



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 07:36 PM EDT

PDB ID : 8G6Y / pdb_00008g6y
EMDB ID : EMD-29788
Title : Structure of WT E.coli ribosome 50S subunit with complexed with mRNA, P-site fMet-NH-tRNA^{fMet} and A-site 3-aminopyridine-4-carboxylic acid charged NH-tRNA^{Phe}
Authors : Majumdar, C.; Cate, J.H.D.
Deposited on : 2023-02-16
Resolution : 2.09 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 ⓘ 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:

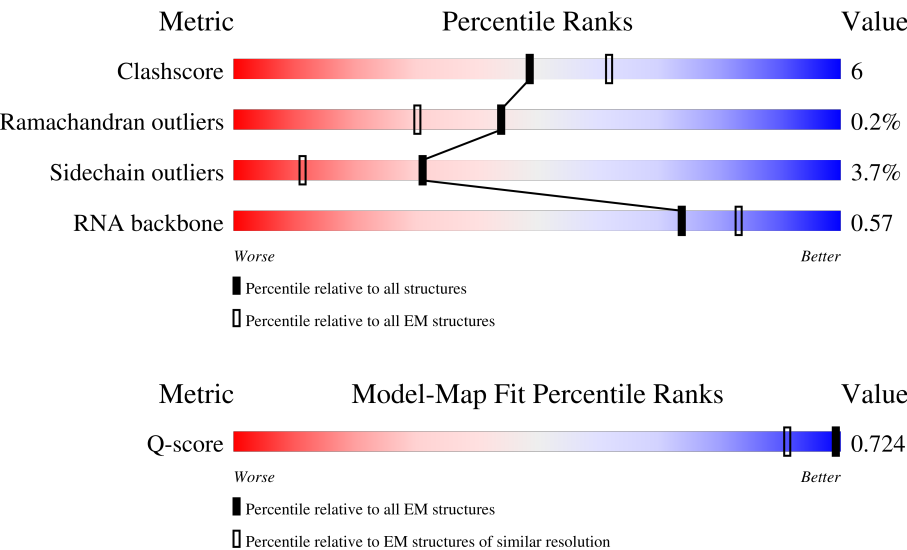
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 2.09 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	2022 (1.60 - 2.59)

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 $\leq 5\%$. 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	0	55	
2	1	46	
3	2	65	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	X	28	
7	Y	76	
8	Z	76	
9	a	2904	
10	b	120	
11	c	273	
12	d	209	
13	e	201	
14	f	179	
15	g	177	
16	h	149	
17	i	142	
18	j	123	
19	k	144	
20	l	136	
21	m	127	
22	n	117	
23	o	115	
24	p	118	
25	q	103	
26	r	110	
27	s	100	
28	t	104	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	u	94	84% 16%
30	v	85	76% 13% 11%
31	w	78	82% 17%
32	x	63	5% 86% 11%
33	y	59	5% 92% 7%
34	z	57	72% 26%

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 93683 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 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called mRNA.

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

- Molecule 7 is a RNA chain called A-site tRNA Phe.

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

- Molecule 8 is a RNA chain called P-site tRNA fMet.

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

- Molecule 9 is a RNA chain called 23S rRNA.

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

- Molecule 10 is a RNA chain called 5S rRNA.

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

- Molecule 11 is a protein called 50S ribosomal protein L2.

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

- Molecule 12 is a protein called 50S ribosomal protein L3.

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

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

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

- Molecule 15 is a protein called 50S ribosomal protein L6.

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

- Molecule 16 is a protein called 50S ribosomal protein L9.

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

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

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

- Molecule 19 is a protein called 50S ribosomal protein L15.

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

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	conflict	UNP A1AGK1

- Molecule 21 is a protein called 50S ribosomal protein L17.

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

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called Ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	v	76	Total	C	N	O	S	0	0
			576	357	114	104	1		

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

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

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

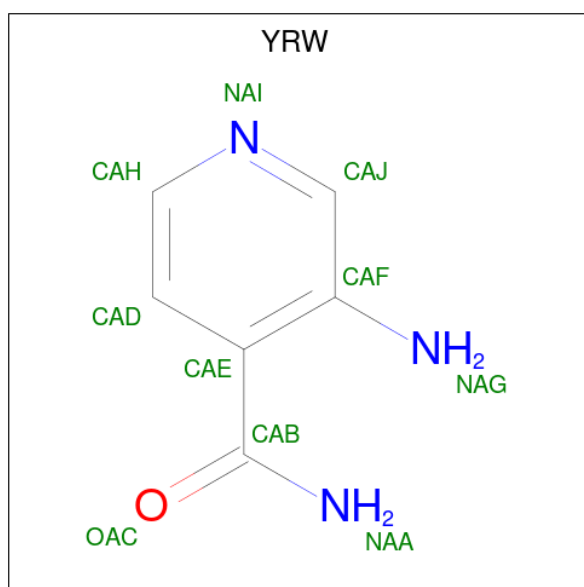
- Molecule 34 is a protein called 50S ribosomal protein L32.

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

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

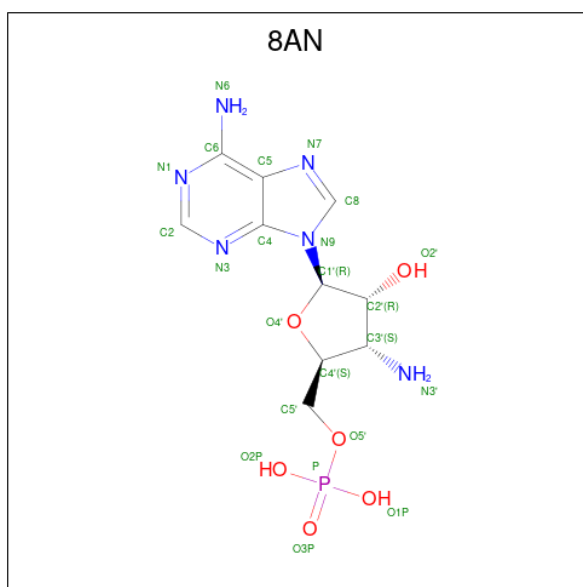
Mol	Chain	Residues	Atoms		AltConf
35	3	1	Total	Zn	0
			1	1	
35	4	1	Total	Zn	0
			1	1	

- Molecule 36 is 3-aminopyridine-4-carboxamide (CCD ID: YRW) (formula: C₆H₇N₃O) (labeled as "Ligand of Interest" by depositor).



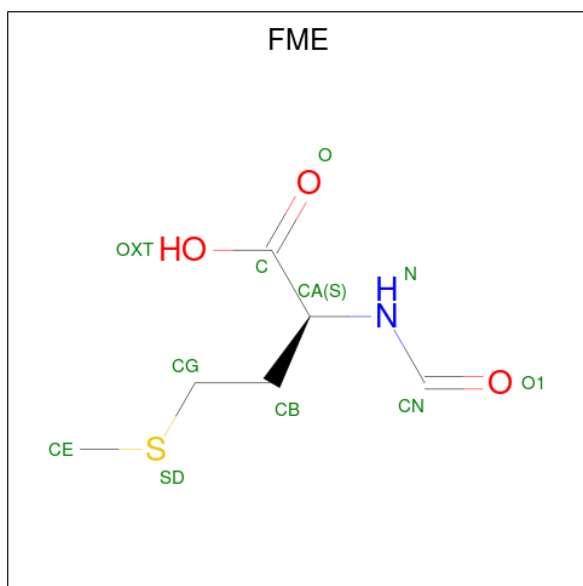
Mol	Chain	Residues	Atoms				AltConf
36	Y	1	Total	C	N	O	0
			10	6	3	1	

- Molecule 37 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (CCD ID: 8AN) (formula: C₁₀H₁₅N₆O₆P).



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

- Molecule 38 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
38	Z	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	a	224	Total 224	Mg 224	0
39	b	5	Total 5	Mg 5	0
39	d	1	Total 1	Mg 1	0
39	z	1	Total 1	Mg 1	0

- Molecule 40 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
40	a	13	Total 13	K 13	0
40	c	2	Total 2	K 2	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	0	1	Total 1	O 1	0
41	1	16	Total 16	O 16	0
41	2	22	Total 22	O 22	0
41	3	2	Total 2	O 2	0
41	Z	1	Total 1	O 1	0
41	a	3019	Total 3019	O 3019	0
41	b	38	Total 38	O 38	0
41	c	84	Total 84	O 84	0
41	d	36	Total 36	O 36	0
41	e	28	Total 28	O 28	0
41	i	9	Total 9	O 9	0
41	j	12	Total 12	O 12	0

Continued on next page...

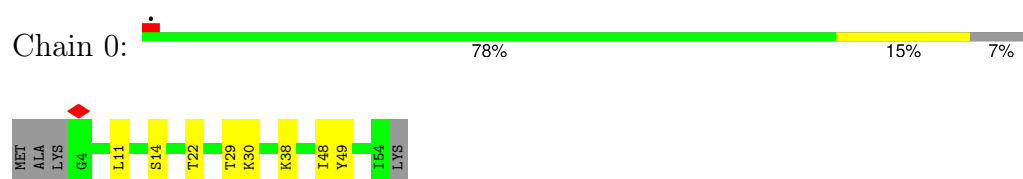
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
41	k	26	Total 26	O 26	0
41	l	24	Total 24	O 24	0
41	m	21	Total 21	O 21	0
41	o	9	Total 9	O 9	0
41	p	20	Total 20	O 20	0
41	q	12	Total 12	O 12	0
41	r	24	Total 24	O 24	0
41	s	7	Total 7	O 7	0
41	t	1	Total 1	O 1	0
41	u	4	Total 4	O 4	0
41	v	10	Total 10	O 10	0
41	w	9	Total 9	O 9	0
41	x	1	Total 1	O 1	0
41	z	24	Total 24	O 24	0

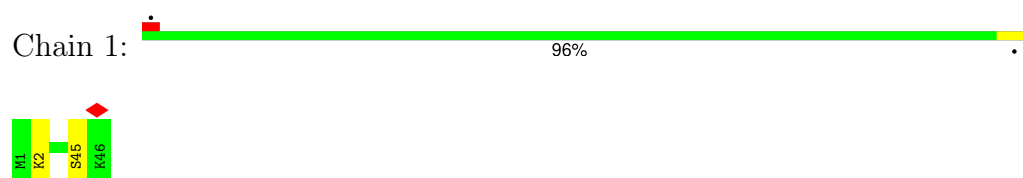
3 Residue-property plots [i](#)

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.

