0	0	0
40	4	1	0	0	0	0
41	Y	20	0	14	0	0
42	Z	22	0	12	0	0
43	1	17	0	0	0	0
43	2	24	0	0	0	0
43	3	3	0	0	0	0
43	Z	2	0	0	0	0
43	a	3013	0	0	47	0
43	b	40	0	0	2	0
43	c	86	0	0	2	0
43	d	33	0	0	1	0
43	e	27	0	0	1	0
43	h	1	0	0	0	0
43	i	12	0	0	0	0
43	j	12	0	0	0	0
43	k	32	0	0	0	0
43	l	20	0	0	0	0
43	m	20	0	0	0	0
43	o	10	0	0	0	0
43	p	19	0	0	0	0
43	q	14	0	0	0	0
43	r	24	0	0	3	0
43	s	5	0	0	0	0
43	t	1	0	0	0	0
43	u	3	0	0	0	0
43	v	12	0	0	0	0
43	w	9	0	0	0	0
43	x	1	0	0	0	0
43	y	1	0	0	1	0
43	z	21	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	93873	0	59265	1142	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 8.

The worst 5 of 1142 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:1968:G:OP1	36:a:6216:SPD:H22	1.20	1.34
32:Y:26:A:N6	32:Y:44:G:H1	1.49	1.10
1:a:1968:G:OP1	36:a:6216:SPD:C2	2.04	1.05
1:a:1868:C:O2	1:a:1873:G:N2	2.07	0.87
1:a:95:A:HO2'	24:x:41:HIS:HD1	1.21	0.85

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
3	c	269/273 (98%)	262 (97%)	7 (3%)	0	100 100
4	d	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24 30
5	e	199/201 (99%)	196 (98%)	3 (2%)	0	100 100
6	f	175/179 (98%)	159 (91%)	16 (9%)	0	100 100
7	g	174/177 (98%)	154 (88%)	18 (10%)	2 (1%)	11 12
8	h	39/149 (26%)	32 (82%)	7 (18%)	0	100 100
9	i	140/142 (99%)	138 (99%)	2 (1%)	0	100 100
10	j	121/123 (98%)	113 (93%)	8 (7%)	0	100 100
11	k	142/144 (99%)	137 (96%)	4 (3%)	1 (1%)	18 22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
13	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
14	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
15	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
16	p	115/118 (98%)	115 (100%)	0	0	100	100
17	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
18	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
19	s	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
20	t	100/104 (96%)	95 (95%)	4 (4%)	1 (1%)	12	14
21	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
22	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
23	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
24	x	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
25	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
26	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
27	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
28	1	44/46 (96%)	44 (100%)	0	0	100	100
29	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	7
30	3	36/38 (95%)	36 (100%)	0	0	100	100
31	4	56/70 (80%)	49 (88%)	7 (12%)	0	100	100
All	All	3114/3337 (93%)	2981 (96%)	127 (4%)	6 (0%)	44	53

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	g	47	ASP
7	g	48	ASN
29	2	32	ILE
11	k	36	LYS
20	t	99	ASN

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	
3	c	216/218 (99%)	212 (98%)	4 (2%)	50	67
4	d	163/163 (100%)	160 (98%)	3 (2%)	51	69
5	e	165/165 (100%)	159 (96%)	6 (4%)	31	45
6	f	148/150 (99%)	120 (81%)	28 (19%)	1	1
7	g	137/138 (99%)	114 (83%)	23 (17%)	2	2
8	h	32/114 (28%)	23 (72%)	9 (28%)	0	0
9	i	116/116 (100%)	112 (97%)	4 (3%)	32	47
10	j	104/104 (100%)	100 (96%)	4 (4%)	29	43
11	k	103/103 (100%)	100 (97%)	3 (3%)	37	53
12	l	107/107 (100%)	103 (96%)	4 (4%)	30	44
13	m	98/103 (95%)	97 (99%)	1 (1%)	68	81
14	n	86/87 (99%)	79 (92%)	7 (8%)	11	14
15	o	99/100 (99%)	92 (93%)	7 (7%)	13	18
16	p	89/90 (99%)	87 (98%)	2 (2%)	45	63
17	q	84/84 (100%)	77 (92%)	7 (8%)	10	13
18	r	93/93 (100%)	88 (95%)	5 (5%)	20	28
19	s	80/84 (95%)	80 (100%)	0	100	100
20	t	83/85 (98%)	78 (94%)	5 (6%)	17	24
21	u	78/78 (100%)	74 (95%)	4 (5%)	21	31
22	v	58/63 (92%)	57 (98%)	1 (2%)	53	70
23	w	67/68 (98%)	62 (92%)	5 (8%)	12	16
24	x	54/55 (98%)	50 (93%)	4 (7%)	13	16
25	y	48/49 (98%)	45 (94%)	3 (6%)	16	22
26	z	47/48 (98%)	46 (98%)	1 (2%)	47	65
27	0	46/49 (94%)	44 (96%)	2 (4%)	26	38
28	1	38/38 (100%)	38 (100%)	0	100	100
29	2	51/52 (98%)	49 (96%)	2 (4%)	28	42
30	3	34/34 (100%)	31 (91%)	3 (9%)	9	12
31	4	55/62 (89%)	51 (93%)	4 (7%)	13	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2579/2700 (96%)	2428 (94%)	151 (6%)	19 25

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	r	108	SER
29	2	52	LYS
20	t	60	GLU
23	w	66	THR
31	4	57	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
18	r	9	HIS
26	z	42	HIS
21	u	5	ASN
9	i	80	HIS
15	o	66	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	2749/2904 (94%)	354 (12%)	0
2	b	118/120 (98%)	23 (19%)	0
32	Y	71/76 (93%)	29 (40%)	2 (2%)
33	Z	74/76 (97%)	26 (35%)	0
34	X	14/28 (50%)	5 (35%)	1 (7%)
All	All	3026/3204 (94%)	437 (14%)	3 (0%)

5 of 437 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	A
1	a	12	U
1	a	13	A
1	a	34	U
1	a	42	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	Y	13	C
32	Y	57	G
34	X	24	A

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

27 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
1	PSU	a	2457	1	18,21,22	1.40	3 (16%)	21,30,33	2.11	5 (23%)
12	4D4	l	81	12	9,11,12	2.07	2 (22%)	7,13,15	0.80	0
1	3TD	a	1915	1	19,22,23	1.59	5 (26%)	23,32,35	2.26	4 (17%)
12	MS6	l	82	12	5,7,8	0.19	0	2,7,9	0.16	0
1	5MU	a	747	1	19,22,23	1.41	5 (26%)	27,32,35	2.21	9 (33%)
1	5MU	a	1939	1	19,22,23	1.41	5 (26%)	27,32,35	2.22	6 (22%)
1	6MZ	a	2030	1	22,25,26	1.50	4 (18%)	29,36,39	2.47	11 (37%)
1	6MZ	a	1618	1	22,25,26	1.41	4 (18%)	29,36,39	2.21	11 (37%)
1	PSU	a	1917	1	18,21,22	1.40	3 (16%)	21,30,33	2.03	3 (14%)
1	OMC	a	2498	1,35	19,22,23	0.82	0	25,31,34	0.96	1 (4%)
1	2MG	a	1835	1	23,26,27	1.26	3 (13%)	33,38,41	2.10	5 (15%)
1	PSU	a	955	1	18,21,22	1.54	5 (27%)	21,30,33	2.01	4 (19%)
1	PSU	a	2504	38,1	18,21,22	1.49	3 (16%)	21,30,33	2.18	4 (19%)
1	PSU	a	746	1,35	18,21,22	1.40	2 (11%)	21,30,33	2.17	4 (19%)
1	OMU	a	2552	1,35	19,22,23	1.26	3 (15%)	25,31,34	1.81	5 (20%)
1	PSU	a	2604	1	18,21,22	1.38	3 (16%)	21,30,33	2.18	4 (19%)
1	G7M	a	2069	1	23,26,27	1.49	4 (17%)	34,39,42	1.75	5 (14%)
1	2MG	a	2445	1	23,26,27	1.26	3 (13%)	33,38,41	2.23	7 (21%)
1	PSU	a	1911	1	18,21,22	1.47	3 (16%)	21,30,33	2.11	5 (23%)
1	H2U	a	2449	1	18,21,22	1.18	2 (11%)	19,30,33	0.85	0
1	PSU	a	2605	1	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	a	2580	1	18,21,22	1.47	4 (22%)	21,30,33	2.18	5 (23%)
1	1MG	a	745	1	23,26,27	1.19	3 (13%)	33,39,42	1.77	7 (21%)
1	5MC	a	1962	1	19,22,23	1.63	3 (15%)	26,32,35	1.12	3 (11%)
1	OMG	a	2251	38,1,33	23,26,27	1.21	4 (17%)	32,38,41	2.00	7 (21%)
4	MEQ	d	150	4	8,9,10	0.43	0	5,10,12	0.45	0
1	2MA	a	2503	38,1,35	22,25,26	1.47	4 (18%)	32,37,40	2.44	8 (25%)

