wwPDB EM Validation Summary Report

Sep 16, 2026 – 04:30 PM EDT

PDB ID	:	7S1I / pdb_00007s1i
EMDB ID	:	EMD-24802
Title	:	Wild-type Escherichia coli stalled ribosome with antibiotic radezolid
Authors	:	Young, I.D.; Stojkovic, V.; Tsai, K.; Lee, D.J.; Fraser, J.S.; Galonic Fujimori, D.
Deposited on	:	2021-09-02
Resolution	:	2.48 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:

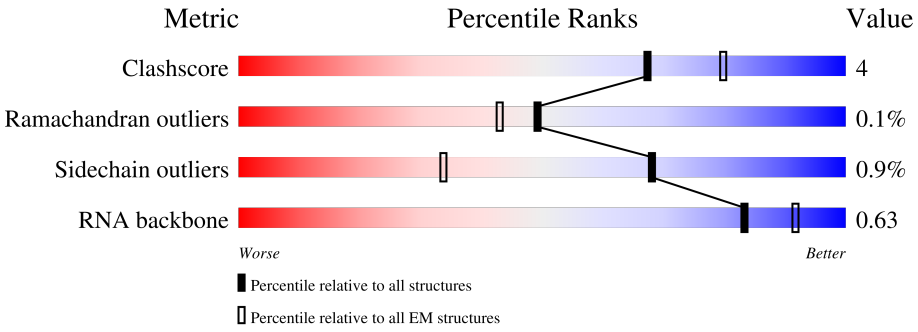
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

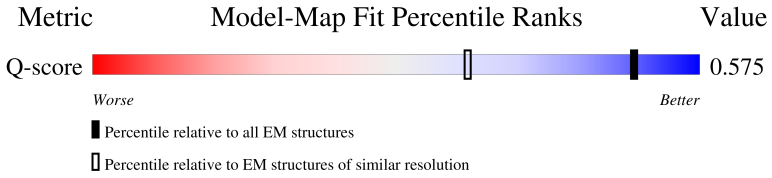
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.48 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	6178 (1.98 - 2.98)

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	1	92	71% 15% 14%
2	2	87	78% 18%
3	3	71	15% 89% 10%

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Mol	Chain	Length	Quality of chain
4	4	15	40% 60%
5	A	76	63% 26% 11%
6	C	1540	80% 18%
7	D	241	10% 72% 17% 10%
8	E	233	76% 12% 12%
9	F	206	83% 16%
10	G	167	77% 12% 10%
11	H	135	60% 14% 26%
12	I	2904	79% 17%
13	J	120	83% 15%
14	K	273	90% 10%
15	L	209	89% 11%
16	M	201	88% 11%
17	N	179	79% 19%
18	O	177	87% 11%
19	P	149	9% 75% 25%
20	Q	70	69% 17% 14%
21	R	142	92% 8%
22	S	123	85% 13%
23	T	144	91% 9%
24	U	136	93% 7%
25	V	127	87% 8% 6%
26	W	117	88% 11%
27	X	115	90% 10%
28	Y	118	97%

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Mol	Chain	Length	Quality of chain
29	Z	103	90% 10%
30	a	110	90% 10%
31	b	100	78% 14% 7%
32	c	104	85% 13%
33	d	94	95% 5%
34	e	85	78% 11% 12%
35	f	78	92% 6%
36	g	63	83% 16%
37	h	59	90% 7%
38	i	57	91% 7%
39	j	55	82% 62% 27% 9%
40	k	46	96%
41	l	65	94% 5%
42	m	38	89% 11%
43	n	179	70% 14% 16%
44	o	130	90% 9%
45	p	130	5% 75% 22%
46	q	103	10% 69% 26% 5%
47	r	129	79% 12% 9%
48	s	5	20% 100%
49	t	124	85% 15%
50	u	118	87% 9%
51	v	101	77% 17% 5%
52	w	89	89% 10%
53	x	82	88% 12%

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Mol	Chain	Length	Quality of chain
54	y	84	
55	z	75	

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 240853 atoms, of which 96700 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 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	79	Total	C	H	N	O	S	0	0
			1303	408	666	120	107	2		

- Molecule 2 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	85	Total	C	H	N	O	S	0	0
			1380	411	715	137	114	3		

- Molecule 3 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	3	70	Total	C	H	N	O	S	0	0
			1219	366	629	125	98	1		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	4	6	Total	C	H	N	O	P	0	0
			190	56	65	20	43	6		

- Molecule 5 is a RNA chain called tRNA(PHE).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	76	Total	C	H	N	O	P	0	0
			2444	724	820	292	532	76		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	C	1540	Total	C	H	N	O	P	0	0
			49665	14735	16628	6057	10705	1540		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D	218	Total	C	H	N	O	S	0	0
			3438	1081	1734	305	311	7		

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	E	206	Total	C	H	N	O	S	0	0
			3321	1028	1697	305	288	3		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	F	205	Total	C	H	N	O	S	0	0
			3352	1026	1709	315	298	4		

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	G	150	Total	C	H	N	O	S	0	0
			2254	687	1149	211	201	6		

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	H	100	Total	C	H	N	O	S	0	0
			1625	515	808	148	148	6		

- Molecule 12 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	I	2898	Total	C	H	N	O	P	0	0
			93548	27768	31319	11448	20115	2898		

- Molecule 13 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	J	118	Total	C	H	N	O	P	0	0
			3809	1126	1280	464	821	118		

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	K	271	Total	C	H	N	O	S	2	0
			4263	1294	2170	427	365	7		

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	L	209	Total	C	H	N	O	S	0	0
			3184	979	1619	288	294	4		

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	M	201	Total	C	H	N	O	S	0	0
			3172	974	1620	283	290	5		

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	N	177	Total	C	H	N	O	S	0	0
			2855	899	1445	249	256	6		

- Molecule 18 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	O	176	Total	C	H	N	O	S	0	0
			2696	832	1373	243	246	2		

- Molecule 19 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	P	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 20 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	Q	60	Total	C	H	N	O	S	0	0
			964	299	484	90	85	6		

- Molecule 21 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	R	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 22 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	S	122	Total	C	H	N	O	S	0	0
			1950	587	1012	180	165	6		

- Molecule 23 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	T	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 24 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	U	136	Total	C	H	N	O	S	0	0
			2231	686	1156	205	178	6		

- Molecule 25 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	V	120	Total	C	H	N	O	S	0	0
			1960	593	1000	196	166	5		

- Molecule 26 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	116	Total	C	H	N	O	0	0
			1817	552	925	178	162		

- Molecule 27 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	X	114	Total	C	H	N	O	S	0	0
			1880	574	963	179	163	1		

- Molecule 28 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	117	Total	C	H	N	O	0	0
			1968	604	1021	192	151		

- Molecule 29 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Z	103	Total	C	H	N	O	S	0	0
			1657	516	841	153	145	2		

- Molecule 30 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	a	110	Total	C	H	N	O	S	0	0
			1780	532	923	166	156	3		

- Molecule 31 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	b	93	Total	C	H	N	O	S	0	0
			1546	466	808	139	131	2		

- Molecule 32 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	102	Total	C	H	N	O	0	0
			1611	492	832	146	141		

- Molecule 33 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	d	94	Total	C	H	N	O	S	0	0
			1534	479	781	137	134	3		

- Molecule 34 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	e	75	Total	C	H	N	O	S	0	0
			1168	356	593	116	102	1		

- Molecule 35 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	f	77	Total	C	H	N	O	S	0	0
			1278	388	653	129	106	2		