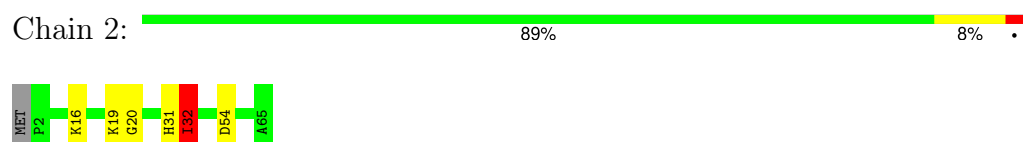
- Molecule 1: 50S ribosomal protein L33



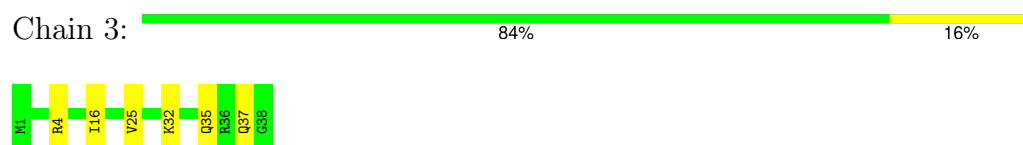
- Molecule 2: 50S ribosomal protein L34



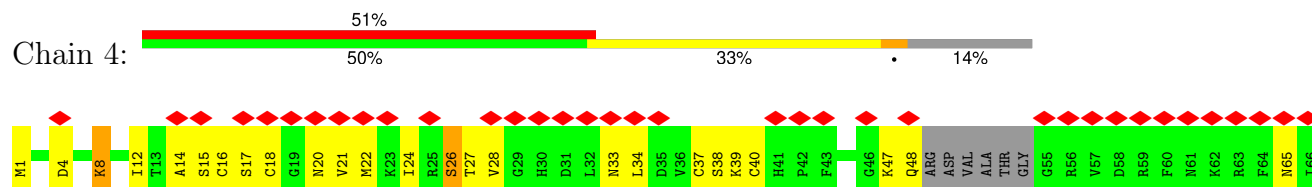
- Molecule 3: 50S ribosomal protein L35



- Molecule 4: 50S ribosomal protein L36

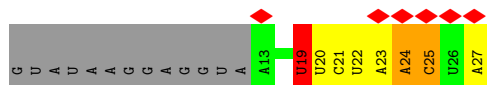


- Molecule 5: 50S ribosomal protein L31

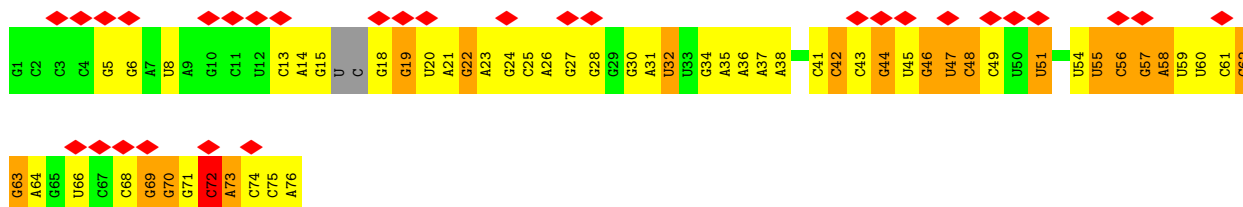


PRO
GLY
SER
LYS

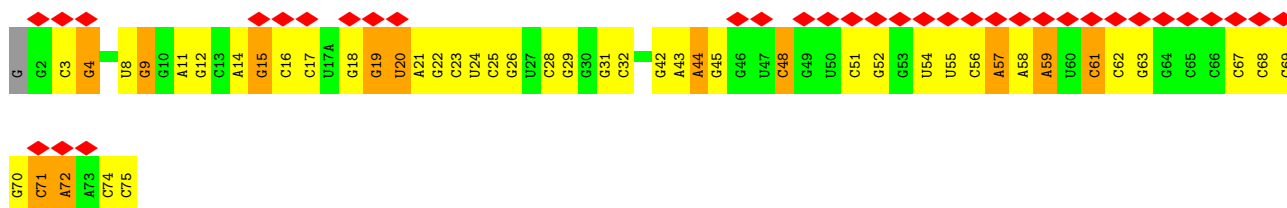
• Molecule 6: mRNA



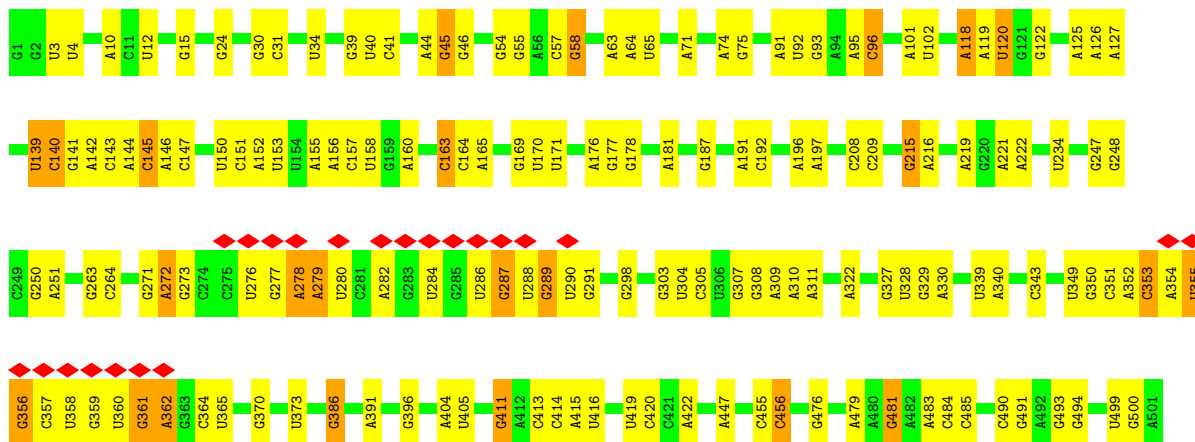
• Molecule 7: A-site tRNA Phe



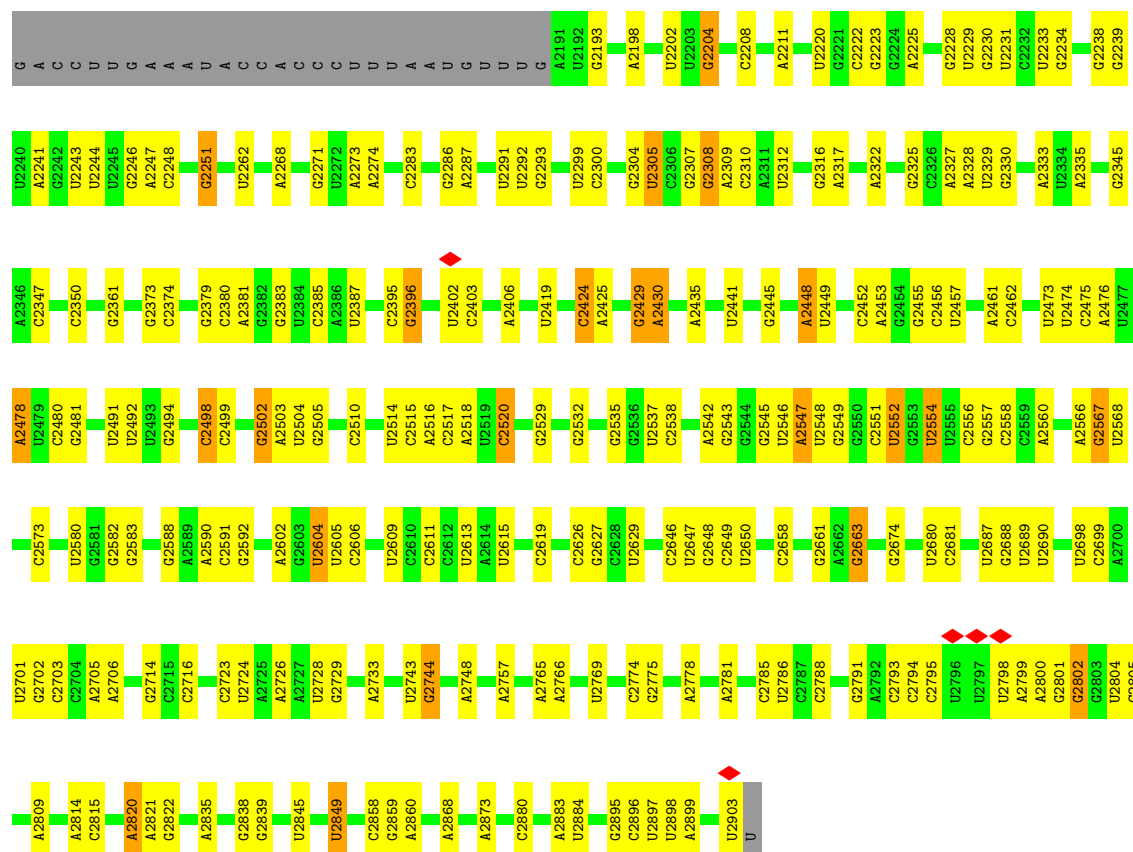
• Molecule 8: P-site tRNA fMet



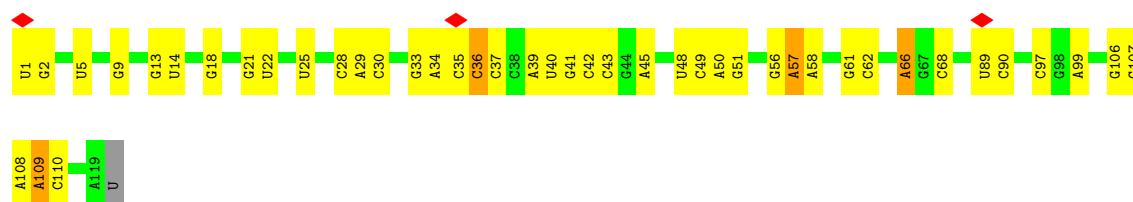
• Molecule 9: 23S rRNA



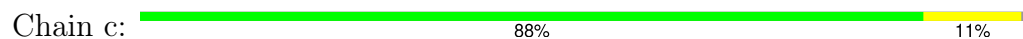
G	U1991	G1869	A1744	C1592	C1498	U1400	G1187	A	U999	G881	U755	A613	A502
C	G1992	C1870	A1745	A1593	A1504	U1405	G1197	A	A1000	G882	G760	A614	A503
U	U1993	A1871	U1746	U1594	A1505	U1406	G1198	C	G1001	G883	A761	U615	A504
C	C1997	G1872	U1747	U1599	U1506	G1407	U1199	G	C1005	U884	G775	A626	A505
U	U1998	C1873	C1748	C1600	U1507	G1408	C1200	A	U1012	C885	G776	C634	C609
A	G2012	G1874	A1754	A1603	A1508	U1412	U1224	A	U1013	A886	A782	C635	G530
U	A2013	G1875	A1762	C1604	A1509	A1413	G1225	U	C1013	U887	G783	C636	G531
G	A2014	A1876	G1763	A1605	G1510	U1414	A1226	A	G1026	C888	G784	G637	A532
U	A2015	G1878	C1764	C1607	G1511	U1415	A1227	G	U1027	C889	G785	G638	G533
C	A2020	C1879	A1773	A1608	U1513	G1416	G1250	C	A1028	C990	U639	U534	U534
U	C2021	G1884	U1778	A1614	G1514	C1417	A1253	U	A1029	G891	A788	U637	G537
G	U2022	A1889	U1779	A1618	A1515	G1418	A1256	A	U1033	A892	A789	A538	A538
A	G2023	A1890	U1782	G1622	U1523	A1419	G1257	C	U1040	C893	U790	A644	C644
U	U2026	G1906	A1783	G1627	C1526	C1428	U1263	U	C1045	U895	G905	U646	U646
C	A2030	C1907	A1784	U1647	G1527	A1432	A1268	A	A896	C897	U657	G647	U645
U	A2031	G1908	A1785	U1648	A1528	A1433	A1269	A	A1046	A898	U658	G651	U647
G	G2032	U1911	A1786	G1649	G1529	A1434	C1270	A	G1047	C898	U659	U652	U648
U	A2033	U1912	A1787	U1653	C1533	A1435	G1271	A	C1052	A899	U660	U653	G548
G	G2038	A1915	A1788	G1660	U1534	G1436	A1272	A	C	A900	U661	A654	G549
A	U2039	U1917	A1791	A1664	A1535	C1437	A1273	A	G	G907	U662	A655	C550
G	C2043	G1922	A1794	U1665	C1536	U1438	C1289	A	A	C908	C914	G656	A563
U	C2044	U1923	C1795	A1666	G1537	U1442	C1290	G	G	C909	U668	U657	U568
U	C2055	C1924	U1796	A1672	U1538	A1443	G1300	A	A	A910	U669	U658	U569
U	G2056	C1925	G1797	G1673	U1539	G1444	A1301	U	U	A911	U670	A685	G570
G	U2060	U1929	C1800	G1674	A1544	G1445	C1306	U	G	C912	U671	U686	U571
A	G2061	G1930	A1801	U1681	A1545	G1452	A1307	U	U	U913	U672	A572	A572
G	A2062	U1931	A1802	G1682	A1546	A1453	A1308	U	U	U914	U673	U573	U573
U	C2063	A1932	A1803	U1683	C1547	U1460	U1329	A	G	G915	G703	A574	A574
U	C2064	G1933	C1804	G1684	A1548	C1461	U1332	U	C	A918	G704	A575	A575
U	C2065	U1937	A1805	U1685	A1549	U1462	U1333	U	U	A927	U680	U580	U580
G	C2066	A1938	A1808	C1704	C1550	U1465	A1334	U	U	A928	U681	C581	C581
A	G2069	U1939	C1816	G1710	C1561	U1466	G1352	A	A	U929	U682	A582	A582
C	A2070	C1947	A1829	U1714	U1562	A1469	A1353	U	G	G930	U683	G585	G585
C	C2072	U1955	G1835	G1715	U1563	A1470	G1354	U	A	U931	A715	A586	A586
C	C2073	U1956	A	U1720	C1564	G1478	C1357	U	G	U932	C717	C587	C587
A	U2074	C1957	U1842	G1721	C1565	U1484	G1358	U	A	A933	U689	U588	U588
G	U2075	C1958	C1843	A1722	A1566	U1485	C1361	U	C	U934	A590	U589	U589
U	U2086	C1962	A1847	G1728	A1569	U1486	C1362	U	C	C935	G729	A592	A592
U	C2087	C1963	A1853	U1729	U1578	U1487	A1365	U	A	C937	A730	U593	U593
C	G2093	C1965	A1858	C1730	G1581	U1488	U1379	U	U	A945	G738	U594	U594
U	A2094	A1866	U1859	G1731	C1582	U1489	A1383	A	A	A946	A742	G600	G600
U	C2096	C1967	U1860	C1732	U1584	A1493	C1386	U	U	A947	A743	C801	C801
G	A2097	A1968	G1860	G1733	C1585	A1494	A1387	U	U	C948	U744	A802	A802
A	U2098	A1970	G1867	G1734	A1586	A1495	U1394	A	A	U955	U745	A603	A603
G	U	U1971	C1868	G1738	G1587	A1496	U1399	A	A	C961	U746	U747	U747
C	A	G1972			U1589	U1497	C1399	A	A	G974	A877	A378	A608
					A1590			A	A	A983	G879	A609	A609
					A1591			A	A	A996	G880	U754	C810
								A	A	G997			
								A	A	C998			