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
1	PSU	a	2457	1	-	0/7/25/26	0/2/2/2
12	4D4	l	81	12	-	2/11/12/14	-
1	3TD	a	1915	1	-	2/7/25/26	0/2/2/2
12	MS6	l	82	12	-	0/4/6/8	-
1	5MU	a	747	1	-	0/7/25/26	0/2/2/2
1	5MU	a	1939	1	-	0/7/25/26	0/2/2/2
1	6MZ	a	2030	1	-	2/9/27/28	0/3/3/3
1	6MZ	a	1618	1	-	0/9/27/28	0/3/3/3
1	PSU	a	1917	1	-	0/7/25/26	0/2/2/2
1	OMC	a	2498	1,35	-	1/9/27/28	0/2/2/2
1	2MG	a	1835	1	-	0/9/27/28	0/3/3/3
1	PSU	a	955	1	-	0/7/25/26	0/2/2/2
1	PSU	a	2504	38,1	-	2/7/25/26	0/2/2/2
1	PSU	a	746	1,35	-	2/7/25/26	0/2/2/2
1	OMU	a	2552	1,35	-	1/9/27/28	0/2/2/2
1	PSU	a	2604	1	-	0/7/25/26	0/2/2/2
1	G7M	a	2069	1	-	0/7/25/26	0/3/3/3
1	2MG	a	2445	1	-	0/9/27/28	0/3/3/3
1	PSU	a	1911	1	-	2/7/25/26	0/2/2/2
1	H2U	a	2449	1	-	1/7/38/39	0/2/2/2
1	PSU	a	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	a	2580	1	-	0/7/25/26	0/2/2/2
1	1MG	a	745	1	-	0/7/25/26	0/3/3/3
1	5MC	a	1962	1	-	2/7/25/26	0/2/2/2
1	OMG	a	2251	38,1,33	-	1/9/27/28	0/3/3/3
4	MEQ	d	150	4	-	2/8/9/11	-
1	2MA	a	2503	38,1,35	-	1/7/25/26	0/3/3/3

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1962	5MC	C5-C4	5.85	1.48	1.44
1	a	2069	G7M	C5-N7	-4.73	1.33	1.39
12	l	81	4D4	CZ-NE	4.59	1.42	1.33
1	a	2030	6MZ	C5-C4	4.24	1.46	1.39
1	a	1618	6MZ	C5-C4	4.23	1.46	1.39

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	2503	2MA	C5-C4-N3	-8.53	118.19	127.18
1	a	1915	3TD	N1-C2-N3	8.49	122.30	116.13
1	a	2504	PSU	N1-C2-N3	7.20	122.76	115.17
1	a	1835	2MG	C2-N3-C4	7.17	120.97	112.00
1	a	2445	2MG	C2-N3-C4	7.07	120.85	112.00

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1911	PSU	O4'-C4'-C5'-O5'
1	a	2251	OMG	C1'-C2'-O2'-CM2
1	a	2498	OMC	C1'-C2'-O2'-CM2
1	a	1915	3TD	O4'-C4'-C5'-O5'
1	a	1911	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	747	5MU	1	0
1	a	1939	5MU	1	0
1	a	2030	6MZ	3	0
1	a	1917	PSU	1	0
1	a	2498	OMC	1	0
1	a	1835	2MG	1	0
1	a	2552	OMU	1	0
1	a	2604	PSU	1	0
1	a	2251	OMG	1	0
4	d	150	MEQ	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 254 ligands modelled in this entry, 232 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
36	SPD	a	6212	-	9,9,9	0.14	0	8,8,8	0.27	0
36	SPD	a	6203	-	9,9,9	0.18	0	8,8,8	0.31	0
36	SPD	a	6210	-	9,9,9	0.18	0	8,8,8	0.18	0
36	SPD	a	6209	-	9,9,9	0.17	0	8,8,8	0.40	0
41	3AB	Y	101[B]	32	10,10,10	2.48	1 (10%)	13,13,13	0.63	0
36	SPD	a	6204	-	9,9,9	0.16	0	8,8,8	0.30	0
36	SPD	a	6202	-	9,9,9	0.18	0	8,8,8	0.20	0
36	SPD	a	6207	-	9,9,9	0.17	0	8,8,8	0.18	0
36	SPD	a	6217	-	9,9,9	0.15	0	8,8,8	0.19	0
36	SPD	a	6199	-	9,9,9	0.18	0	8,8,8	0.39	0
37	SPM	a	6213	-	13,13,13	0.35	0	12,12,12	0.76	0
41	3AB	Y	101[A]	32	10,10,10	2.53	1 (10%)	13,13,13	0.82	0
36	SPD	a	6200	-	9,9,9	0.18	0	8,8,8	0.29	0
36	SPD	a	6205	-	9,9,9	0.17	0	8,8,8	0.22	0
42	8AN	Z	101	35,33,39	21,24,25	0.66	1 (4%)	26,35,38	0.49	0
36	SPD	a	6216	-	9,9,9	0.16	0	8,8,8	0.19	0
36	SPD	a	6214	-	9,9,9	0.14	0	8,8,8	0.18	0
36	SPD	a	6211	-	9,9,9	0.17	0	8,8,8	0.29	0
36	SPD	a	6201	-	9,9,9	0.16	0	8,8,8	0.28	0
36	SPD	a	6206	-	9,9,9	0.15	0	8,8,8	0.28	0
39	FME	a	6222	42	8,9,10	1.00	0	8,9,11	0.94	0
36	SPD	a	6208	-	9,9,9	0.14	0	8,8,8	0.22	0

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
36	SPD	a	6212	-	-	1/7/7/7	-
36	SPD	a	6203	-	-	2/7/7/7	-
36	SPD	a	6210	-	-	0/7/7/7	-
36	SPD	a	6209	-	-	0/7/7/7	-
41	3AB	Y	101[B]	32	-	0/4/4/4	0/1/1/1
36	SPD	a	6204	-	-	2/7/7/7	-
36	SPD	a	6202	-	-	0/7/7/7	-
36	SPD	a	6207	-	-	2/7/7/7	-
36	SPD	a	6217	-	-	6/7/7/7	-
36	SPD	a	6199	-	-	1/7/7/7	-
37	SPM	a	6213	-	-	5/11/11/11	-
41	3AB	Y	101[A]	32	-	0/4/4/4	0/1/1/1
36	SPD	a	6200	-	-	1/7/7/7	-
36	SPD	a	6205	-	-	0/7/7/7	-
42	8AN	Z	101	35,33,39	-	1/7/25/26	0/3/3/3
36	SPD	a	6216	-	-	5/7/7/7	-
36	SPD	a	6214	-	-	5/7/7/7	-
36	SPD	a	6211	-	-	0/7/7/7	-
36	SPD	a	6201	-	-	1/7/7/7	-
36	SPD	a	6206	-	-	0/7/7/7	-
39	FME	a	6222	42	-	2/7/9/11	-
36	SPD	a	6208	-	-	0/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	Y	101[A]	3AB	C1-C1'	-7.82	1.38	1.50
41	Y	101[B]	3AB	C1-C1'	-7.64	1.39	1.50
42	Z	101	8AN	C3'-N3'	-2.50	1.43	1.47

There are no bond angle outliers.

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	a	6216	SPD	C4-C5-N6-C7
36	a	6217	SPD	C4-C5-N6-C7
39	a	6222	FME	N-CA-CB-CG
39	a	6222	FME	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
42	Z	101	8AN	C4'-C5'-O5'-P

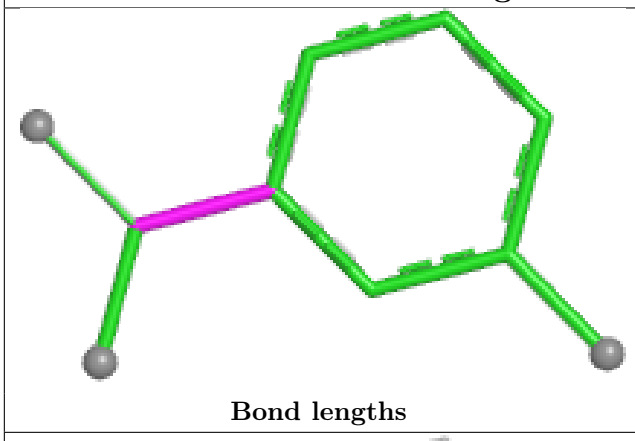
There are no ring outliers.

13 monomers are involved in 41 short contacts:

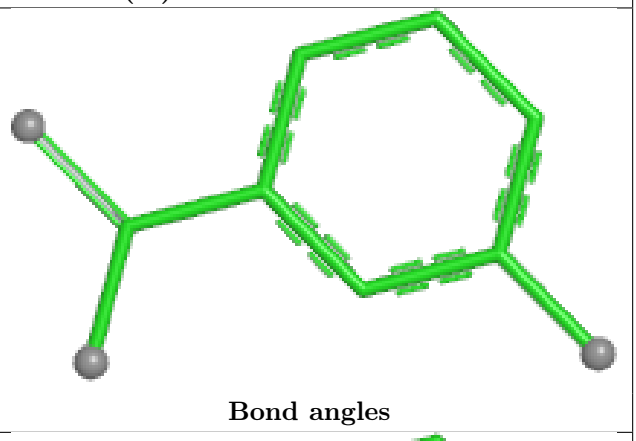
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	a	6212	SPD	1	0
36	a	6203	SPD	1	0
36	a	6209	SPD	2	0
36	a	6204	SPD	1	0
36	a	6207	SPD	1	0
36	a	6217	SPD	1	0
36	a	6200	SPD	3	0
36	a	6205	SPD	2	0
36	a	6216	SPD	23	0
36	a	6214	SPD	2	0
36	a	6211	SPD	1	0
36	a	6201	SPD	1	0
36	a	6206	SPD	2	0

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.

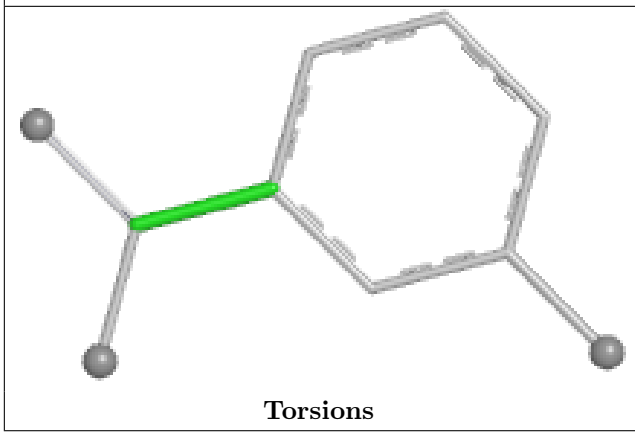
Ligand 3AB Y 101 (B)



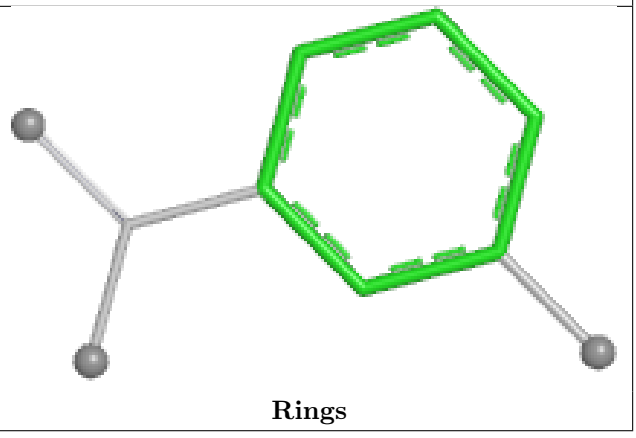
Bond lengths



Bond angles

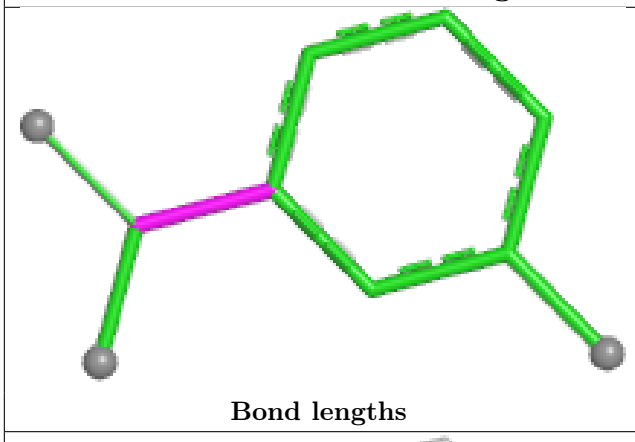


Torsions

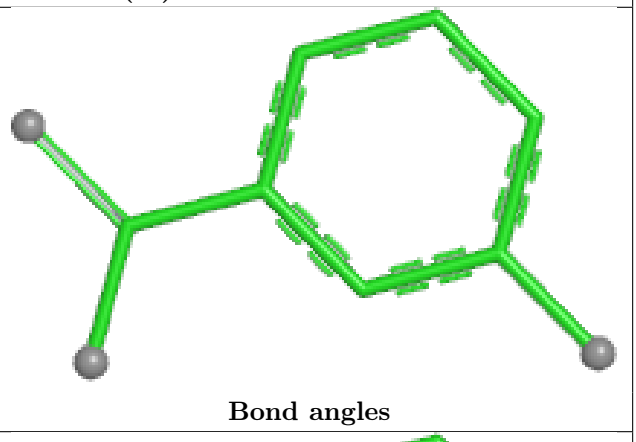


Rings

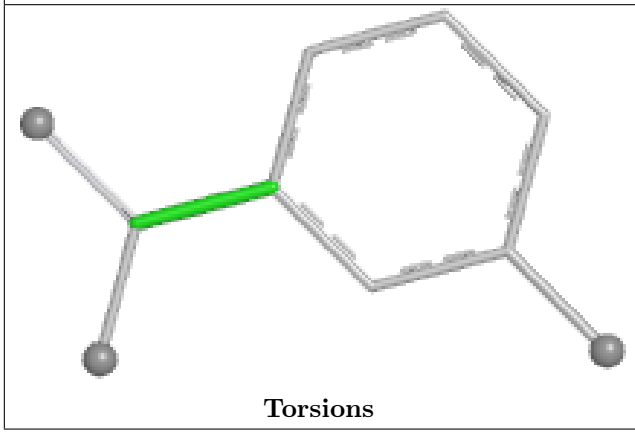
Ligand 3AB Y 101 (A)