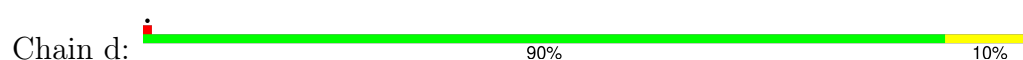
• Molecule 10: 5S rRNA



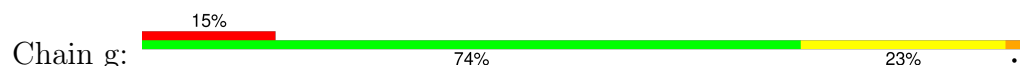
• Molecule 11: 50S ribosomal protein L2



• Molecule 12: 50S ribosomal protein L3



Chain e: 83% 17%



- Molecule 17: 50S ribosomal protein L13

Chain i:  85% 15%



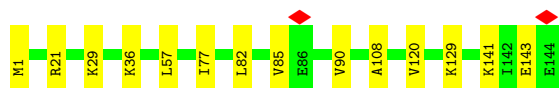
- Molecule 18: 50S ribosomal protein L14

Chain j:  79% 21%



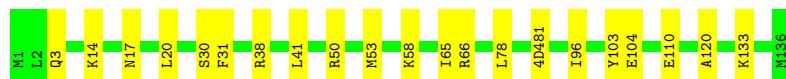
- Molecule 19: 50S ribosomal protein L15

Chain k:  90% 10%



- Molecule 20: 50S ribosomal protein L16

Chain l:  85% 15%



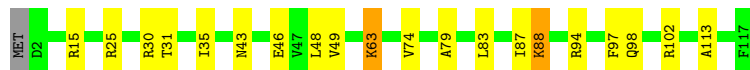
- Molecule 21: 50S ribosomal protein L17

Chain m:  83% 10% 7%



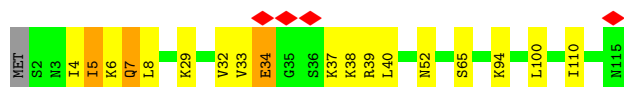
- Molecule 22: 50S ribosomal protein L18

Chain n:  82% 15%



- Molecule 23: 50S ribosomal protein L19

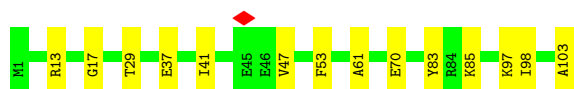
Chain o:  83% 13%



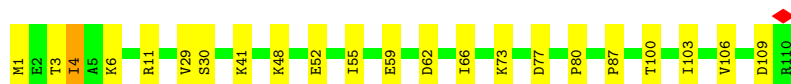
• Molecule 24: 50S ribosomal protein L20

Chain p:  87% 12%

• Molecule 25: Ribosomal protein L21

Chain q:  86% 14%

• Molecule 26: 50S ribosomal protein L22

Chain r:  80% 19%

• Molecule 27: 50S ribosomal protein L23

Chain s:  84% 9% 7%

• Molecule 28: 50S ribosomal protein L24

Chain t:  5% 79% 15%

• Molecule 29: 50S ribosomal protein L25

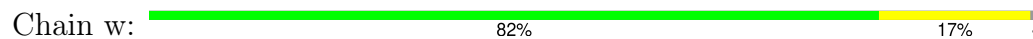
Chain u:  84% 16%

• Molecule 30: 50S ribosomal protein L27

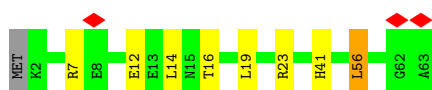
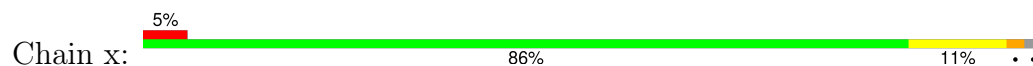
Chain v:  76% 13% 11%



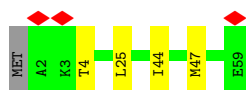
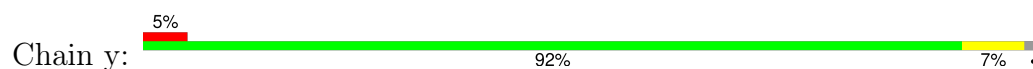
- Molecule 31: 50S ribosomal protein L28



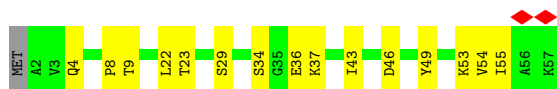
- Molecule 32: 50S ribosomal protein L29



- Molecule 33: 50S ribosomal protein L30



- Molecule 34: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288552	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 ($e^-/\text{\AA}^2$)	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	0.377	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0265	Depositor
Map size ($\text{\AA}$)	408.704, 408.704, 408.704	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.824, 0.824, 0.824	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.26	0/424	0.50	0/565
2	1	0.27	0/380	0.51	0/498
3	2	0.28	0/513	0.50	0/676
4	3	0.30	0/303	0.53	0/397
5	4	0.24	0/488	0.60	0/649
6	X	0.44	1/354 (0.3%)	0.43	0/548
7	Y	0.72	4/1763 (0.2%)	0.74	4/2745 (0.1%)
8	Z	0.22	0/1788	0.45	2/2786 (0.1%)
9	a	0.31	7/65651 (0.0%)	0.41	3/102413 (0.0%)
10	b	0.24	0/2850	0.36	0/4444
11	c	0.27	0/2121	0.51	0/2852
12	d	0.27	0/1576	0.49	0/2119
13	e	0.26	0/1571	0.48	0/2113
14	f	0.22	0/1434	0.56	0/1926
15	g	0.25	0/1343	0.61	0/1816
16	h	0.26	0/306	0.76	0/413
17	i	0.26	0/1152	0.47	0/1551
18	j	0.27	0/955	0.46	0/1279
19	k	0.30	0/1062	0.57	0/1413
20	l	0.26	0/1073	0.47	0/1433
21	m	0.29	0/958	0.57	0/1281
22	n	0.23	0/902	0.54	0/1209
23	o	0.31	0/929	0.52	0/1242
24	p	0.28	0/960	0.50	0/1278
25	q	0.27	0/829	0.53	0/1107
26	r	0.28	0/864	0.46	0/1156
27	s	0.24	0/744	0.49	0/994
28	t	0.26	0/787	0.58	2/1051 (0.2%)
29	u	0.25	0/766	0.50	0/1025
30	v	0.25	0/583	0.46	0/772
31	w	0.27	0/635	0.51	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	x	0.22	0/502	0.49	0/667
33	y	0.25	0/453	0.46	0/605
34	z	0.26	0/450	0.44	0/599
All	All	0.31	12/97469 (0.0%)	0.45	11/146470 (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
3	2	0	1
15	g	0	1
31	w	0	1
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	8	U	C4-O4	17.84	1.59	1.23
7	Y	73	A	P-OP2	-13.11	1.22	1.49
9	a	2588	G	O3'-P	-10.76	1.45	1.61
7	Y	73	A	P-O5'	10.54	1.75	1.59
9	a	2510	C	O3'-P	9.26	1.75	1.61

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	72	C	O3'-P-O5'	-26.09	64.86	104.00
7	Y	73	A	P-O5'-C5'	-9.58	106.53	120.90
7	Y	73	A	OP1-P-OP2	8.59	145.38	119.60
9	a	2605	PSU	P-O3'-C3'	-8.23	107.86	120.20
9	a	2606	C	P-O3'-C3'	-7.70	108.65	120.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	31	HIS	Peptide
15	g	47	ASP	Peptide
31	w	16	ASN	Peptide

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	0	417	0	451	5	0
2	1	377	0	418	2	0
3	2	504	0	572	4	0
4	3	302	0	340	6	0
5	4	480	0	478	15	0
6	X	317	0	161	5	0
7	Y	1578	0	800	54	0
8	Z	1601	0	813	29	0
9	a	59130	0	29764	483	0
10	b	2549	0	1290	26	0
11	c	2082	0	2154	19	0
12	d	1566	0	1618	15	0
13	e	1552	0	1619	21	0
14	f	1410	0	1444	44	0
15	g	1323	0	1371	21	0
16	h	303	0	327	5	0
17	i	1129	0	1162	12	0
18	j	946	0	1023	16	0
19	k	1053	0	1129	13	0
20	l	1075	0	1146	10	0
21	m	945	0	989	8	0
22	n	892	0	923	10	0
23	o	917	0	962	11	0
24	p	947	0	1019	13	0
25	q	816	0	839	9	0
26	r	857	0	922	14	0
27	s	738	0	807	3	0
28	t	779	0	831	13	0
29	u	753	0	780	9	0
30	v	576	0	588	8	0
31	w	625	0	652	9	0
32	x	501	0	531	5	0
33	y	449	0	488	2	0
34	z	444	0	458	10	0
35	3	1	0	0	0	0
35	4	1	0	0	0	0
36	Y	10	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	Z	22	0	11	1	0
38	Z	10	0	10	1	0
39	a	224	0	0	1	0
39	b	5	0	0	0	0
39	d	1	0	0	0	0
39	z	1	0	0	0	0
40	a	13	0	0	0	0
40	c	2	0	0	0	0
41	0	1	0	0	0	0
41	1	16	0	0	0	0
41	2	22	0	0	0	0
41	3	2	0	0	0	0
41	Z	1	0	0	0	0
41	a	3019	0	0	36	0
41	b	38	0	0	0	0
41	c	84	0	0	3	0
41	d	36	0	0	1	0
41	e	28	0	0	0	0
41	i	9	0	0	0	0
41	j	12	0	0	0	0
41	k	26	0	0	0	0
41	l	24	0	0	0	0
41	m	21	0	0	1	0
41	o	9	0	0	0	0
41	p	20	0	0	0	0
41	q	12	0	0	0	0
41	r	24	0	0	0	0
41	s	7	0	0	0	0
41	t	1	0	0	0	0
41	u	4	0	0	0	0
41	v	10	0	0	0	0
41	w	9	0	0	0	0
41	x	1	0	0	1	0
41	z	24	0	0	0	0
All	All	93683	0	58890	847	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 6.