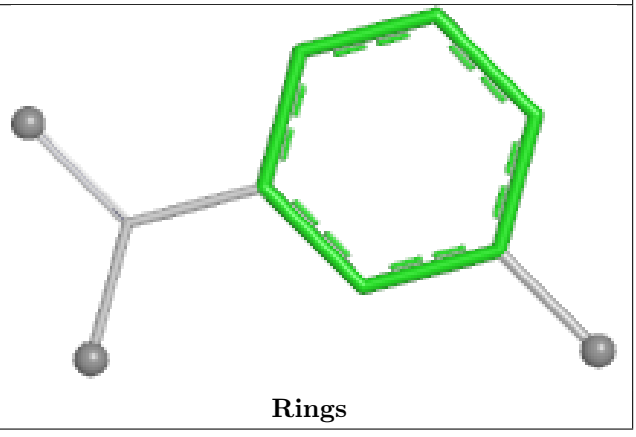
Bond lengths



Bond angles

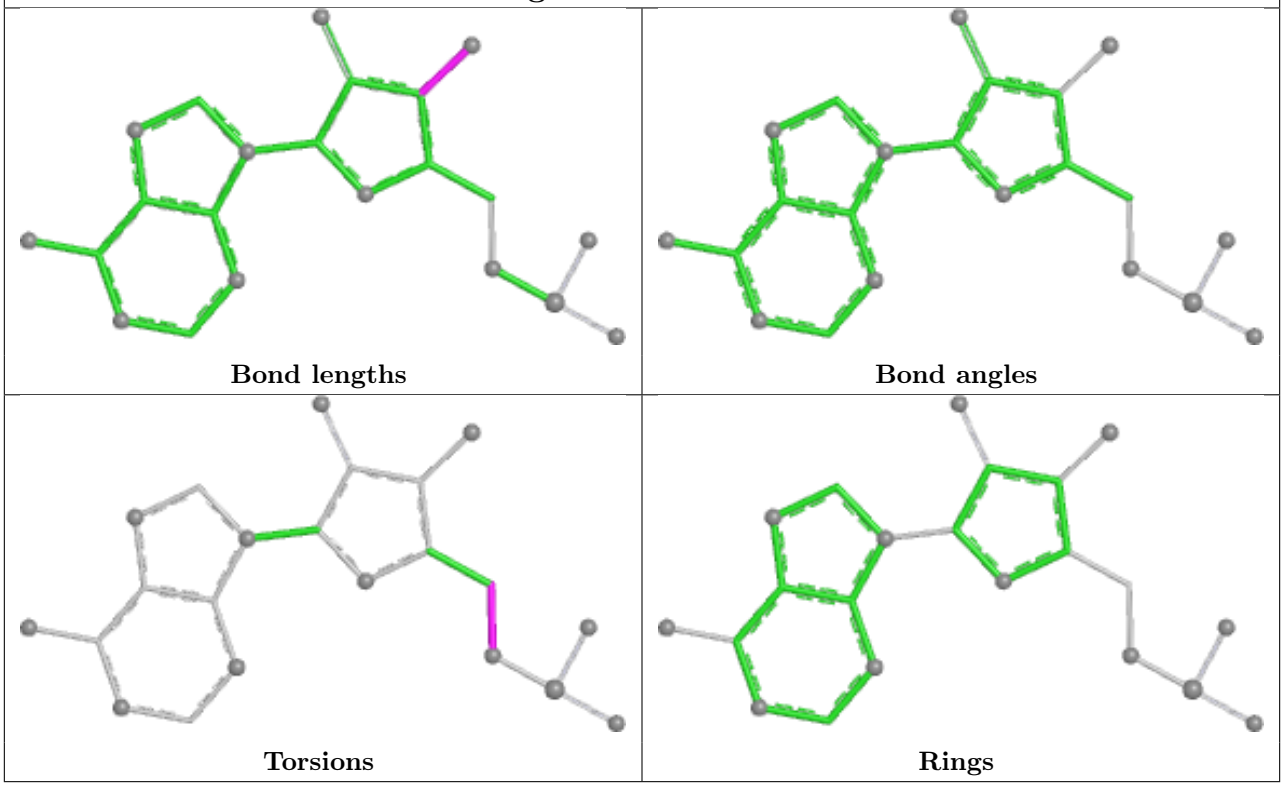


Torsions



Rings

Ligand 8AN Z 101



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.

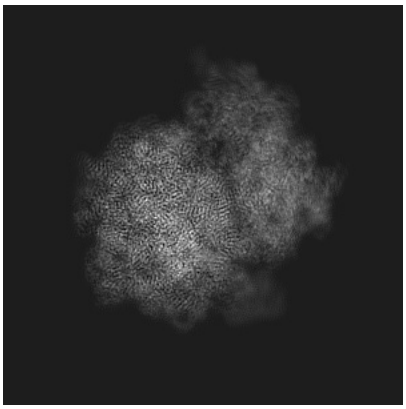
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29787. These allow visual inspection of the internal detail of the map and identification of artifacts.

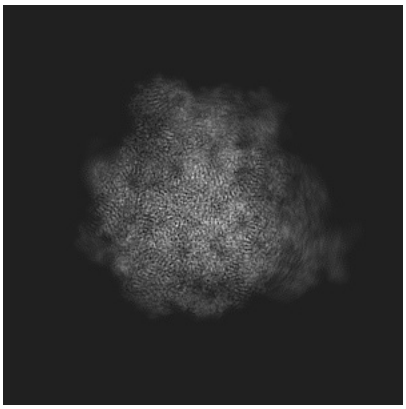
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

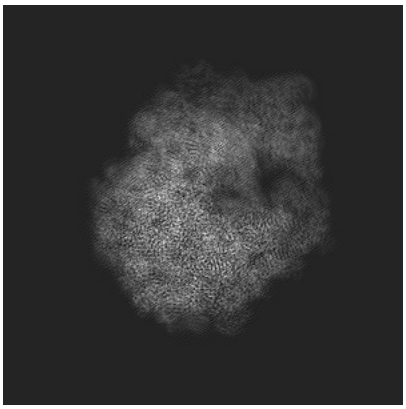
6.1.1 Primary map



X

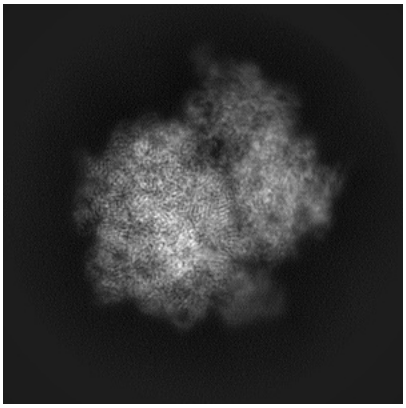


Y

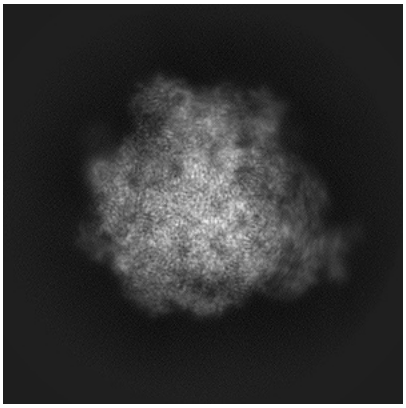


Z

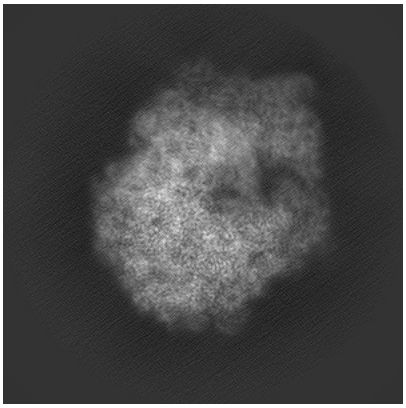
6.1.2 Raw map



X



Y

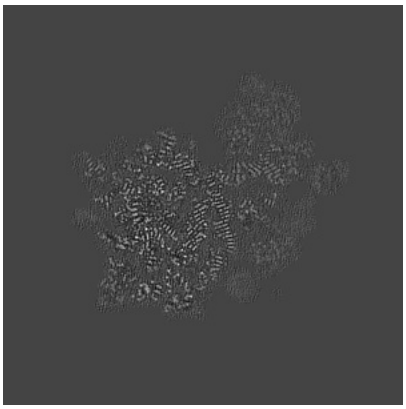


Z

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

6.2 Central slices (i)

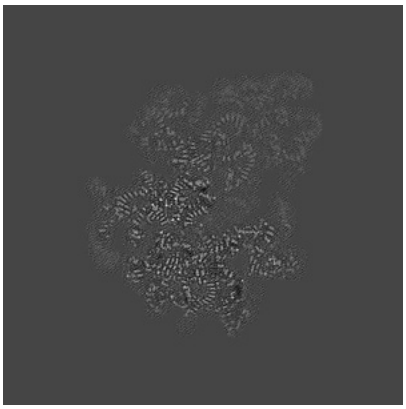
6.2.1 Primary map



X Index: 248

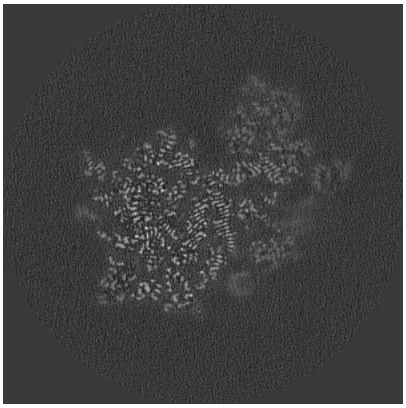


Y Index: 248

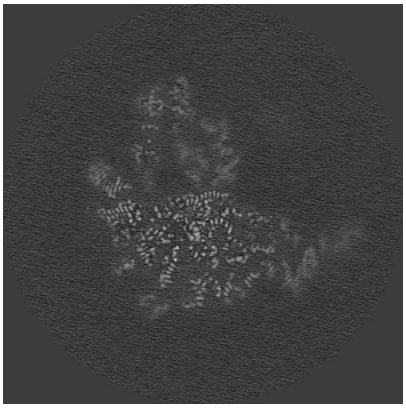


Z Index: 248

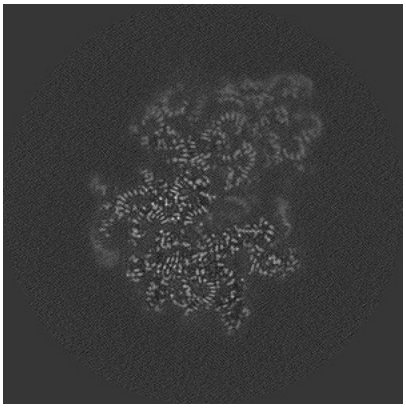
6.2.2 Raw map



X Index: 248



Y Index: 248

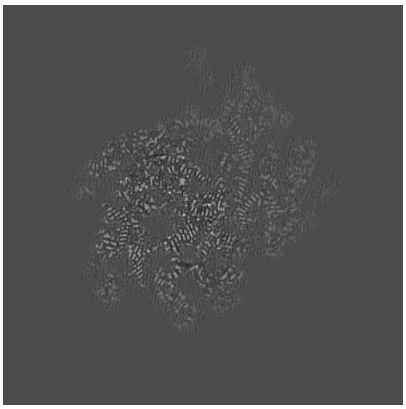


Z Index: 248

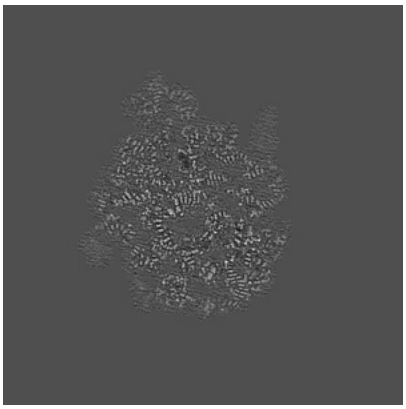
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

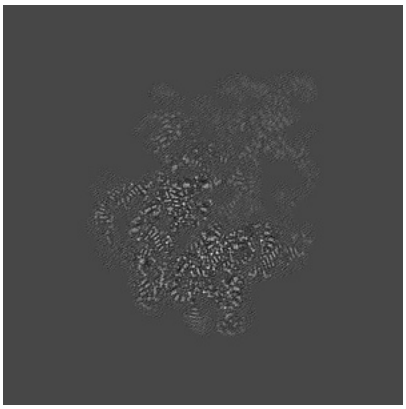
6.3.1 Primary map



X Index: 214

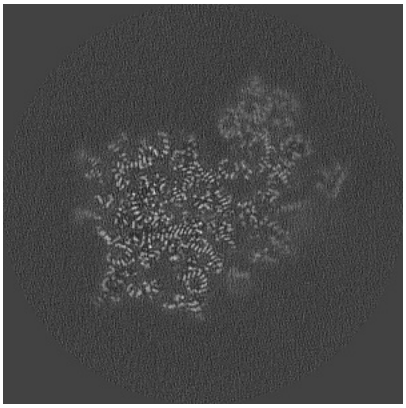


Y Index: 207

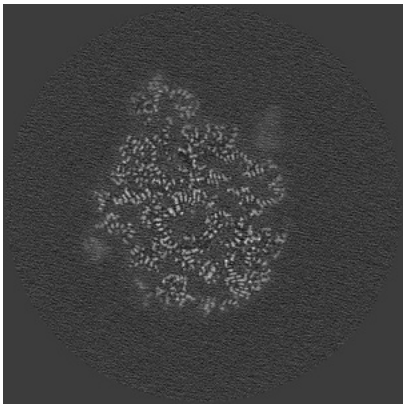


Z Index: 236

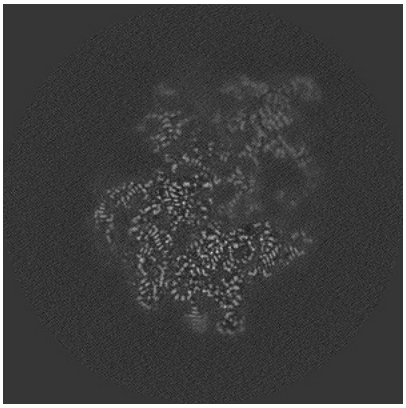
6.3.2 Raw map



X Index: 242



Y Index: 207

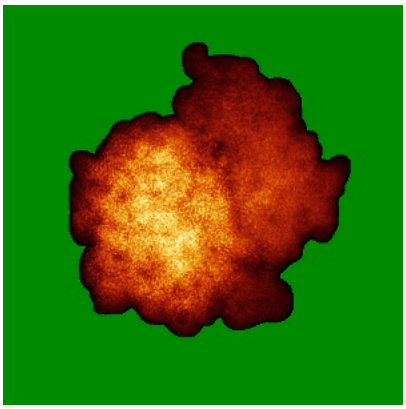


Z Index: 236

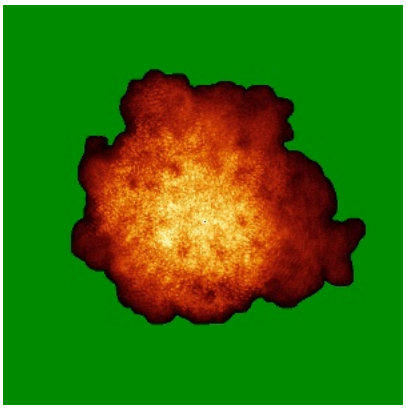
The images above show the largest variance slices of the map in three orthogonal directions.

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

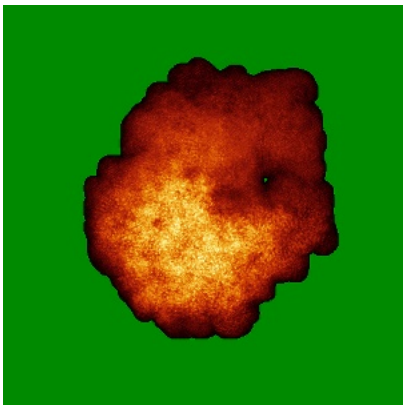
6.4.1 Primary map



X

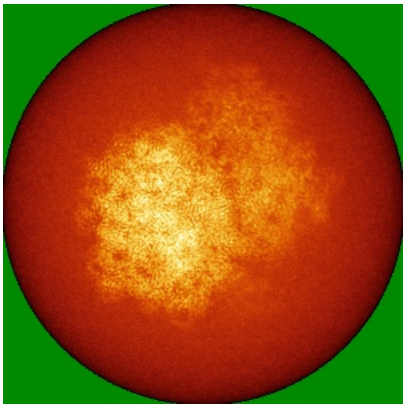


Y

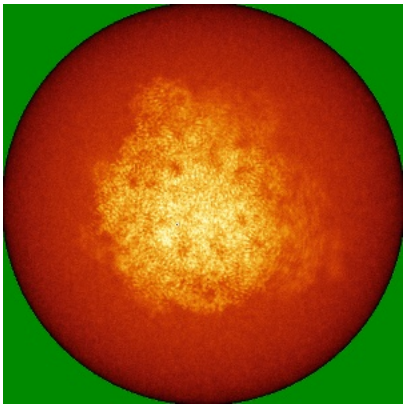


Z

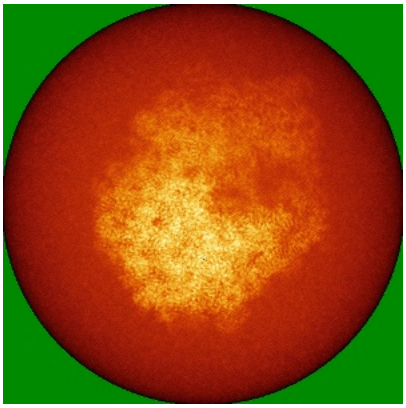
6.4.2 Raw map



X



Y

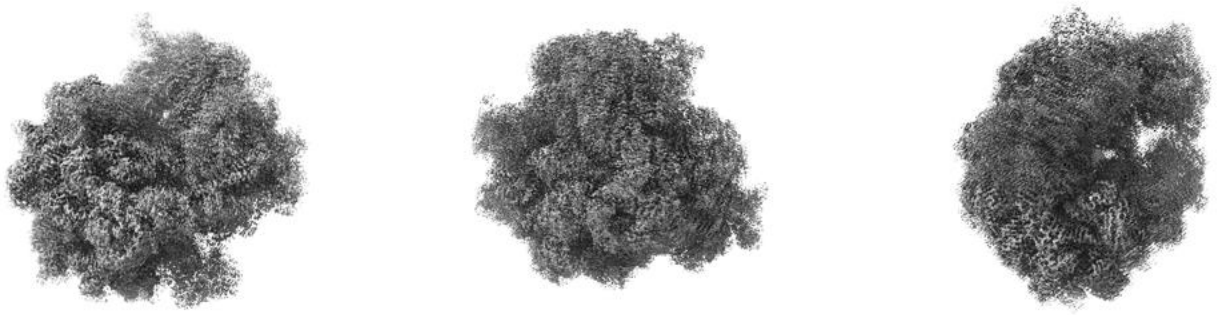


Z

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)

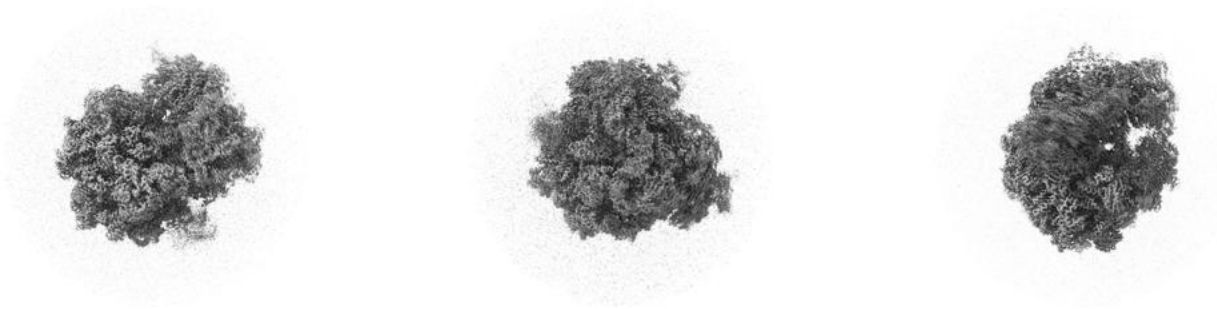
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0246. 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.