The worst 5 of 847 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)
28:t:49:VAL:O	28:t:54:GLN:HA	1.34	1.22
7:Y:26:A:N6	7:Y:44:G:H1	1.59	1.00
7:Y:26:A:H61	7:Y:44:G:H1	0.90	0.89
5:4:16:CYS:SG	5:4:37:CYS:HB3	2.15	0.86
9:a:1482:G:H1'	9:a:1509:A:H61	1.42	0.84

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	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	4
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	50 (89%)	6 (11%)	0	100	100
11	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
12	d	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
13	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
14	f	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
15	g	174/177 (98%)	153 (88%)	20 (12%)	1 (1%)	21	18
16	h	39/149 (26%)	33 (85%)	5 (13%)	1 (3%)	4	1
17	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
18	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
19	k	142/144 (99%)	137 (96%)	4 (3%)	1 (1%)	18	15
20	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
21	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	n	114/117 (97%)	111 (97%)	2 (2%)	1 (1%)	14	10
23	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
24	p	115/118 (98%)	115 (100%)	0	0	100	100
25	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
26	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
27	s	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
28	t	100/104 (96%)	91 (91%)	8 (8%)	1 (1%)	12	9
29	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
30	v	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
31	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
32	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
33	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
34	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	3112/3337 (93%)	2997 (96%)	109 (4%)	6 (0%)	44	44

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	32	ILE
15	g	47	ASP
19	k	36	LYS
16	h	35	LYS
22	n	88	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	45 (98%)	1 (2%)	45	53
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	50 (98%)	1 (2%)	48	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	45 (82%)	10 (18%)	2	1
11	c	216/218 (99%)	210 (97%)	6 (3%)	38	43
12	d	163/163 (100%)	161 (99%)	2 (1%)	63	72
13	e	165/165 (100%)	160 (97%)	5 (3%)	36	41
14	f	148/150 (99%)	132 (89%)	16 (11%)	6	4
15	g	137/138 (99%)	124 (90%)	13 (10%)	8	5
16	h	32/114 (28%)	31 (97%)	1 (3%)	35	39
17	i	116/116 (100%)	113 (97%)	3 (3%)	40	46
18	j	104/104 (100%)	103 (99%)	1 (1%)	68	76
19	k	103/103 (100%)	102 (99%)	1 (1%)	68	76
20	l	107/107 (100%)	103 (96%)	4 (4%)	30	33
21	m	98/103 (95%)	97 (99%)	1 (1%)	68	76
22	n	86/87 (99%)	80 (93%)	6 (7%)	14	11
23	o	99/100 (99%)	94 (95%)	5 (5%)	21	21
24	p	89/90 (99%)	89 (100%)	0	100	100
25	q	84/84 (100%)	81 (96%)	3 (4%)	31	34
26	r	93/93 (100%)	90 (97%)	3 (3%)	34	38
27	s	80/84 (95%)	77 (96%)	3 (4%)	29	32
28	t	83/85 (98%)	78 (94%)	5 (6%)	17	15
29	u	78/78 (100%)	77 (99%)	1 (1%)	61	69
30	v	57/63 (90%)	55 (96%)	2 (4%)	32	35
31	w	67/68 (98%)	67 (100%)	0	100	100
32	x	54/55 (98%)	53 (98%)	1 (2%)	50	58
33	y	48/49 (98%)	47 (98%)	1 (2%)	47	54
34	z	47/48 (98%)	46 (98%)	1 (2%)	47	54
All	All	2578/2700 (96%)	2482 (96%)	96 (4%)	31	33

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	i	12	LYS
23	o	5	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	k	120	VAL
22	n	25	ARG
23	o	37	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
23	o	66	ASN
27	s	70	HIS
29	u	87	GLN
28	t	46	GLN
27	s	48	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	118/120 (98%)	19 (16%)	0
6	X	14/28 (50%)	4 (28%)	1 (7%)
7	Y	71/76 (93%)	27 (38%)	1 (1%)
8	Z	74/76 (97%)	22 (29%)	0
9	a	2749/2904 (94%)	331 (12%)	0
All	All	3026/3204 (94%)	403 (13%)	2 (0%)

5 of 403 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	X	19	U
6	X	24	A
6	X	25	C
6	X	27	A
7	Y	13	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	X	24	A
7	Y	13	C

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

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
9	2MG	a	2445	9	23,26,27	1.26	3 (13%)	33,38,41	2.19	7 (21%)
9	PSU	a	2504	40,9	18,21,22	1.42	3 (16%)	21,30,33	2.06	4 (19%)
9	3TD	a	1915	9	19,22,23	1.57	5 (26%)	23,32,35	2.15	3 (13%)
9	OMG	a	2251	8,40,9	23,26,27	1.19	3 (13%)	32,38,41	2.03	7 (21%)
12	MEQ	d	150	12	8,9,10	0.47	0	5,10,12	0.25	0
9	OMC	a	2498	39,9	19,22,23	0.76	1 (5%)	25,31,34	0.96	1 (4%)
9	PSU	a	1911	9	18,21,22	1.35	2 (11%)	21,30,33	2.11	3 (14%)
9	PSU	a	746	39,9	18,21,22	1.32	3 (16%)	21,30,33	1.94	4 (19%)
9	6MZ	a	1618	9	22,25,26	1.41	5 (22%)	29,36,39	2.30	11 (37%)
9	PSU	a	2457	9	18,21,22	1.48	4 (22%)	21,30,33	2.04	5 (23%)
9	PSU	a	2604	9	18,21,22	1.46	3 (16%)	21,30,33	2.06	5 (23%)
9	6MZ	a	2030	9	22,25,26	1.43	5 (22%)	29,36,39	2.46	12 (41%)
9	PSU	a	1917	9	18,21,22	1.46	2 (11%)	21,30,33	2.17	4 (19%)
9	2MG	a	1835	9	23,26,27	1.26	3 (13%)	33,38,41	2.27	9 (27%)
9	OMU	a	2552	39,9	19,22,23	1.24	3 (15%)	25,31,34	1.83	5 (20%)
9	G7M	a	2069	9	23,26,27	1.50	4 (17%)	34,39,42	1.67	5 (14%)
9	PSU	a	955	9	18,21,22	1.39	3 (16%)	21,30,33	2.07	4 (19%)
9	2MA	a	2503	39,40,9	22,25,26	1.45	4 (18%)	32,37,40	2.33	9 (28%)
9	PSU	a	2605	9	18,21,22	1.40	3 (16%)	21,30,33	2.18	4 (19%)
9	PSU	a	2580	9	18,21,22	1.36	3 (16%)	21,30,33	2.17	4 (19%)
9	5MU	a	747	9	19,22,23	1.39	5 (26%)	27,32,35	2.16	6 (22%)
9	H2U	a	2449	9	18,21,22	1.13	2 (11%)	19,30,33	1.07	2 (10%)
20	MS6	l	82	20	5,7,8	0.24	0	2,7,9	0.06	0
20	4D4	l	81	20	9,11,12	2.02	2 (22%)	7,13,15	1.05	0
9	5MU	a	1939	9	19,22,23	1.37	5 (26%)	27,32,35	2.14	6 (22%)
9	1MG	a	745	9	23,26,27	1.18	4 (17%)	33,39,42	1.71	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	5MC	a	1962	9	19,22,23	1.62	3 (15%)	26,32,35	1.09	2 (7%)

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
9	2MG	a	2445	9	-	0/9/27/28	0/3/3/3
9	PSU	a	2504	40,9	-	0/7/25/26	0/2/2/2
9	3TD	a	1915	9	-	0/7/25/26	0/2/2/2
9	OMG	a	2251	8,40,9	-	0/9/27/28	0/3/3/3
12	MEQ	d	150	12	-	2/8/9/11	-
9	OMC	a	2498	39,9	-	0/9/27/28	0/2/2/2
9	PSU	a	1911	9	-	0/7/25/26	0/2/2/2
9	PSU	a	746	39,9	-	2/7/25/26	0/2/2/2
9	6MZ	a	1618	9	-	0/9/27/28	0/3/3/3
9	PSU	a	2457	9	-	0/7/25/26	0/2/2/2
9	PSU	a	2604	9	-	0/7/25/26	0/2/2/2
9	6MZ	a	2030	9	-	1/9/27/28	0/3/3/3
9	PSU	a	1917	9	-	0/7/25/26	0/2/2/2
9	2MG	a	1835	9	-	0/9/27/28	0/3/3/3
9	OMU	a	2552	39,9	-	1/9/27/28	0/2/2/2
9	G7M	a	2069	9	-	1/7/25/26	0/3/3/3
9	PSU	a	955	9	-	0/7/25/26	0/2/2/2
9	2MA	a	2503	39,40,9	-	1/7/25/26	0/3/3/3
9	PSU	a	2605	9	-	0/7/25/26	0/2/2/2
9	PSU	a	2580	9	-	0/7/25/26	0/2/2/2
9	5MU	a	747	9	-	1/7/25/26	0/2/2/2
9	H2U	a	2449	9	-	0/7/38/39	0/2/2/2
20	MS6	l	82	20	-	1/4/6/8	-
20	4D4	l	81	20	-	1/11/12/14	-
9	5MU	a	1939	9	-	0/7/25/26	0/2/2/2
9	1MG	a	745	9	-	0/7/25/26	0/3/3/3
9	5MC	a	1962	9	-	2/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	1962	5MC	C5-C4	6.01	1.48	1.44
9	a	2069	G7M	C5-N7	-4.88	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	2503	2MA	C5-C4	4.35	1.46	1.39
9	a	1618	6MZ	C5-C4	4.14	1.46	1.39
9	a	2030	6MZ	C5-C4	4.09	1.46	1.39

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	1915	3TD	N1-C2-N3	8.06	121.99	116.13
9	a	2503	2MA	C5-C4-N3	-7.84	118.92	127.18
9	a	1835	2MG	C2-N3-C4	7.35	121.20	112.00
9	a	2445	2MG	C2-N3-C4	6.98	120.73	112.00
9	a	1917	PSU	N1-C2-N3	6.84	122.38	115.17

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	d	150	MEQ	NE2-CD-CG-CB
12	d	150	MEQ	OE1-CD-CG-CB
9	a	747	5MU	C3'-C4'-C5'-O5'
20	l	81	4D4	NE-CD-CG-CB
9	a	1962	5MC	C2'-C1'-N1-C6

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	a	2251	OMG	1	0
12	d	150	MEQ	3	0
9	a	2498	OMC	1	0
9	a	2604	PSU	1	0
9	a	2030	6MZ	2	0
9	a	2552	OMU	1	0
9	a	2069	G7M	1	0
9	a	1939	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 251 ligands modelled in this entry, 248 are monoatomic - leaving 3 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	YRW	Y	101	7	10,10,10	2.74	3 (30%)	12,13,13	1.70	1 (8%)
38	FME	Z	102	37	8,9,10	0.92	0	8,9,11	0.92	0
37	8AN	Z	101	38,8,39	21,24,25	0.71	1 (4%)	26,35,38	0.47	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	YRW	Y	101	7	-	0/4/4/4	0/1/1/1
38	FME	Z	102	37	-	4/7/9/11	-
37	8AN	Z	101	38,8,39	-	1/7/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Y	101	YRW	CAE-CAB	-7.48	1.39	1.50
36	Y	101	YRW	CAJ-NAI	2.91	1.40	1.34
37	Z	101	8AN	C3'-N3'	-2.83	1.43	1.47
36	Y	101	YRW	CAH-NAI	2.32	1.40	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Y	101	YRW	CAE-CAF-NAG	-4.41	116.53	122.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