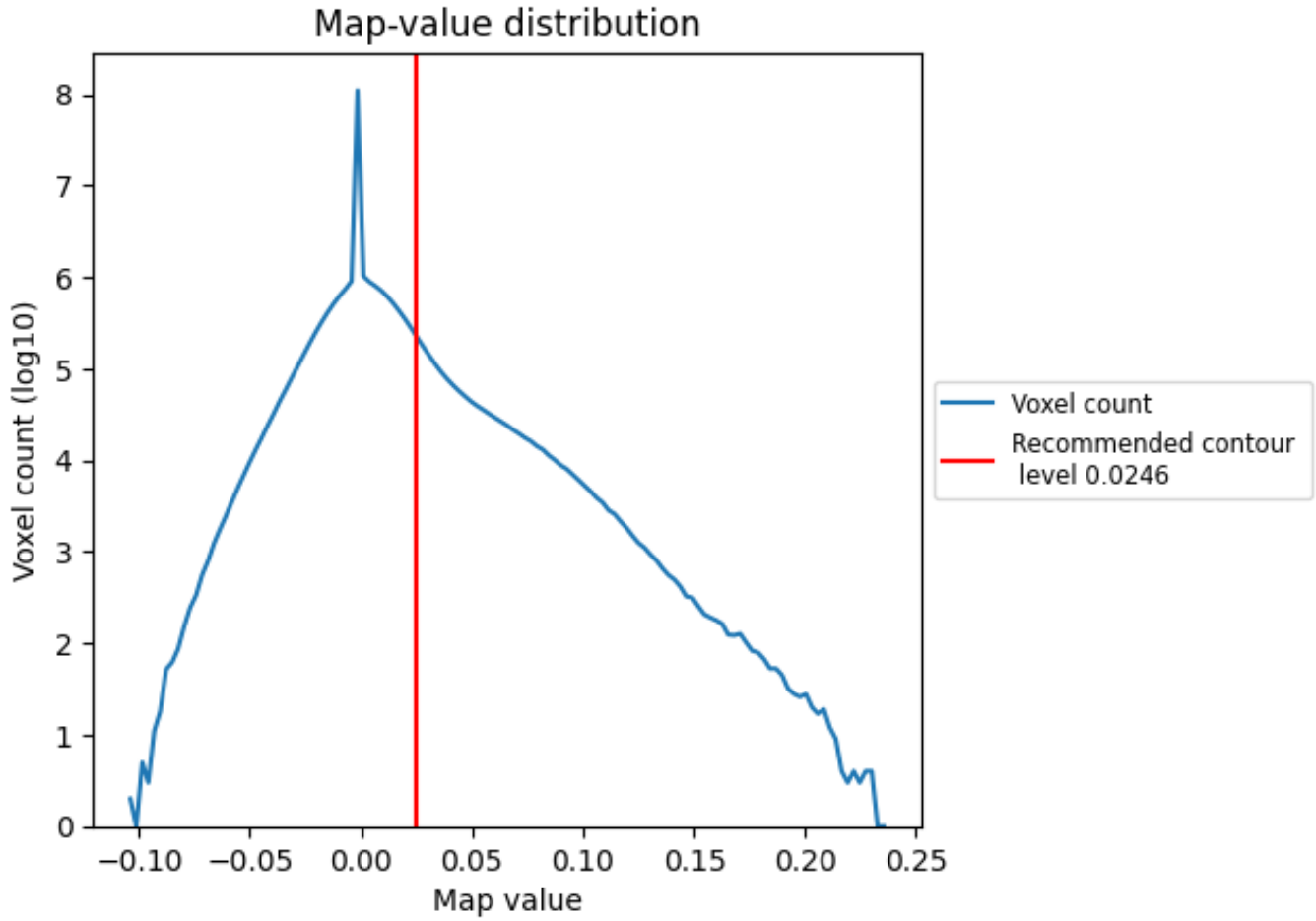
6.6 Mask visualisation (i)

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

7 Map analysis

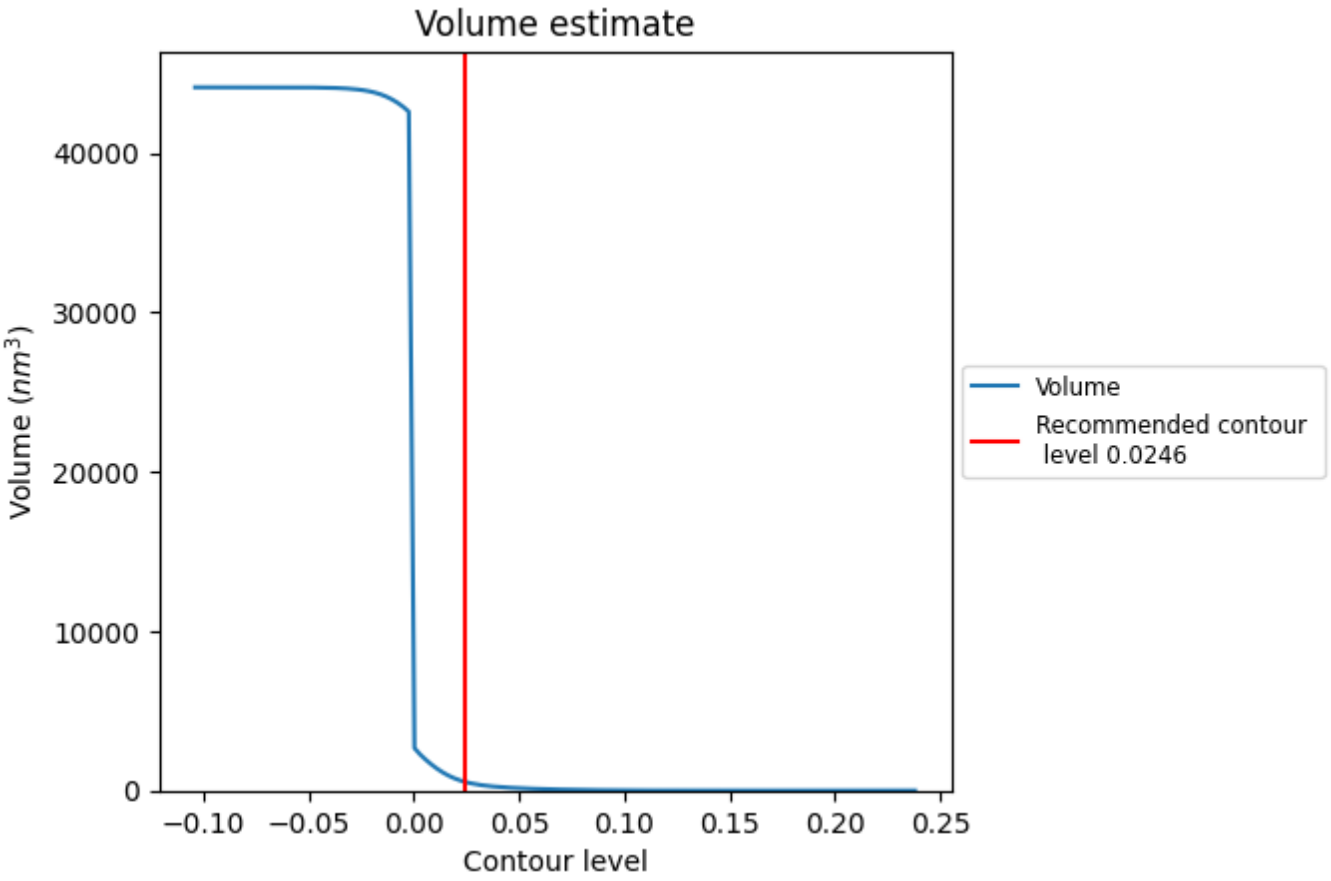
This section contains the results of statistical analysis of the map.

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.