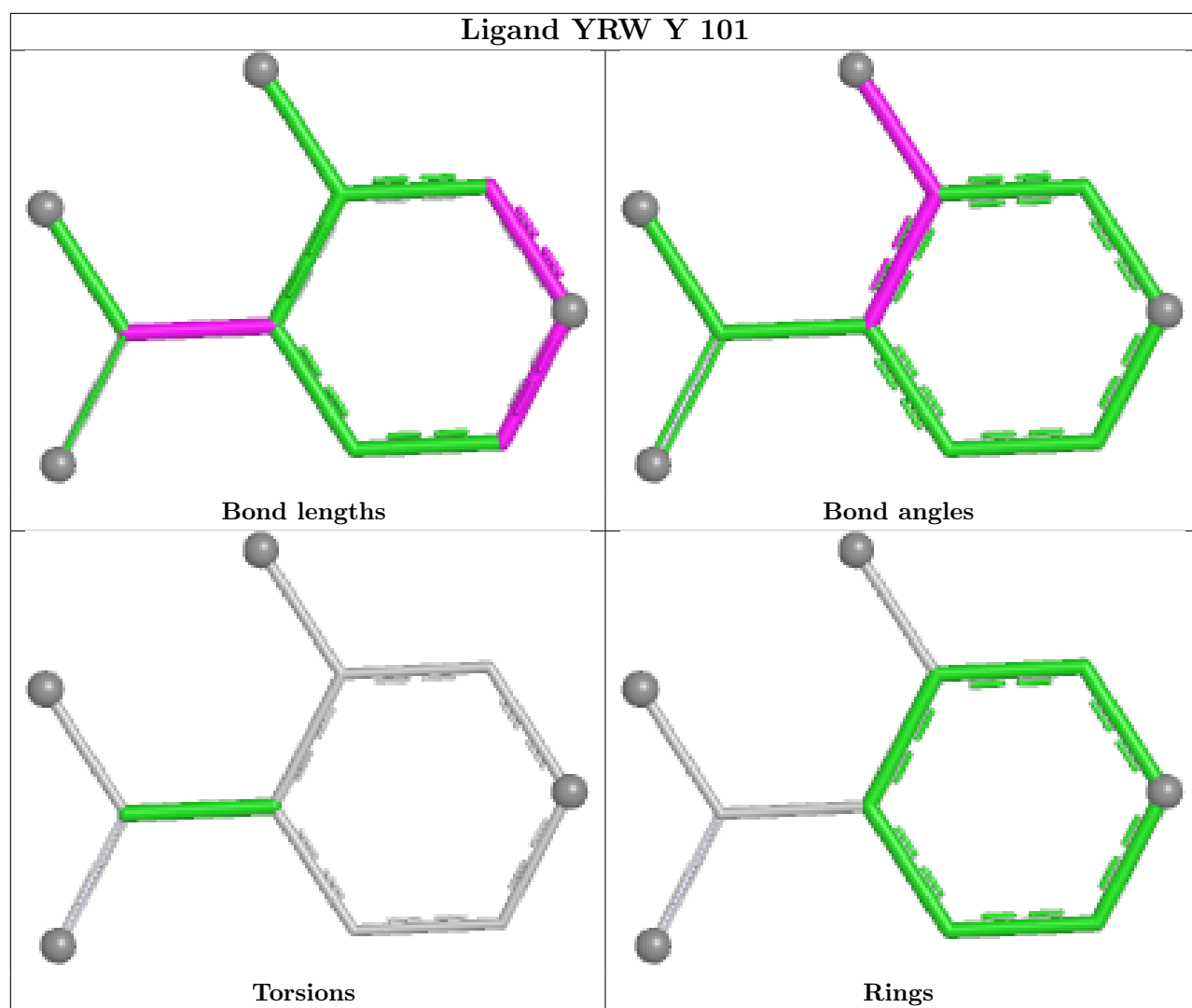
Mol	Chain	Res	Type	Atoms
37	Z	101	8AN	C4'-C5'-O5'-P
38	Z	102	FME	N-CA-CB-CG
38	Z	102	FME	C-CA-CB-CG
38	Z	102	FME	CB-CG-SD-CE
38	Z	102	FME	CA-CB-CG-SD

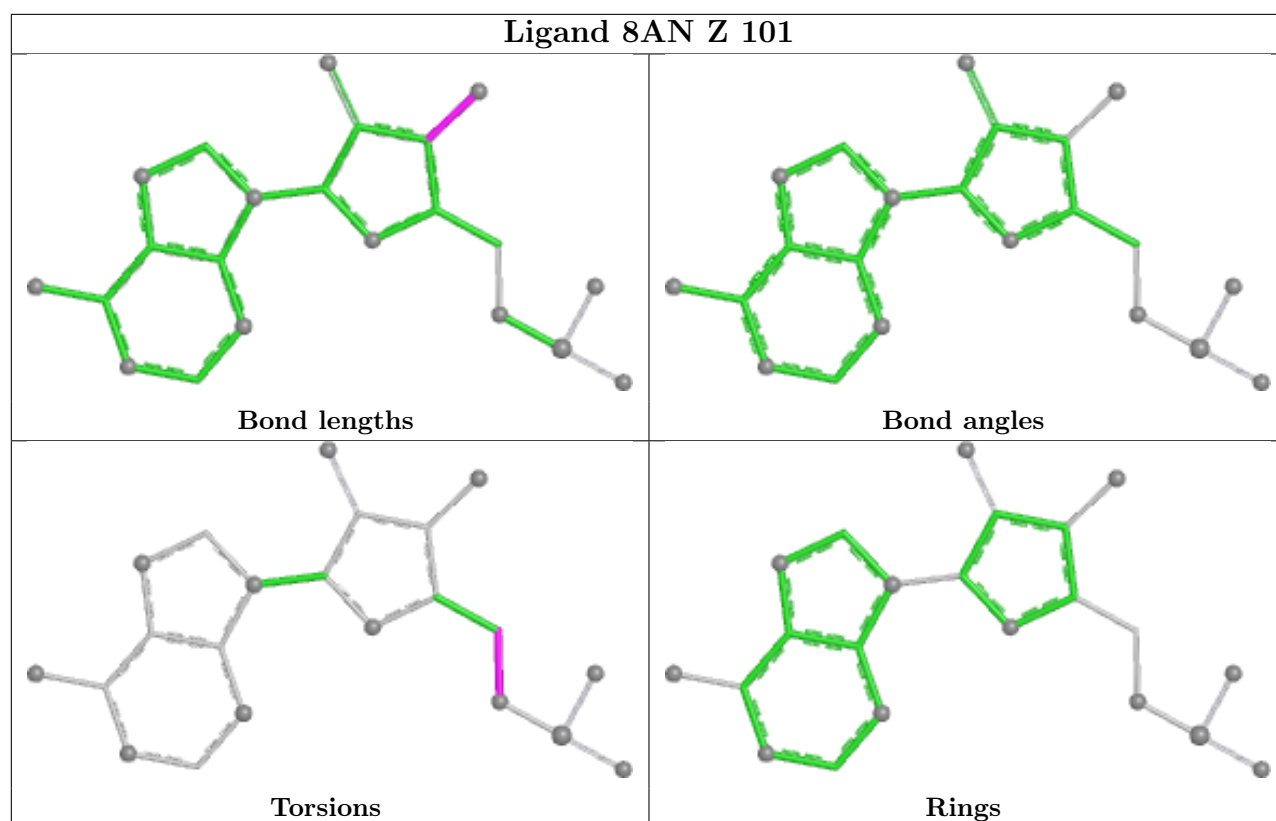
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	Y	101	YRW	1	0
38	Z	102	FME	1	0
37	Z	101	8AN	1	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

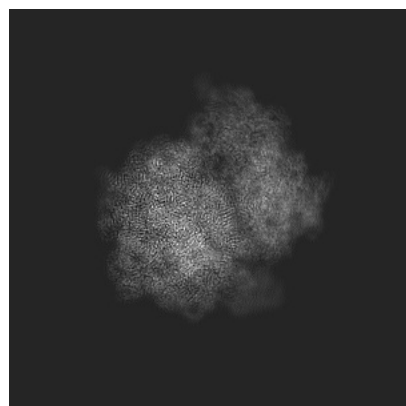
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29788. These allow visual inspection of the internal detail of the map and identification of artifacts.

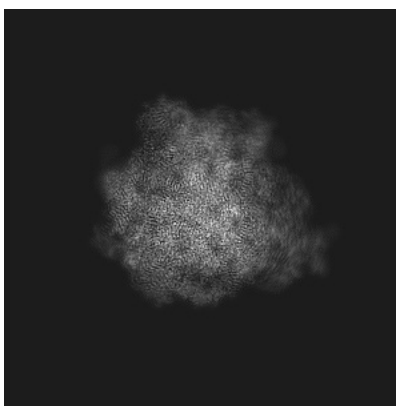
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

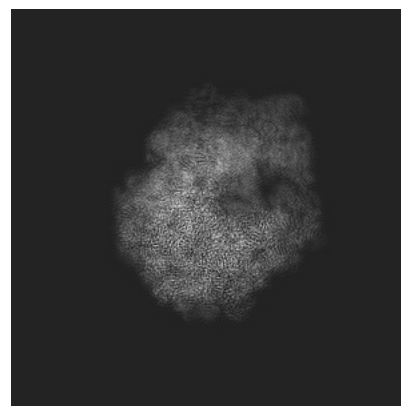
6.1.1 Primary map



X

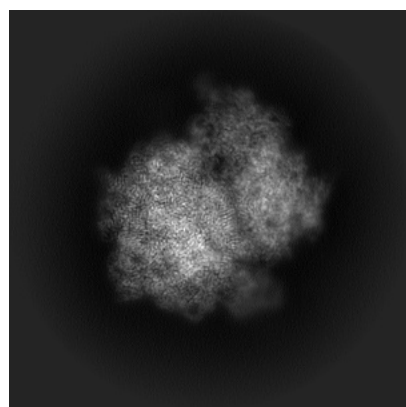


Y

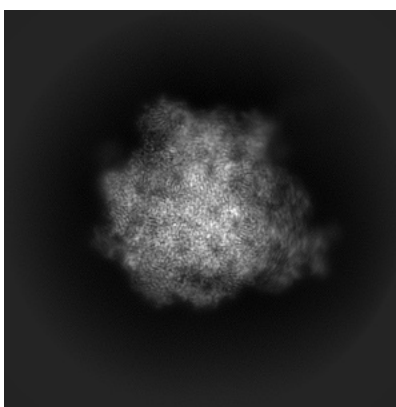


Z

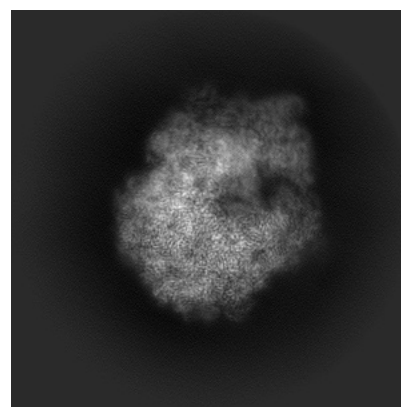
6.1.2 Raw map



X



Y

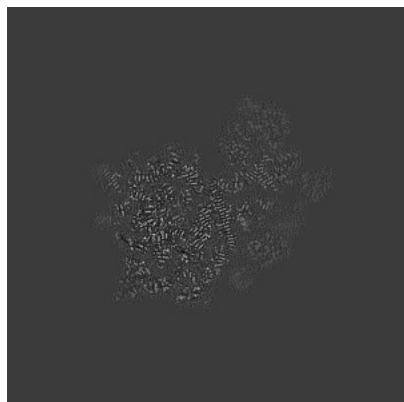


Z

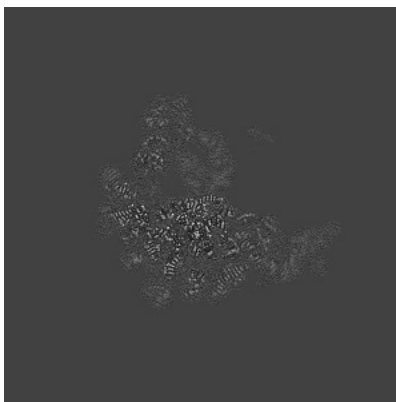
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