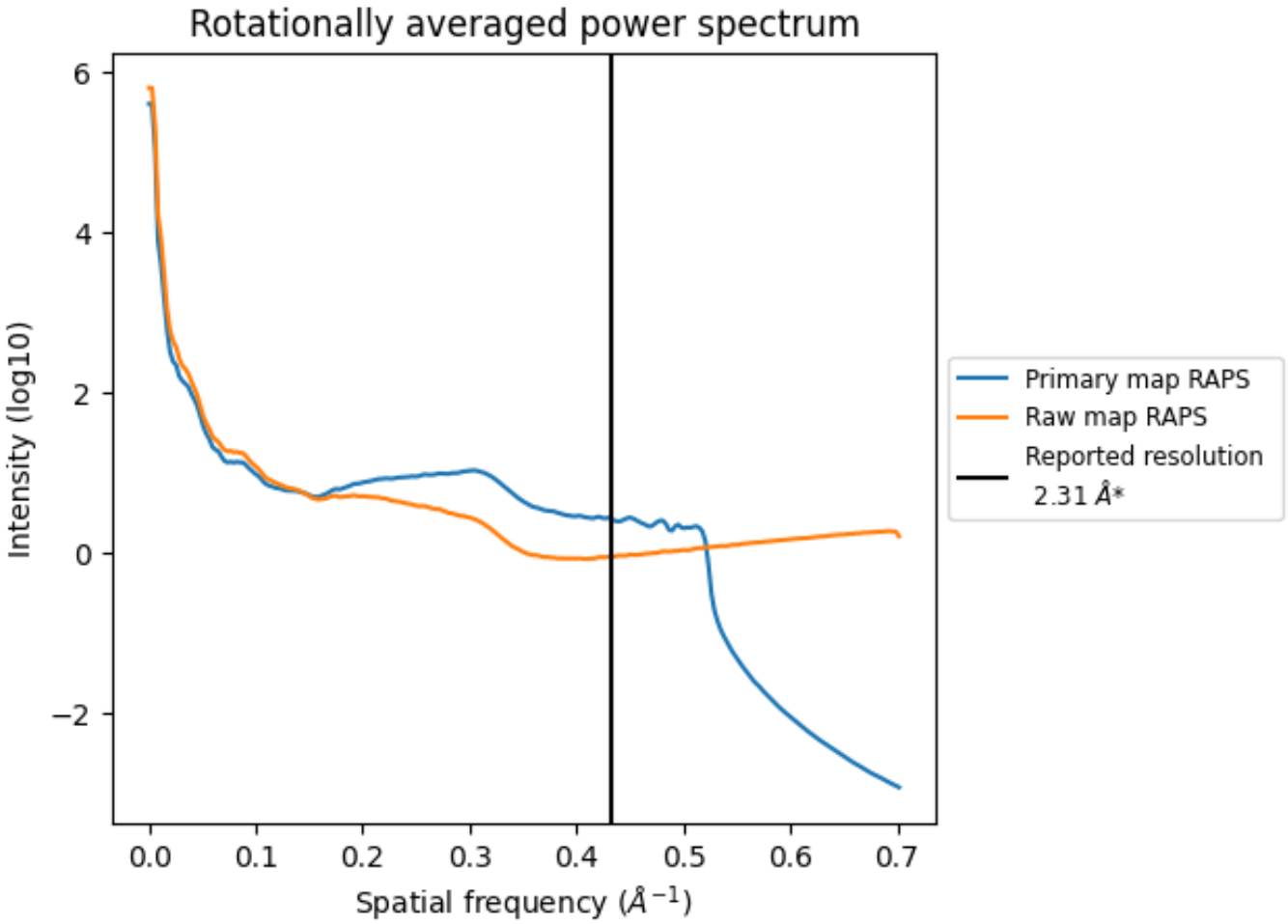
7.2 Volume estimate (i)



The volume at the recommended contour level is 537 nm^3; this corresponds to an approximate mass of 485 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)

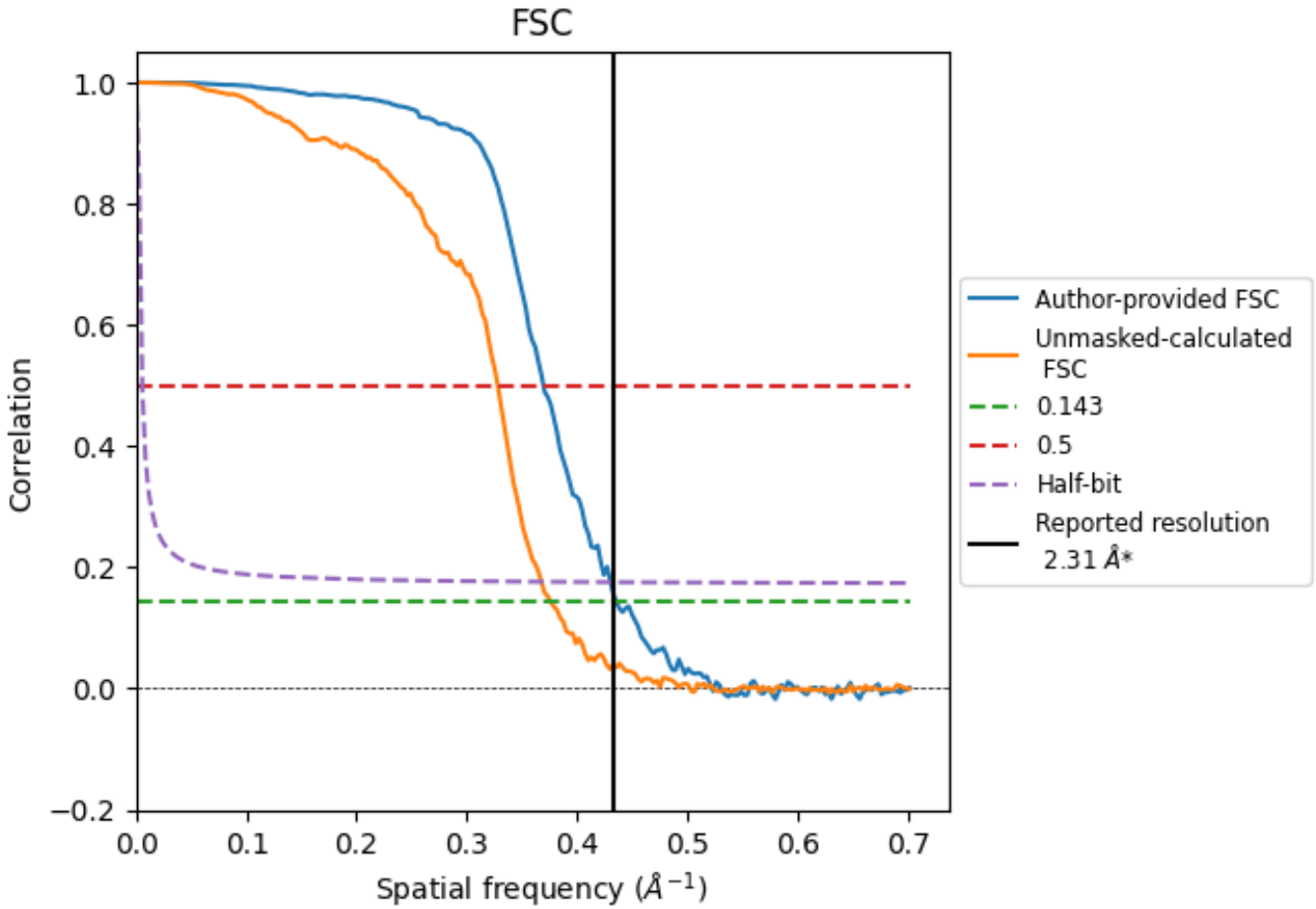


*Reported resolution corresponds to spatial frequency of 0.433 Å^{-1}

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 0.433 Å^{-1}

8.2 Resolution estimates (i)

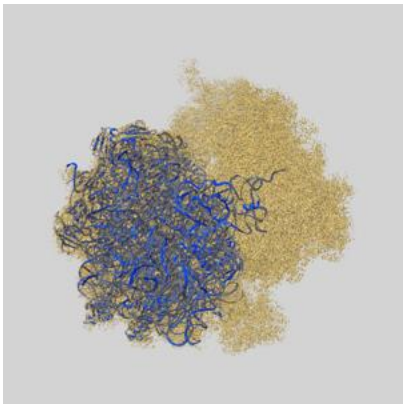
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.30	2.71	2.32
Unmasked-calculated*	2.66	3.05	2.72

*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 2.66 differs from the reported value 2.31 by more than 10 %

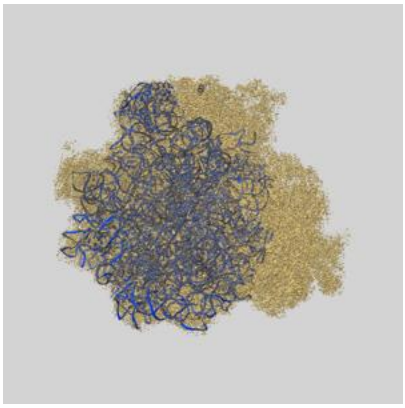
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29787 and PDB model 8G6X. Per-residue inclusion information can be found in section 3 on page 17.

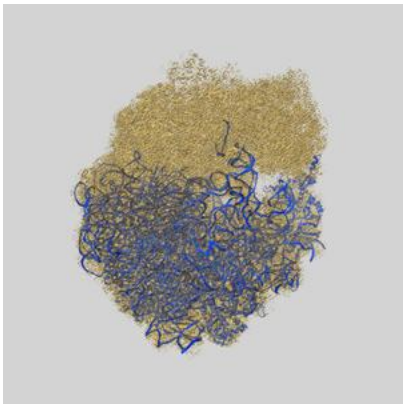
9.1 Map-model overlay



X



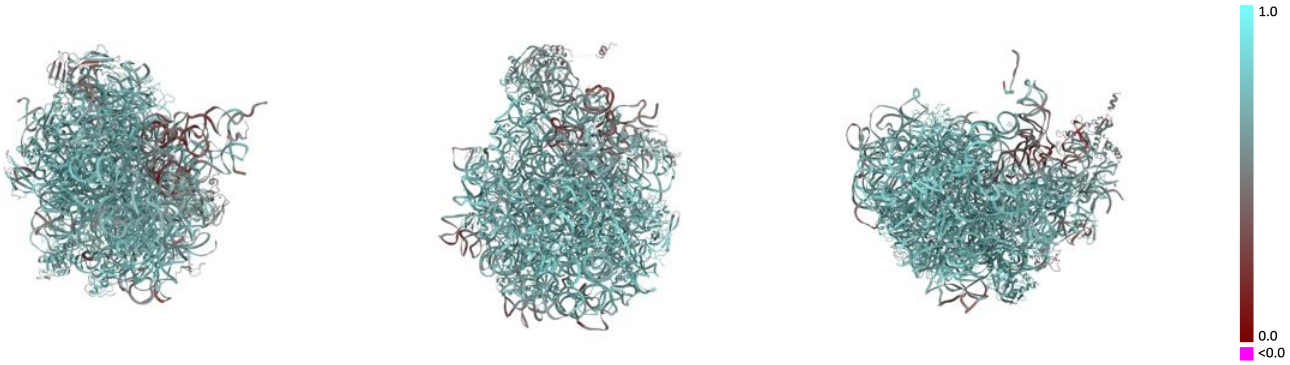
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0246 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.

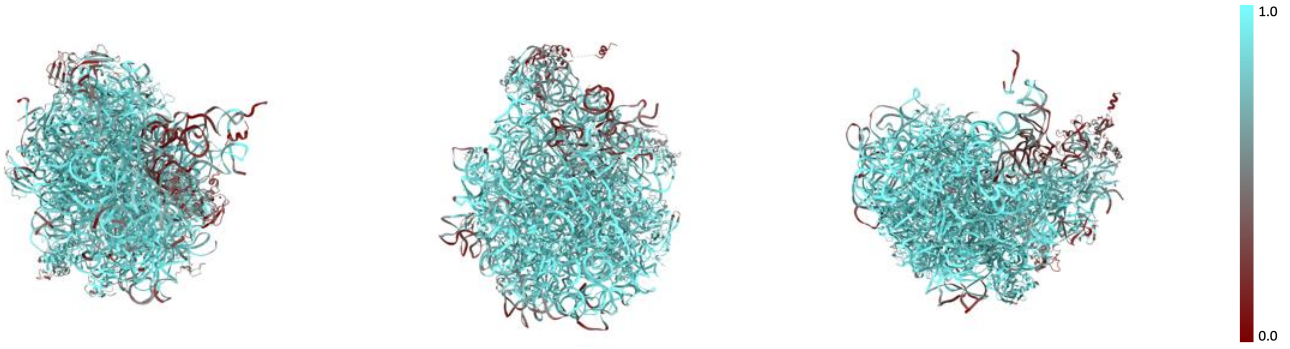
9.2 Q-score mapped to coordinate model (i)



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.

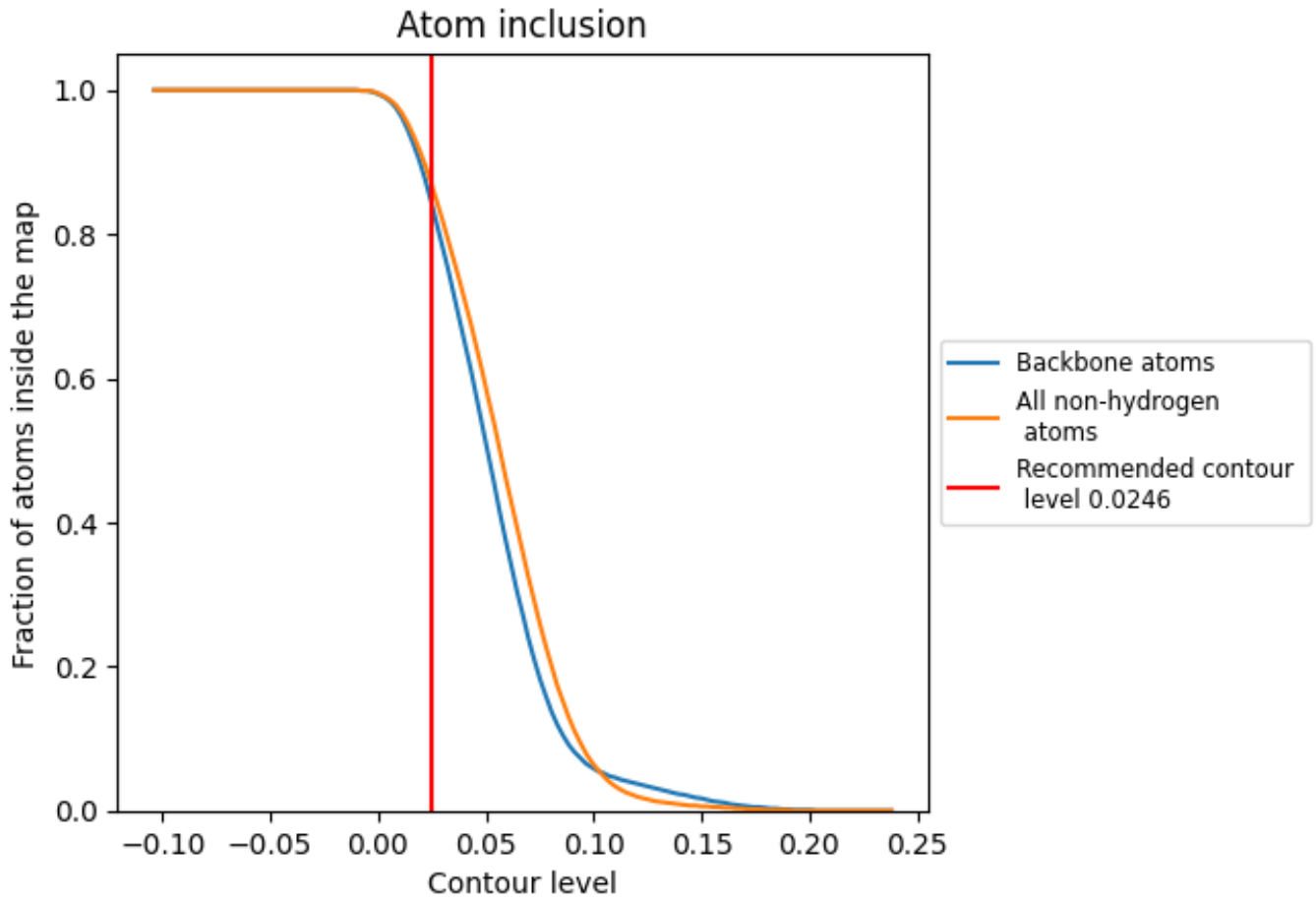
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0246).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 87% 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 (0.0246) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.6930
0	0.8750	0.7110
1	0.9610	0.7710
2	0.9630	0.7710
3	0.9110	0.7190
4	0.2460	0.4640
X	0.4610	0.4910
Y	0.4240	0.4320
Z	0.4760	0.4560
a	0.9150	0.7070
b	0.8240	0.6450
c	0.9460	0.7560
d	0.9300	0.7460
e	0.8350	0.7050
f	0.4600	0.5490
g	0.5200	0.5570
h	0.5600	0.5970
i	0.9250	0.7350
j	0.9120	0.7450
k	0.9060	0.7310
l	0.9260	0.7400
m	0.9750	0.7620
n	0.7600	0.6570
o	0.8720	0.7260
p	0.9420	0.7520
q	0.8420	0.7010
r	0.9150	0.7360
s	0.8350	0.6920
t	0.7520	0.6550
u	0.7720	0.6710
v	0.9390	0.7440
w	0.9070	0.7350
x	0.7380	0.6570
y	0.8900	0.7070
z	0.9040	0.7260