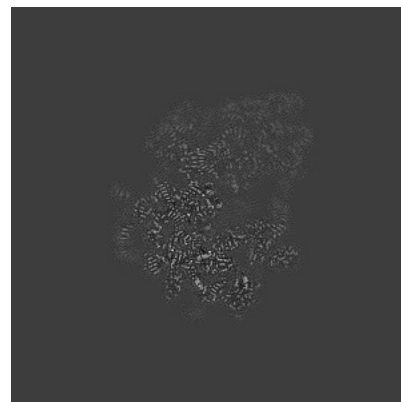
6.2.1 Primary map



X Index: 248

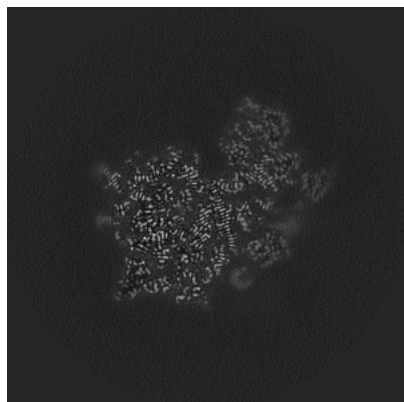


Y Index: 248

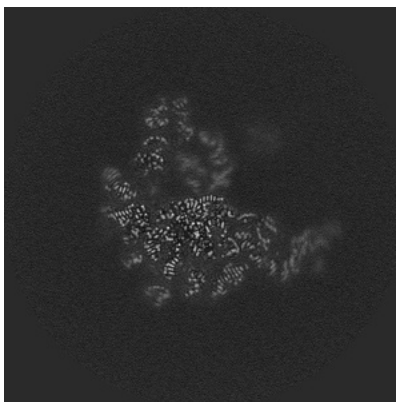


Z Index: 248

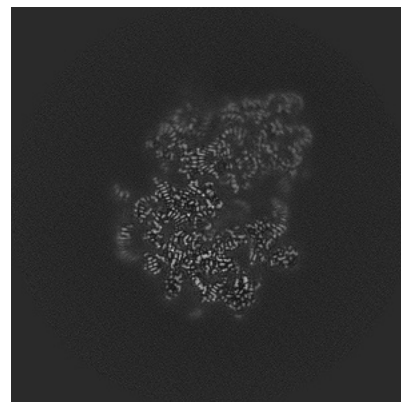
6.2.2 Raw map



X Index: 248



Y Index: 248



Z Index: 248

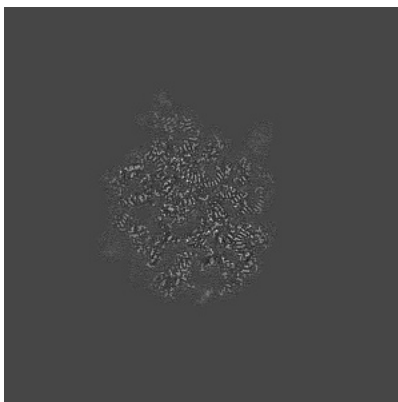
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 218

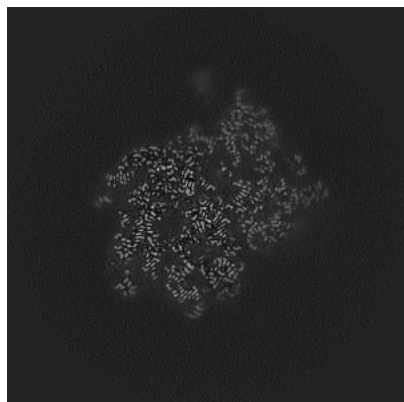


Y Index: 205

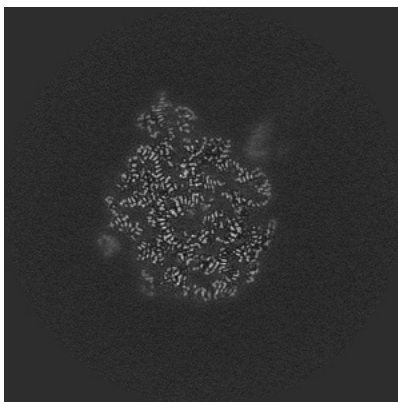


Z Index: 205

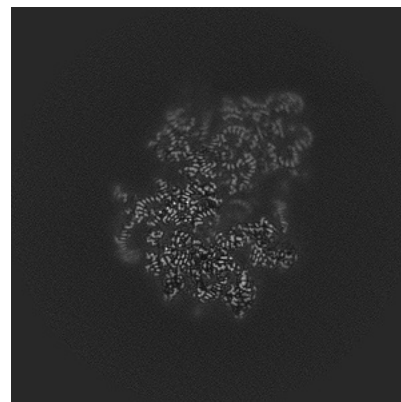
6.3.2 Raw map



X Index: 223



Y Index: 213

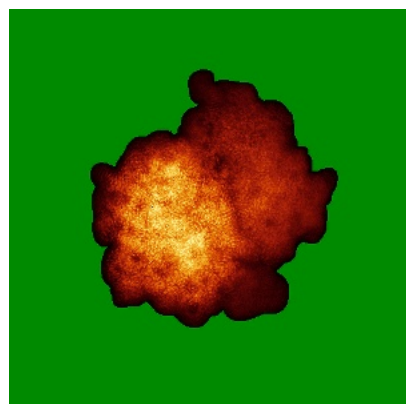


Z Index: 245

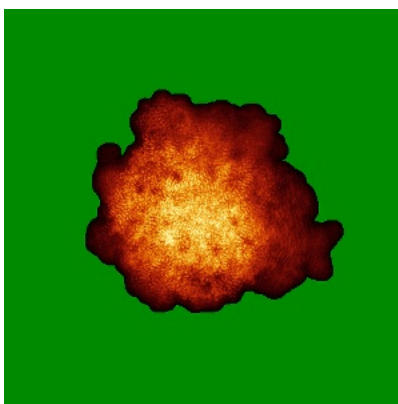
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

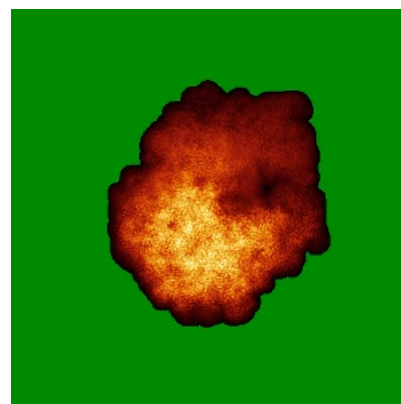
6.4.1 Primary map



X

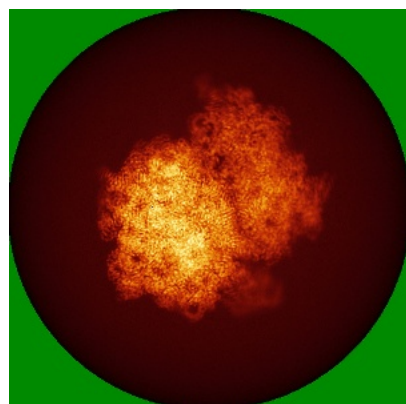


Y

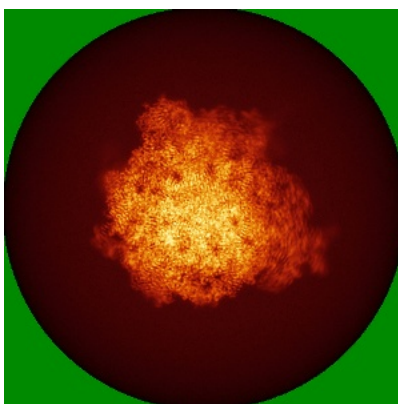


Z

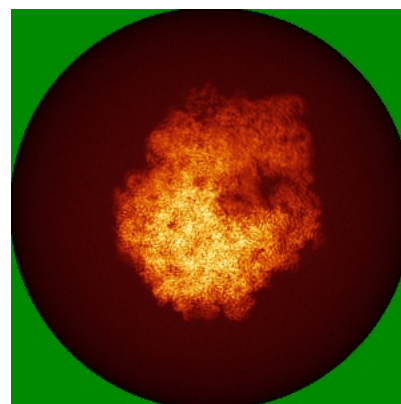
6.4.2 Raw map



X



Y

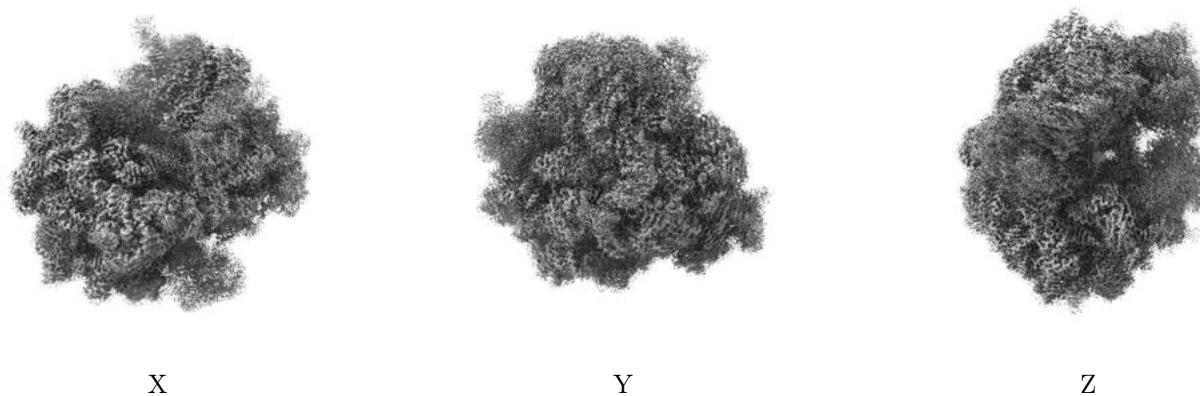


Z

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.

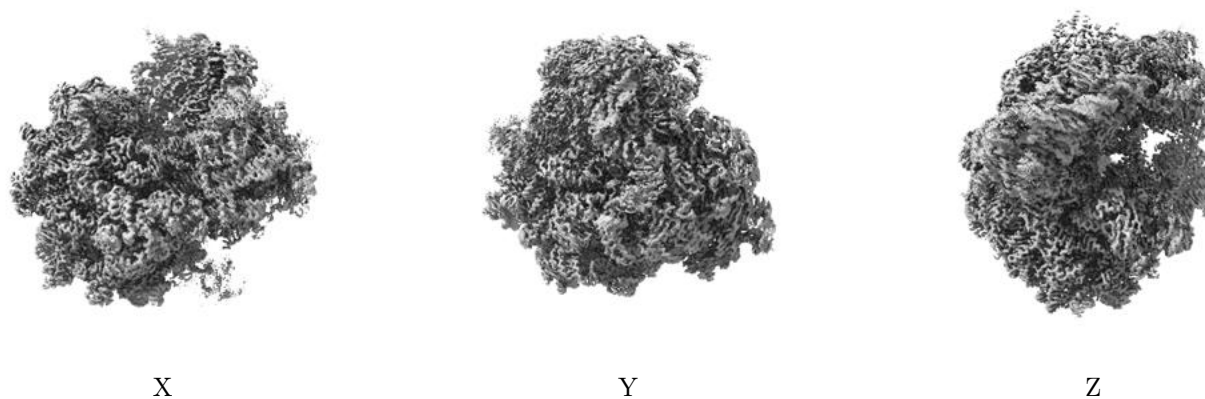
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0265. 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



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.

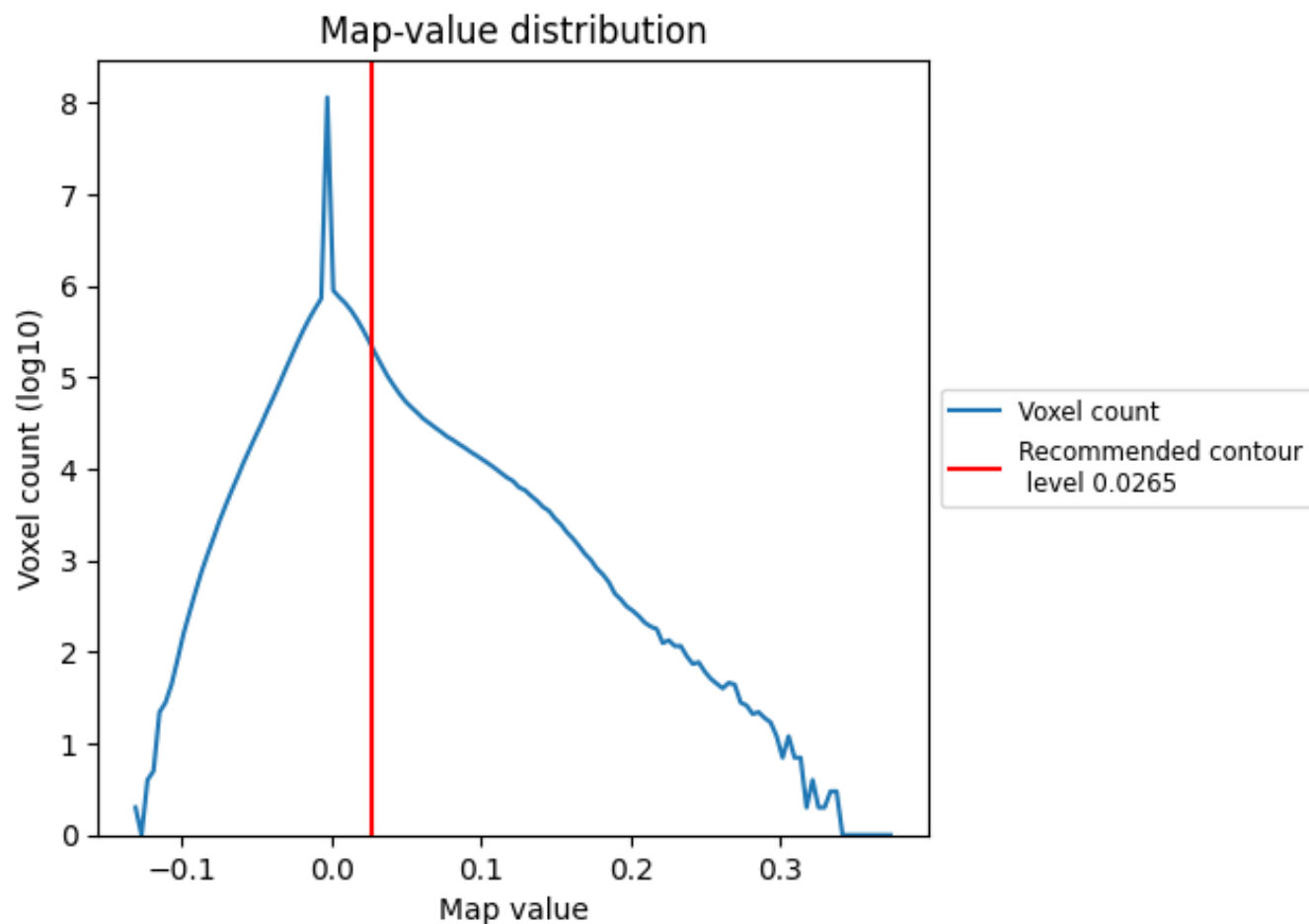
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

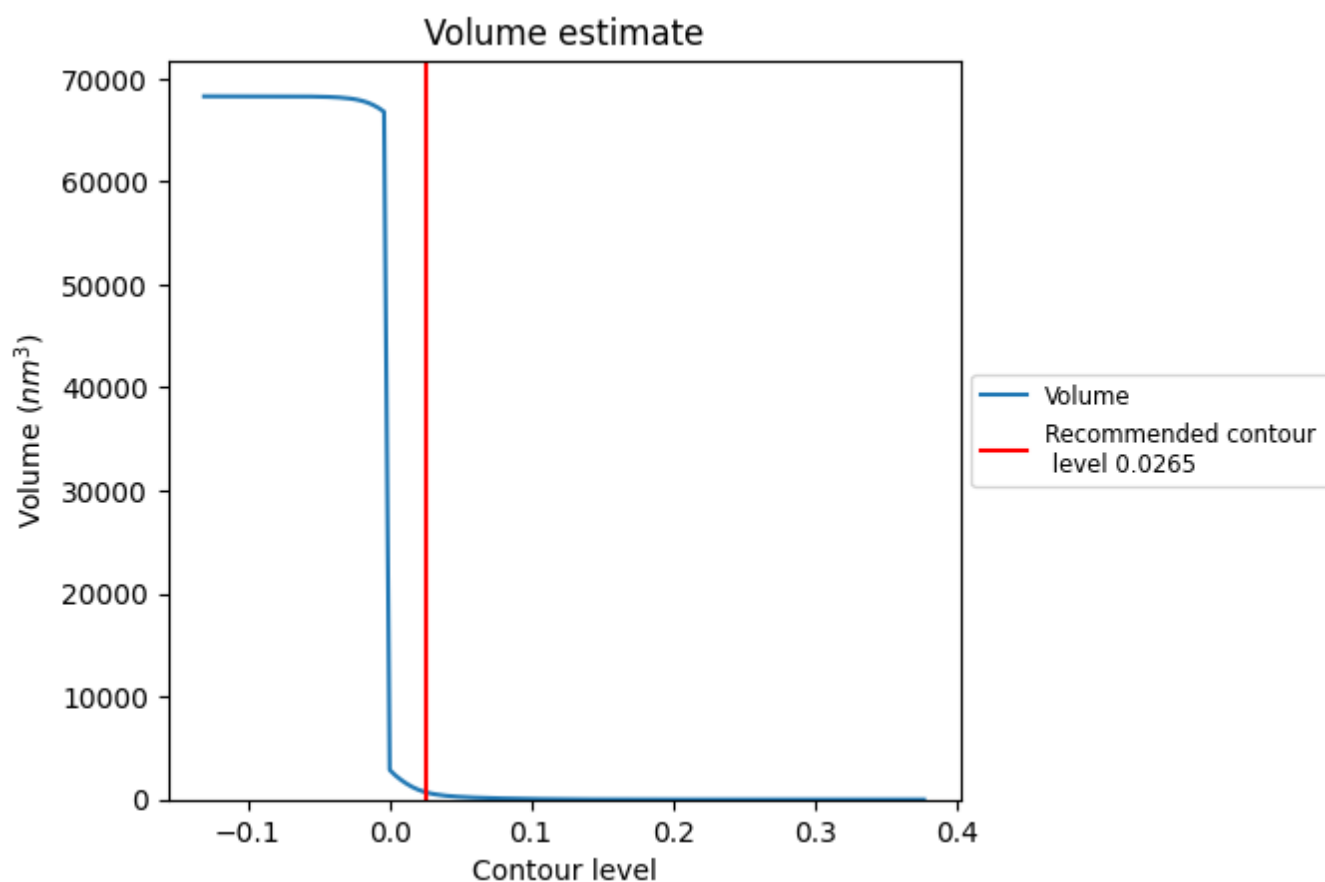
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

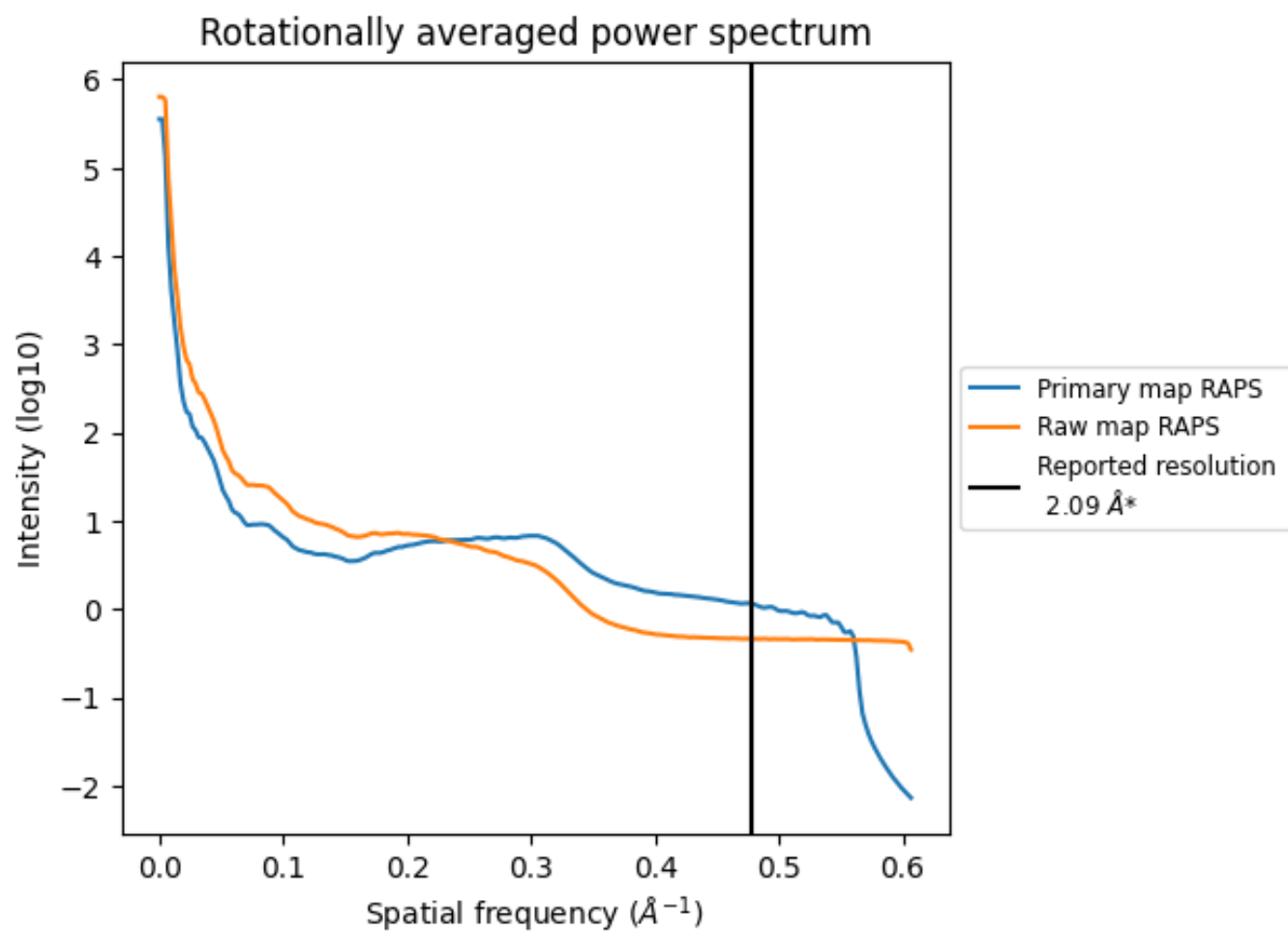
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 687 nm^3 ; this corresponds to an approximate mass of 620 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 ⓘ

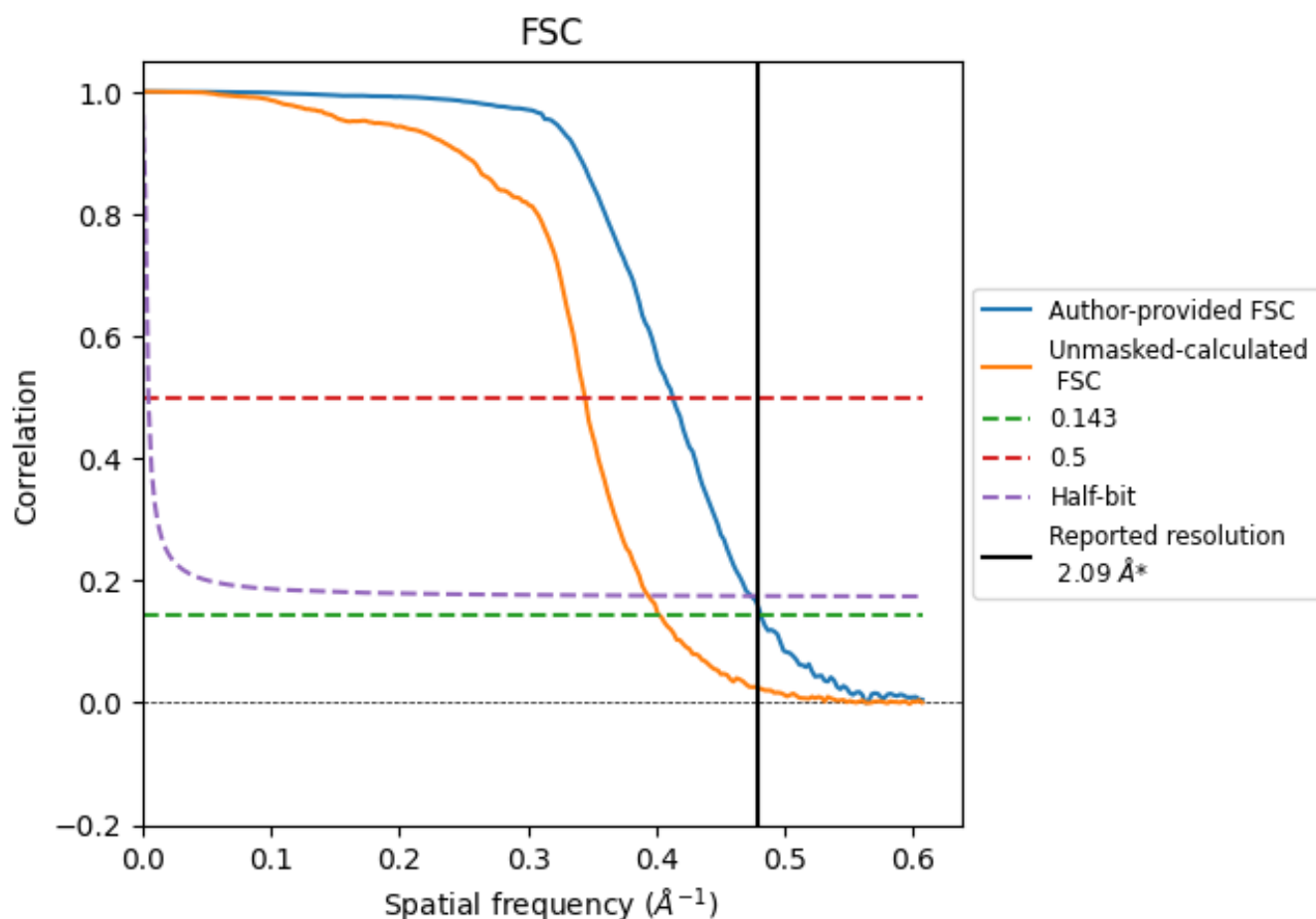


*Reported resolution corresponds to spatial frequency of 0.478 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.478 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

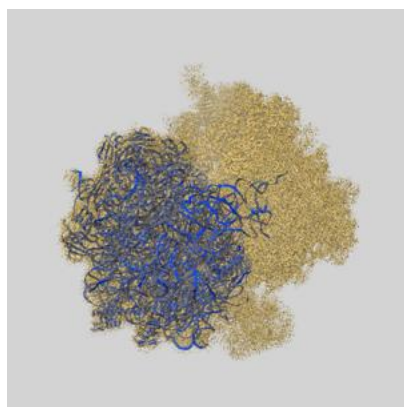
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.09	-	-
Author-provided FSC curve	2.08	2.42	2.11
Unmasked-calculated*	2.49	2.90	2.54

*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 2.49 differs from the reported value 2.09 by more than 10 %

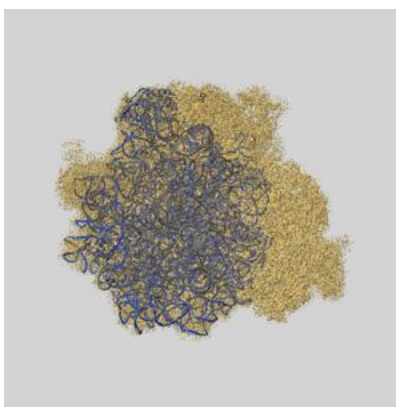
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29788 and PDB model 8G6Y. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

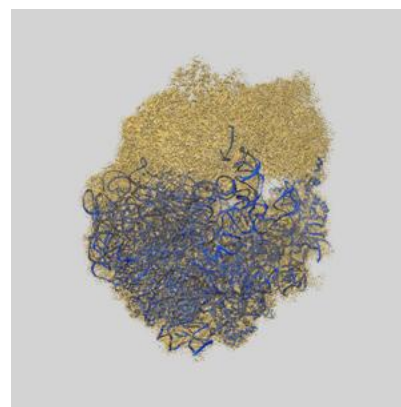
9.1 Map-model overlay [i](#)



X



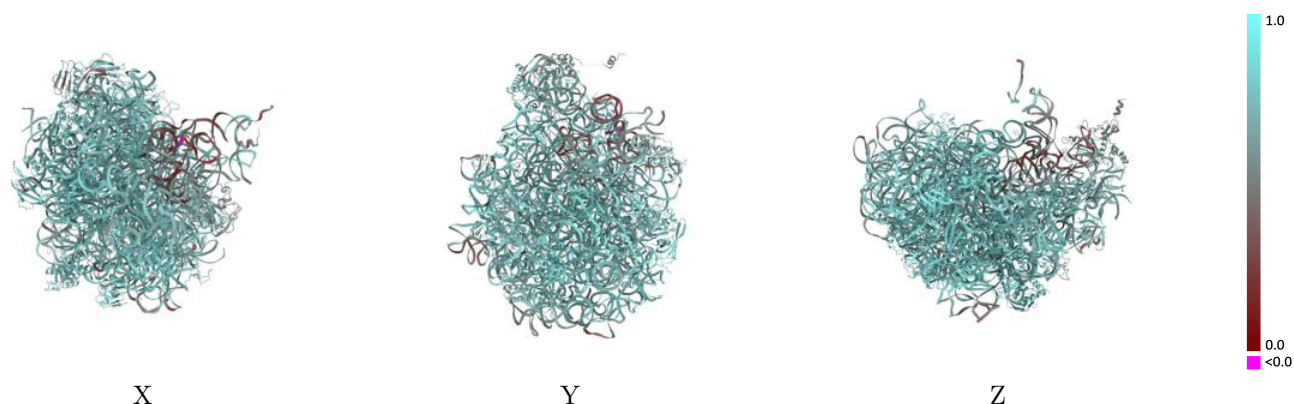
Y



Z

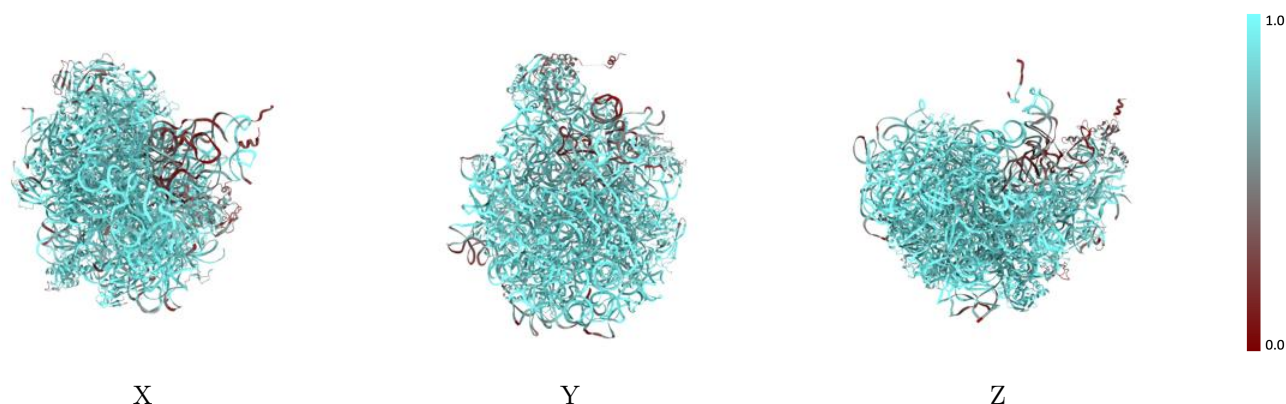
The images above show the 3D surface view of the map at the recommended contour level 0.0265 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



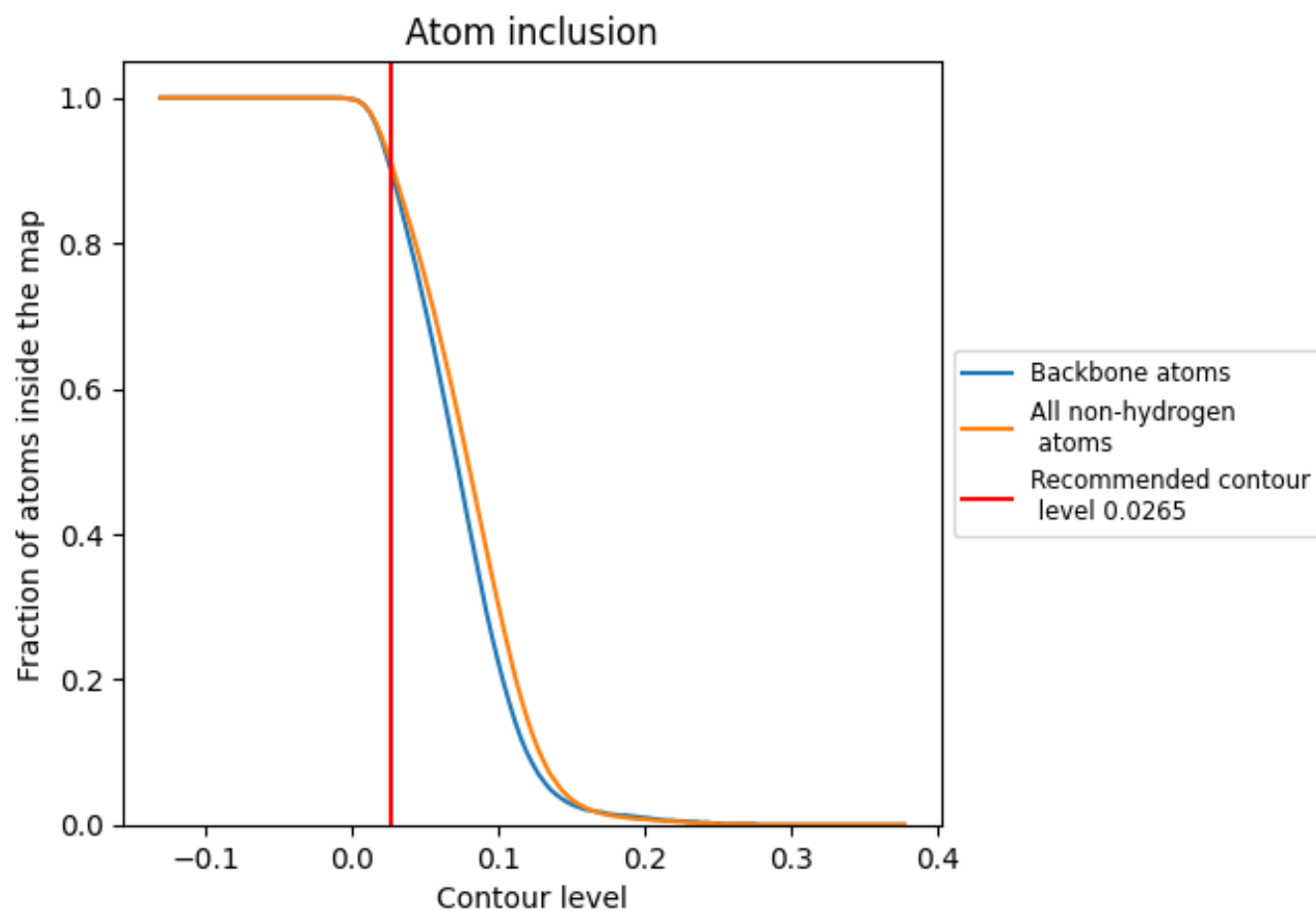
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.0265).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.0265) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9120	 0.7240
0	 0.8920	 0.7380
1	 0.9690	 0.8000
2	 0.9860	 0.7970
3	 0.9490	 0.7580
4	 0.3880	 0.5030
X	 0.5650	 0.5140
Y	 0.4730	 0.4260
Z	 0.5100	 0.4750
a	 0.9460	 0.7360
b	 0.9060	 0.6800
c	 0.9720	 0.7820
d	 0.9500	 0.7820
e	 0.9000	 0.7420
f	 0.5990	 0.5890
g	 0.6930	 0.6070
h	 0.7270	 0.6540
i	 0.9620	 0.7840
j	 0.9490	 0.7730
k	 0.9430	 0.7620
l	 0.9470	 0.7680
m	 0.9900	 0.7930
n	 0.8970	 0.7120
o	 0.9260	 0.7630
p	 0.9760	 0.7950
q	 0.9250	 0.7510
r	 0.9350	 0.7730
s	 0.8880	 0.7270
t	 0.8610	 0.7000
u	 0.8750	 0.7190
v	 0.9400	 0.7790
w	 0.9470	 0.7560
x	 0.8180	 0.6840
y	 0.9150	 0.7540
z	 0.9230	 0.7660