- Molecule 36 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	g	62	Total	C	H	N	O	S	0	0
			1033	308	532	98	94	1		

- Molecule 37 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	h	58	Total	C	H	N	O	S	0	0
			938	281	489	87	79	2		

- Molecule 38 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	i	56	Total	C	H	N	O	S	0	0
			904	269	460	94	80	1		

- Molecule 39 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	50	Total	C	H	N	O	0	0
			851	263	442	75	71		

- Molecule 40 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	k	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 41 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	l	64	Total	C	H	N	O	S	0	0
			1077	323	573	105	74	2		

- Molecule 42 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	m	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 43 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	n	151	Total	C	H	N	O	S	0	0
			2419	735	1238	227	215	4		

- Molecule 44 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	o	129	Total	C	H	N	O	S	0	0
			2011	616	1032	173	184	6		

- Molecule 45 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	p	127	Total	C	H	N	O	S	0	0
			2093	634	1071	206	179	3		

- Molecule 46 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	q	98	Total	C	H	N	O	S	0	0
			1615	493	829	150	142	1		

- Molecule 47 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	r	117	Total	C	H	N	O	S	0	0
			1765	540	888	174	160	3		

- Molecule 48 is a protein called nascent peptide chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	s	5	Total	C	H	N	O	S	0	0
			91	32	47	6	5	1		

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	t	123	Total	C	H	N	O	S	0	0
			1972	590	1017	196	165	4		

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	u	115	Total	C	H	N	O	S	0	0
			1845	552	954	179	157	3		

- Molecule 51 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	v	96	Total	C	H	N	O	S	0	0
			1600	483	826	160	128	3		

- Molecule 52 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	w	88	Total	C	H	N	O	S	0	0
			1441	437	731	143	129	1		

- Molecule 53 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	x	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	y	80	Total	C	H	N	O	S	0	0
			1341	411	693	121	113	3		

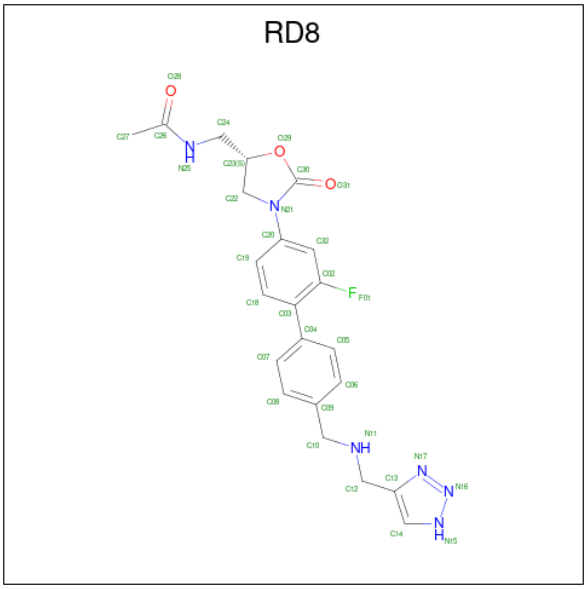
- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	55	Total	C	H	N	O	0	0
			935	288	480	86	81		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	C	93	Total Mg 93 93	0
56	I	113	Total Mg 113 113	0
56	K	1	Total Mg 1 1	0
56	L	1	Total Mg 1 1	0
56	V	1	Total Mg 1 1	0

- Molecule 57 is Radezolid (CCD ID: RD8) (formula: $C_{22}H_{23}FN_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
57	I	1	Total C F H N O 54 22 1 22 6 3	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
58	Q	1	Total Zn 1 1	0
58	m	1	Total Zn 1 1	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	AltConf
59	C	3	Total H O 9 6 3	0
59	I	32	Total H O 96 64 32	0
59	k	1	Total H O 3 2 1	0

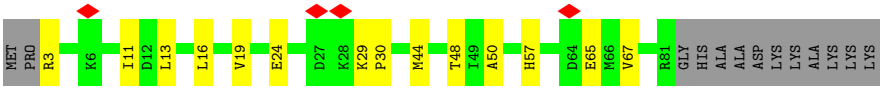
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 30S ribosomal protein S19

Chain 1:

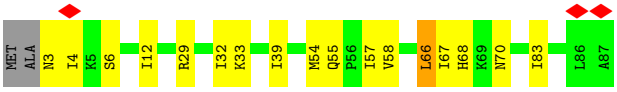




• Molecule 2: 30S ribosomal protein S20

Chain 2:

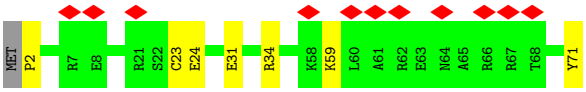




• Molecule 3: 30S ribosomal protein S21

Chain 3:





• Molecule 4: mRNA

Chain 4:

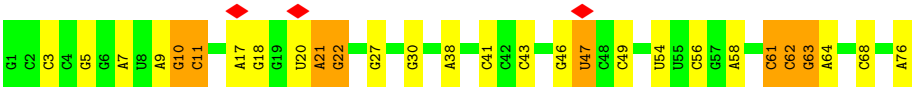




• Molecule 5: tRNA(PHE)

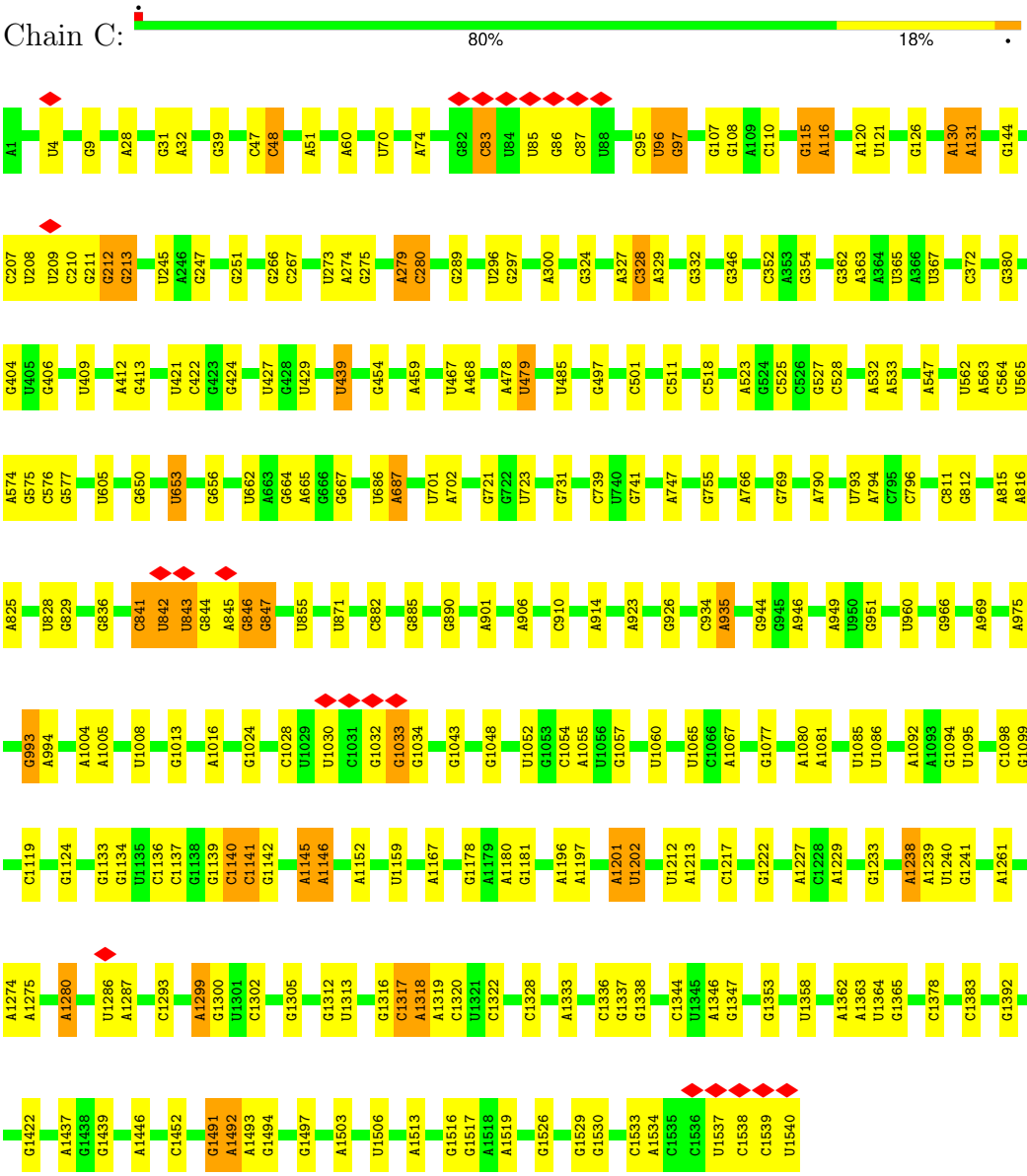
Chain A:





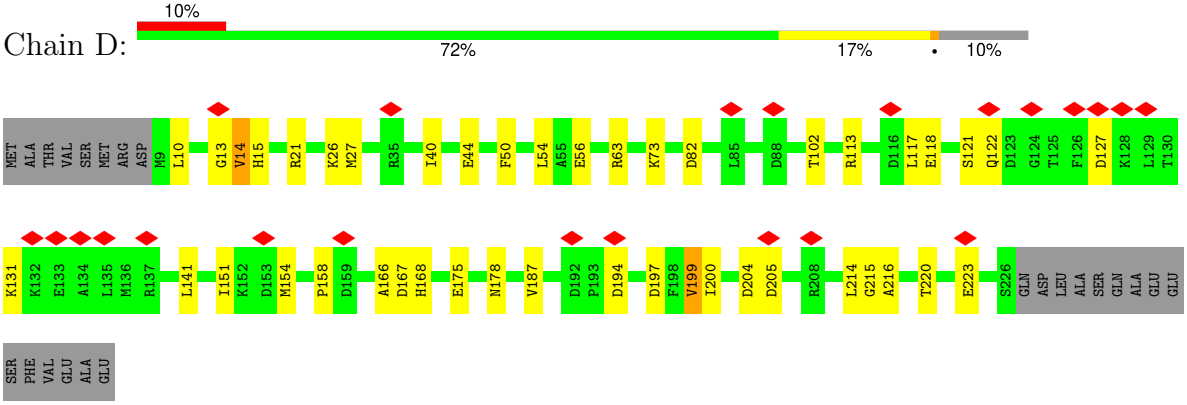
• Molecule 6: 16S rRNA

Chain C:



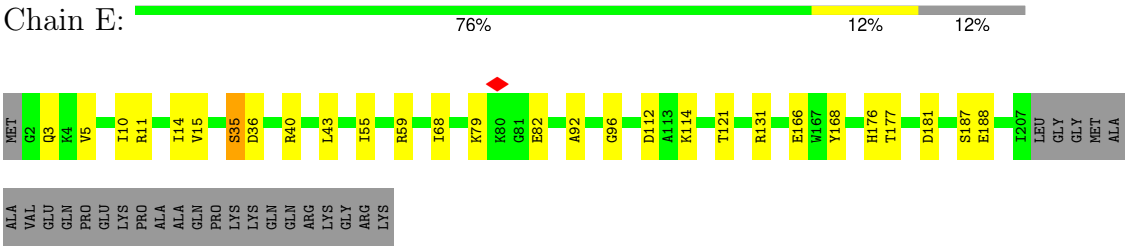
• Molecule 7: 30S ribosomal protein S2

Chain D:



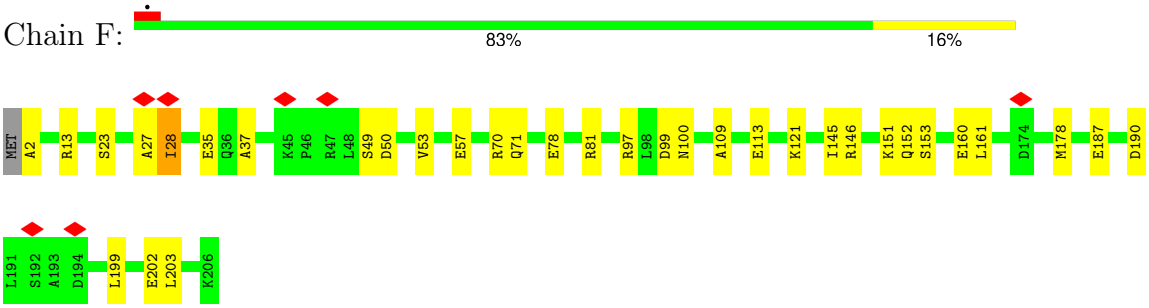
• Molecule 8: 30S ribosomal protein S3

Chain E:



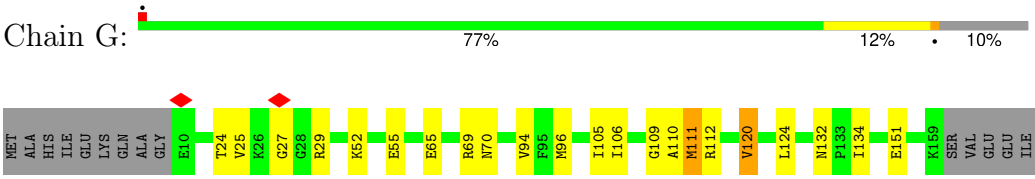
• Molecule 9: 30S ribosomal protein S4

Chain F:



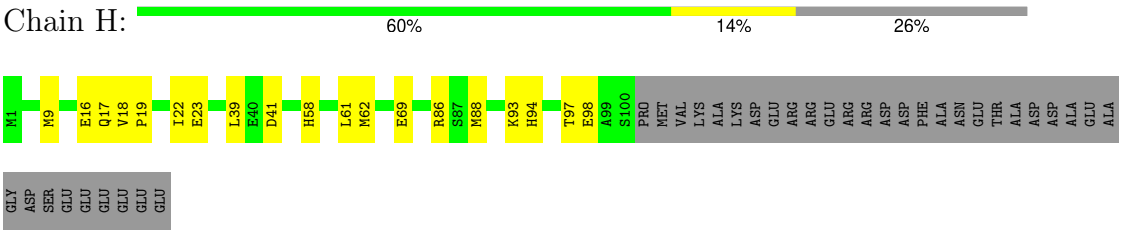
• Molecule 10: 30S ribosomal protein S5

Chain G:



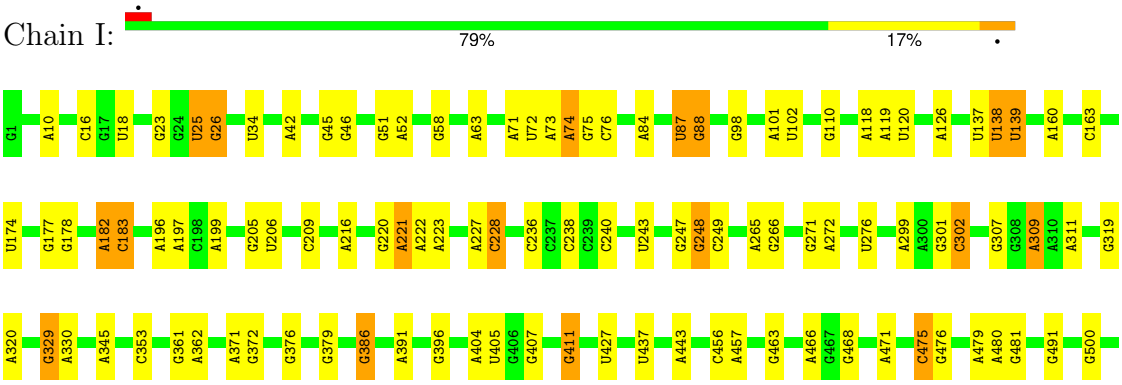
• Molecule 11: 30S ribosomal protein S6

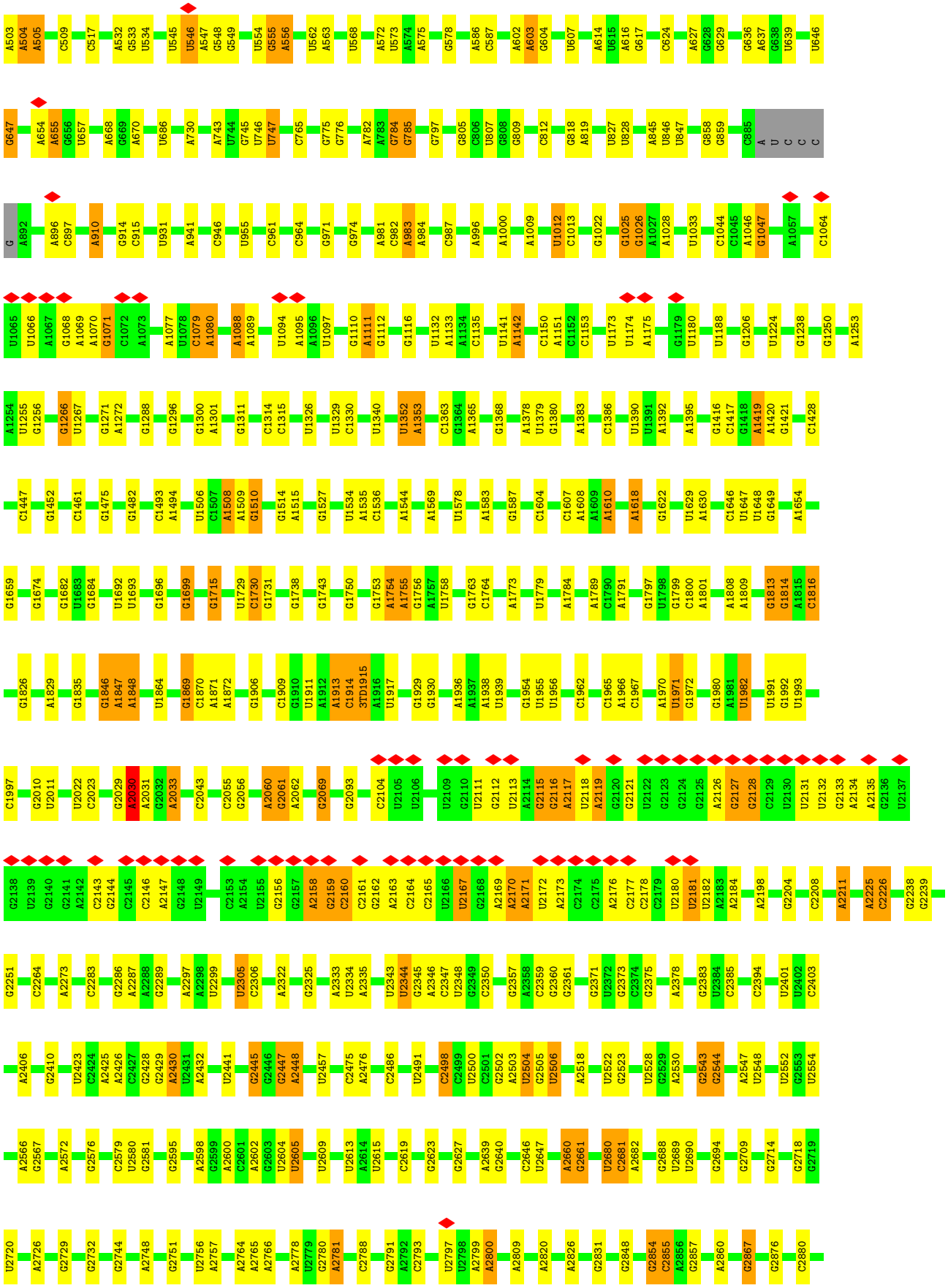
Chain H:

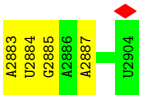


• Molecule 12: 23S rRNA

Chain I:




A503 A504 A505 C509 C517 A532 G533 U534 U545 U546 A547 G548 G549 U554 G555 A556 U562 A563 U568 A572 U573 A574 A575 G578 A586 C587 A602 A603 G604 U607 A614 U615 A616 G617 C624 A627 G628 G629 G636 A637 G638 U639 U646
G647 A654 A655 G656 U657 A668 G669 A670 U686 A730 A743 U744 G745 U746 U747 C765 G775 G776 A782 A783 G784 G785 G797 G805 C806 U807 G808 G809 C812 G818 A819 U827 U828 A845 U846 U847 G858 G859 C885 A U C C C
G A892 A896 C897 A910 G914 C915 U931 A941 C946 U965 C961 C964 G971 G974 A981 C982 A983 A984 C987 A996 A1000 A1009 U1012 C1013 G1022 G1025 G1026 A1027 A1028 U1033 C1044 C1045 A1046 G1047 A1057 C1064
U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 A1077 U1078 C1079 A1080 A1088 A1089 U1094 A1095 A1096 U1097 G1110 A1111 G1112 G1116 U1132 A1133 A1134 C1135 U1141 A1142 C1150 A1151 C1152 C1153 U1173 U1174 A1175 G1179 U1180 U1188 G1206 U1224 G1238 G1250 A1253
A1254 U1255 G1256 G1266 U1267 G1271 A1272 G1288 G1296 G1300 A1301 G1311 C1314 C1315 U1326 U1329 C1330 U1340 U1352 A1353 C1363 G1364 A1365 G1368 A1378 U1379 G1380 A1383 C1386 U1390 U1391 A1392 A1395 G1416 C1417 G1418 A1419 A1420 G1421 C1428
C1447 G1452 C1461 G1475 G1482 C1493 A1494 U1506 C1507 A1508 A1509 G1510 G1514 A1515 G1527 U1534 A1535 C1536 A1544 A1569 U1578 A1583 G1587 C1604 C1607 A1608 A1609 A1610 A1618 G1622 U1629 A1630 C1646 U1647 U1648 G1649 A1654
G1659 G1674 G1682 U1683 G1684 U1692 U1693 G1696 G1699 G1715 U1729 C1730 G1731 G1738 G1743 G1750 G1753 A1754 A1755 G1756 A1757 U1758 G1763 C1764 A1773 U1779 A1784 A1789 C1790 A1791 G1797 U1798 G1799 C1800 A1801 A1808 A1809 G1813 G1814 A1815 C1816
G1826 A1829 G1835 G1846 A1847 A1848 U1864 G1869 C1870 A1871 A1872 G1906 C1909 G1910 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 G1929 G1930 A1936 A1937 A1938 U1939 G1954 U1955 U1956 C1962 C1965 A1966 C1967 A1970 U1971 G1972 G1980 A1981 U1982 U1991 G1992 U1993
C1997 G2010 U2011 U2022 C2023 G2029 A2030 A2031 G2032 A2033 C2043 C2055 G2056 A2060 G2061 A2062 G2069 G2093 C2104 U2105 U2106 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137
G2138 U2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2153 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 A2198 G2204 C2208 A2211 A2225 C2226 G2238 G2239
G2251 C2264 A2273 C2283 G2286 A2287 A2288 G2289 A2297 A2298 U2299 U2305 C2306 A2322 G2325 A2333 U2334 A2335 U2343 U2344 G2345 A2346 C2347 U2348 G2349 C2350 G2357 A2358 C2359 G2360 G2361 G2371 U2372 G2373 C2374 G2375 A2378 G2383 U2384 C2385 C2394 U2401 U2402 C2403
A2406 G2410 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2432 U2441 G2445 G2446 G2447 A2448 U2457 C2475 A2476 C2486 U2491 C2498 C2499 U2500 C2501 G2502 A2503 U2504 G2505 U2506 A2518 U2522 G2523 U2528 G2529 A2530 G2543 G2544 A2547 U2548 U2552 G2553 U2554
A2566 G2567 A2572 G2576 C2579 U2580 G2581 G2595 A2598 G2599 A2600 C2601 A2602 G2603 U2604 U2605 U2609 U2613 A2614 U2615 C2619 G2623 G2627 A2639 G2640 C2646 U2647 A2660 G2661 U2680 C2681 A2682 G2688 U2689 U2690 G2694 G2709 G2714 G2718 G2719
U2720 A2726 G2729 G2732 C2744 A2748 G2751 U2756 A2757 A2764 A2765 A2766 A2778 U2779 G2780 A2781 C2788 G2791 A2792 C2793 U2797 U2798 A2799 A2800 A2809 A2820 A2826 G2831 G2848 G2854 C2855 A2856 G2857 A2860 G2867 G2876 C2880



• Molecule 13: 5S rRNA

Chain J:





• Molecule 14: 50S ribosomal protein L2

Chain K:

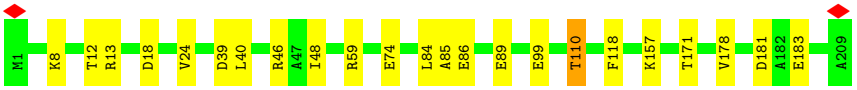




• Molecule 15: 50S ribosomal protein L3

Chain L:

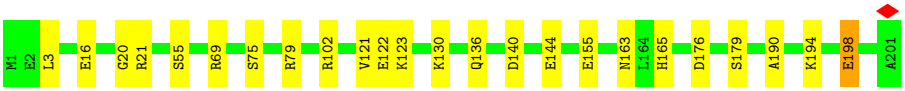




• Molecule 16: 50S ribosomal protein L4

Chain M:

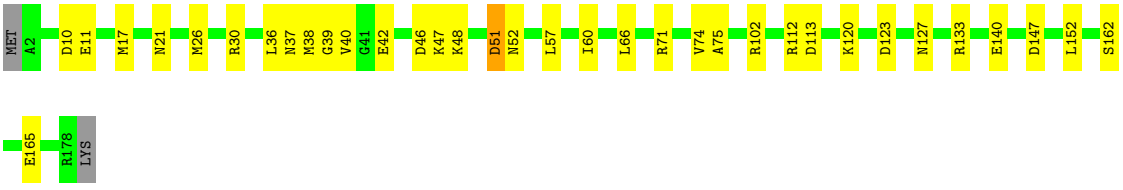




• Molecule 17: 50S ribosomal protein L5

Chain N:

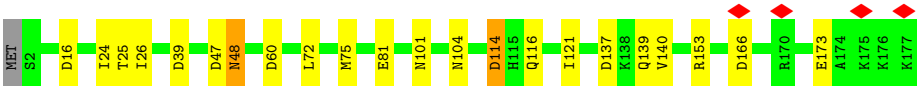




• Molecule 18: 50S ribosomal protein L6

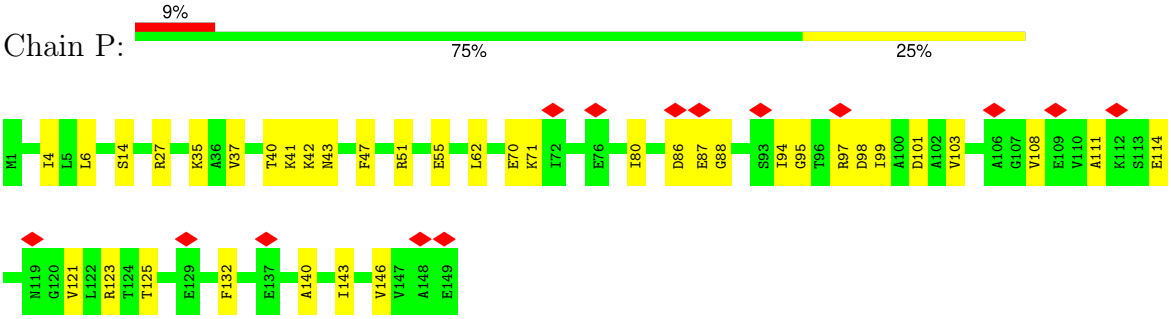
Chain O:





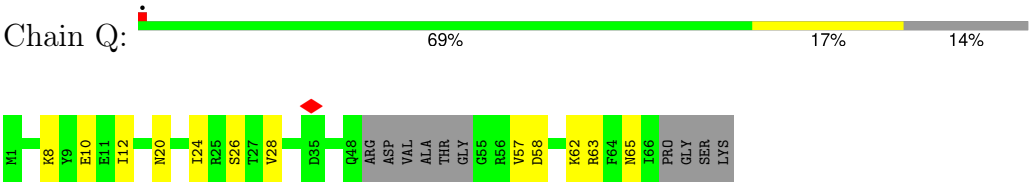
• Molecule 19: 50S ribosomal protein L9

Chain P:



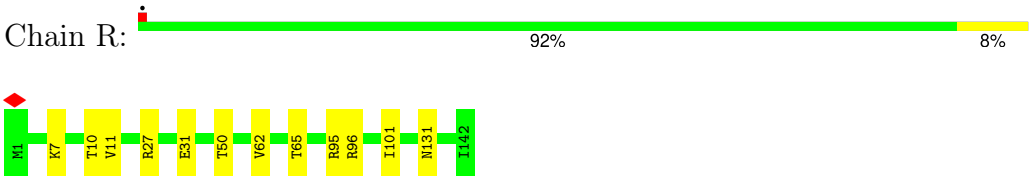
• Molecule 20: 50S ribosomal protein L31

Chain Q:



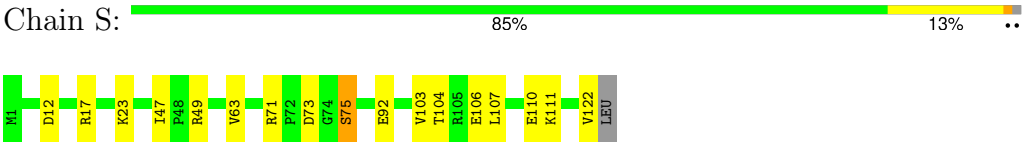
• Molecule 21: 50S ribosomal protein L13

Chain R:



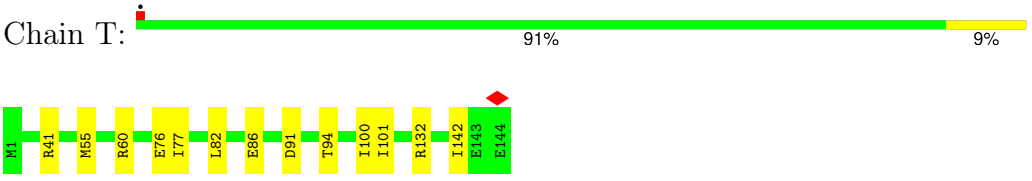
• Molecule 22: 50S ribosomal protein L14

Chain S:



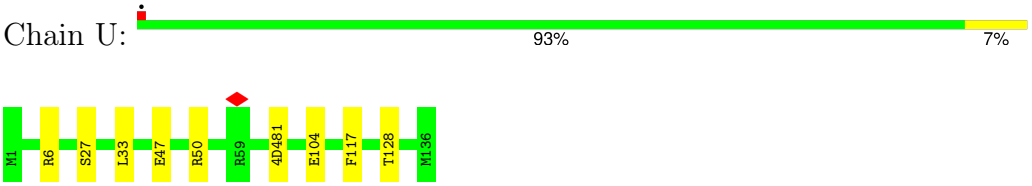
• Molecule 23: 50S ribosomal protein L15

Chain T:



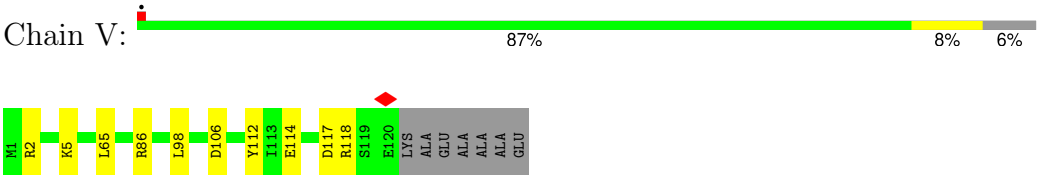
• Molecule 24: 50S ribosomal protein L16

Chain U:



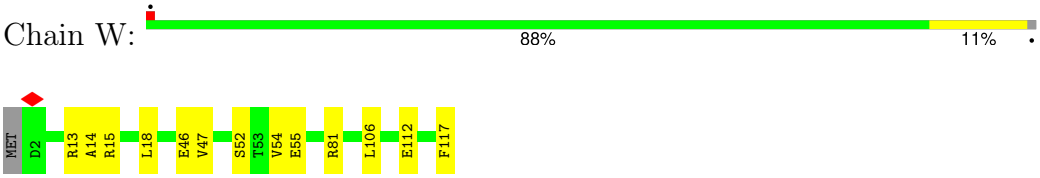
• Molecule 25: 50S ribosomal protein L17

Chain V:



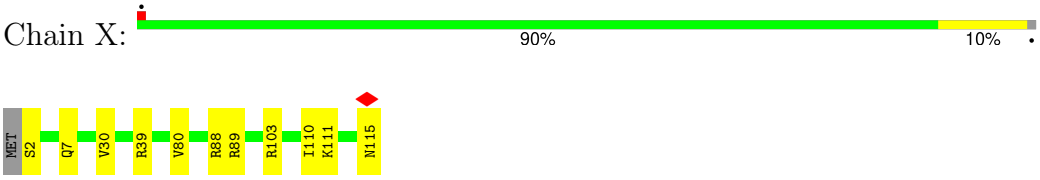
• Molecule 26: 50S ribosomal protein L18

Chain W:



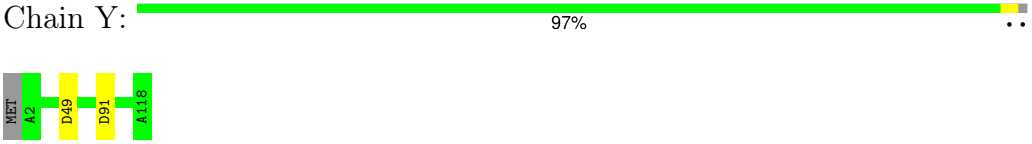
• Molecule 27: 50S ribosomal protein L19

Chain X:



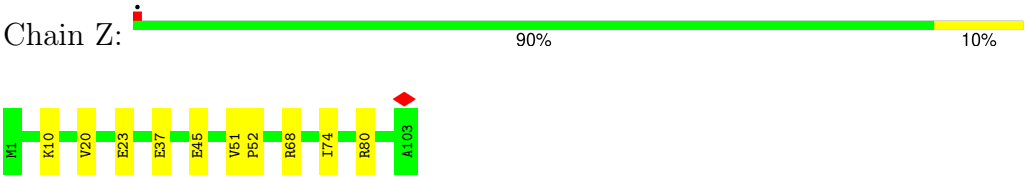
• Molecule 28: 50S ribosomal protein L20

Chain Y:



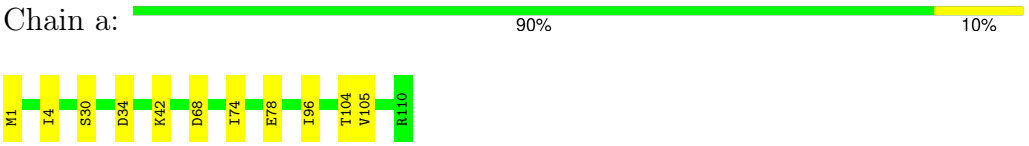
• Molecule 29: Ribosomal protein L21

Chain Z:



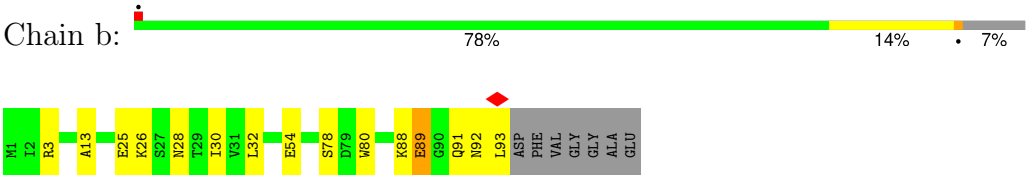
• Molecule 30: 50S ribosomal protein L22

Chain a:



• Molecule 31: 50S ribosomal protein L23

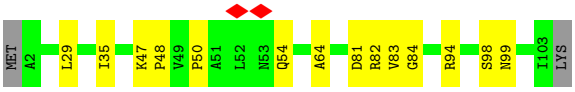
Chain b:



• Molecule 32: 50S ribosomal protein L24

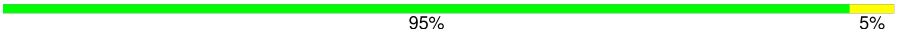
Chain c:





• Molecule 33: 50S ribosomal protein L25

Chain d:

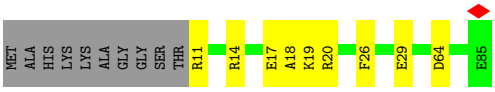




• Molecule 34: 50S ribosomal protein L27

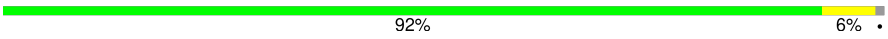
Chain e:

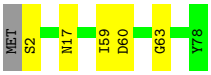




• Molecule 35: 50S ribosomal protein L28

Chain f:

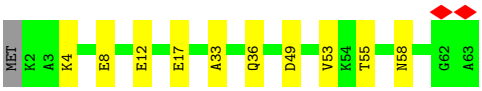




• Molecule 36: 50S ribosomal protein L29

Chain g:

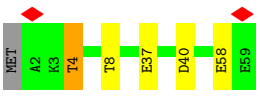




• Molecule 37: 50S ribosomal protein L30

Chain h:

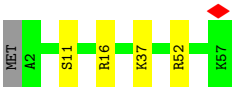




• Molecule 38: 50S ribosomal protein L32

Chain i:

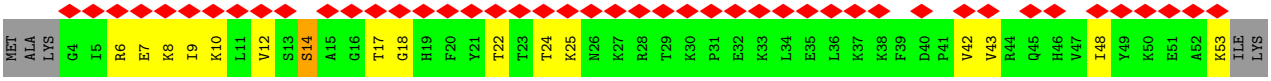




• Molecule 39: 50S ribosomal protein L33

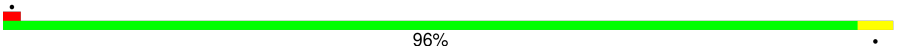
Chain j:

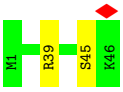




• Molecule 40: 50S ribosomal protein L34

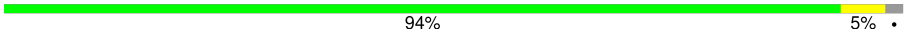
Chain k:





• Molecule 41: 50S ribosomal protein L35

Chain l:

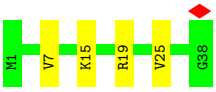




• Molecule 42: 50S ribosomal protein L36

Chain m:

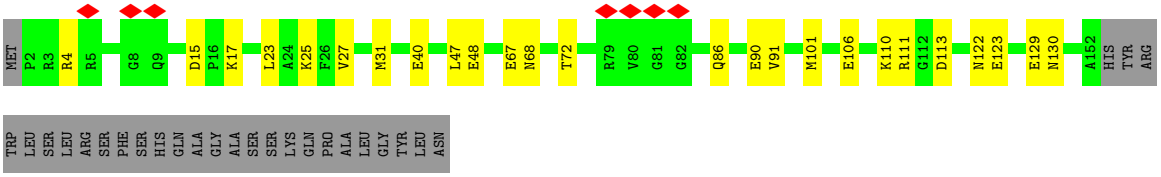




• Molecule 43: 30S ribosomal protein S7

Chain n:

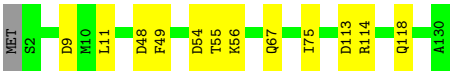




• Molecule 44: 30S ribosomal protein S8

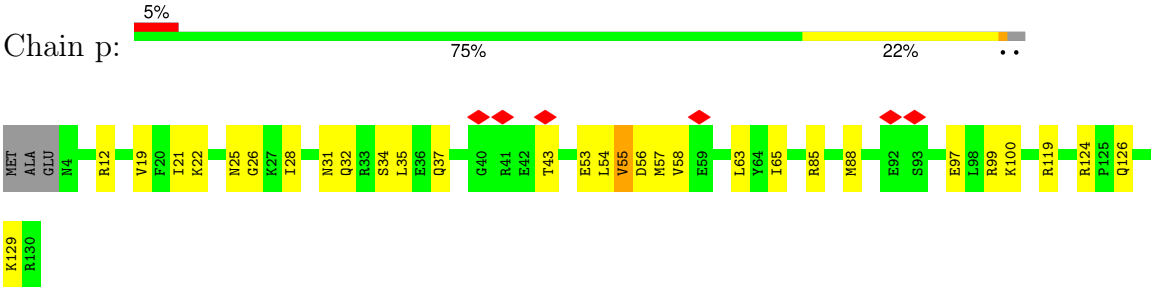
Chain o:





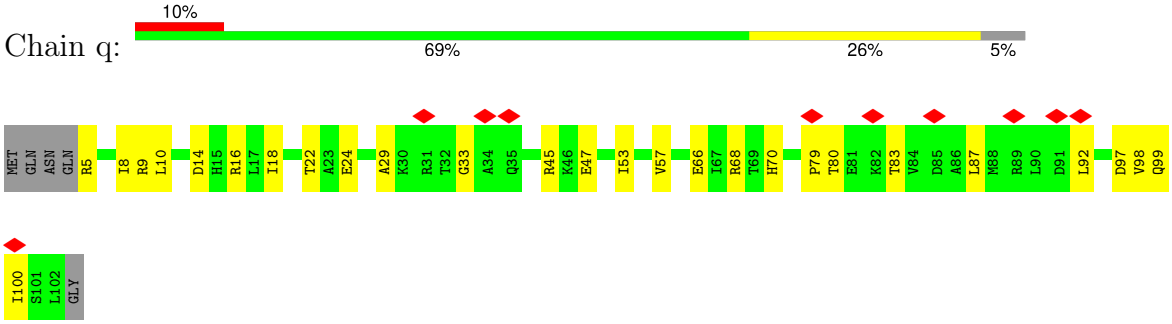
• Molecule 45: 30S ribosomal protein S9

Chain p:



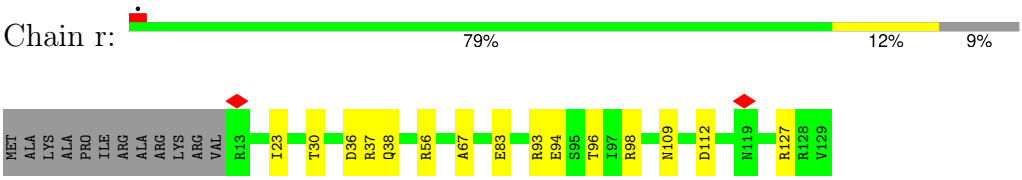
• Molecule 46: 30S ribosomal protein S10

Chain q:



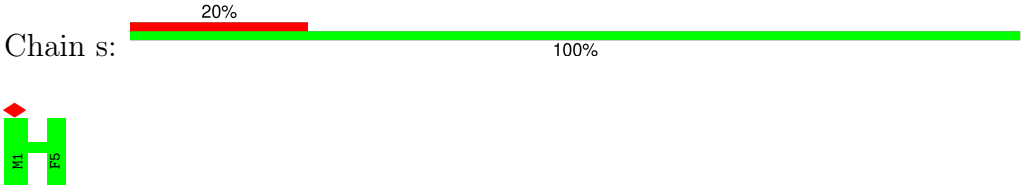
• Molecule 47: 30S ribosomal protein S11

Chain r:



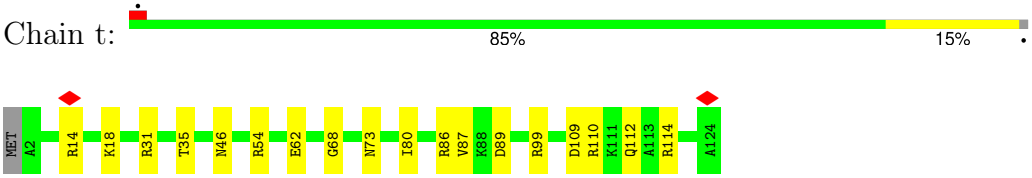
• Molecule 48: nascent peptide chain

Chain s:



• Molecule 49: 30S ribosomal protein S12

Chain t:



• Molecule 50: 30S ribosomal protein S13

Chain u:

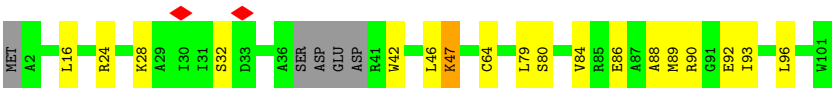




• Molecule 51: 30S ribosomal protein S14

Chain v:

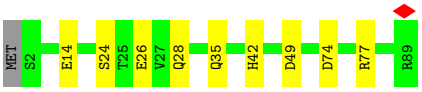




• Molecule 52: 30S ribosomal protein S15

Chain w:

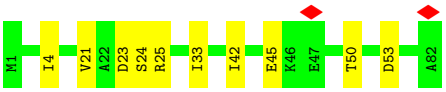




• Molecule 53: 30S ribosomal protein S16

Chain x:

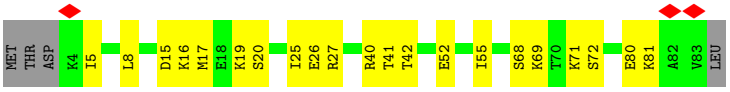




• Molecule 54: 30S ribosomal protein S17

Chain y:

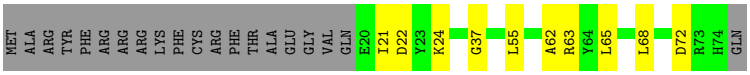




• Molecule 55: 30S ribosomal protein S18

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	240596	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 ($e^-/Å^2$)	52.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	25.561	Depositor
Minimum map value	-9.732	Depositor
Average map value	-0.014	Depositor
Map value standard deviation	0.828	Depositor
Recommended contour level	2	Depositor
Map size (Å)	422.4, 422.4, 422.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, 4D4, OMU, 5MC, G7M, 1MG, 5MU, MG, OMG, ZN, 3TD, RD8, 6MZ, OMC, H2U, PSU, 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	1	0.10	0/652	0.28	0/877
2	2	0.11	0/671	0.32	0/888
3	3	0.13	0/598	0.35	0/792
4	4	0.07	0/138	0.14	0/212
5	A	0.08	0/1815	0.20	0/2828
6	C	0.08	0/36991	0.15	0/57705
7	D	0.12	0/1735	0.32	0/2338
8	E	0.09	0/1651	0.25	0/2225
9	F	0.10	0/1665	0.28	0/2227
10	G	0.10	0/1118	0.29	0/1504
11	H	0.13	0/835	0.34	0/1128
12	I	0.10	0/69121	0.17	1/107828 (0.0%)
13	J	0.07	0/2828	0.14	0/4410
14	K	0.10	0/2139	0.25	0/2876
15	L	0.09	0/1586	0.24	0/2134
16	M	0.10	0/1571	0.27	0/2113
17	N	0.11	0/1434	0.28	0/1926
18	O	0.09	0/1343	0.24	0/1816
19	P	0.11	0/1122	0.29	0/1515
20	Q	0.12	0/488	0.33	0/649
21	R	0.09	0/1152	0.23	0/1551
22	S	0.11	0/947	0.29	0/1268
23	T	0.09	0/1062	0.24	0/1413
24	U	0.10	0/1081	0.26	0/1443
25	V	0.08	0/973	0.21	0/1301
26	W	0.10	0/902	0.28	0/1209
27	X	0.09	0/929	0.22	0/1242
28	Y	0.08	0/960	0.20	0/1278
29	Z	0.10	0/829	0.26	0/1107
30	a	0.08	0/864	0.22	0/1156
31	b	0.11	0/744	0.29	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	c	0.08	0/787	0.24	0/1051
33	d	0.09	0/766	0.25	0/1025
34	e	0.09	0/582	0.25	0/769
35	f	0.10	0/635	0.23	0/848
36	g	0.11	0/502	0.28	0/667
37	h	0.11	0/453	0.24	0/605
38	i	0.11	0/450	0.27	0/599
39	j	0.08	0/416	0.31	0/554
40	k	0.08	0/380	0.19	0/498
41	l	0.09	0/513	0.21	0/676
42	m	0.12	0/303	0.31	0/397
43	n	0.10	0/1195	0.26	0/1602
44	o	0.09	0/989	0.24	0/1326
45	p	0.11	0/1034	0.33	0/1375
46	q	0.10	0/796	0.27	0/1077
47	r	0.12	0/893	0.30	0/1205
48	s	0.06	0/45	0.14	0/57
49	t	0.09	0/969	0.26	0/1300
50	u	0.09	0/900	0.25	0/1204
51	v	0.11	0/785	0.27	0/1043
52	w	0.11	0/718	0.26	0/959
53	x	0.09	0/659	0.25	0/884
54	y	0.12	0/657	0.33	0/881
55	z	0.09	0/462	0.22	0/621
All	All	0.09	0/155833	0.20	1/233176 (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
24	U	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	2506	U	C5'-C4'-C3'	5.83	123.94	115.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	U	6	ARG	Sidechain

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	1	637	666	665	12	0
2	2	665	715	714	14	0
3	3	590	629	629	6	0
4	4	125	65	65	0	0
5	A	1624	820	820	18	0
6	C	33037	16628	16626	123	0
7	D	1704	1734	1732	39	0
8	E	1624	1697	1696	20	0
9	F	1643	1709	1707	26	0
10	G	1105	1149	1148	20	0
11	H	817	808	808	14	0
12	I	62229	31319	31319	234	0
13	J	2529	1280	1281	5	0
14	K	2093	2170	2157	20	0
15	L	1565	1619	1616	17	0
16	M	1552	1620	1619	18	0
17	N	1410	1445	1444	30	0
18	O	1323	1373	1371	19	0
19	P	1111	1148	1148	29	0
20	Q	480	484	478	10	0
21	R	1129	1162	1162	11	0
22	S	938	1012	1012	18	0
23	T	1053	1129	1128	10	0
24	U	1075	1156	1154	5	0
25	V	960	1000	1000	5	0
26	W	892	925	923	12	0
27	X	917	963	962	9	0
28	Y	947	1021	1019	2	0
29	Z	816	841	839	8	0
30	a	857	923	922	7	0
31	b	738	808	807	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	c	779	832	831	8	0
33	d	753	781	780	4	0
34	e	575	593	592	5	0
35	f	625	653	652	4	0
36	g	501	532	531	9	0
37	h	449	489	488	3	0
38	i	444	460	458	4	0
39	j	409	442	440	17	0
40	k	377	418	418	2	0
41	l	504	573	572	3	0
42	m	302	343	340	3	0
43	n	1181	1238	1238	18	0
44	o	979	1032	1031	7	0
45	p	1022	1071	1070	26	0
46	q	786	829	828	17	0
47	r	877	888	887	11	0
48	s	44	47	47	0	0
49	t	955	1017	1016	14	0
50	u	891	954	952	9	0
51	v	774	826	824	13	0
52	w	710	731	728	9	0
53	x	649	666	666	9	0
54	y	648	693	691	18	0
55	z	455	480	478	7	0
56	C	93	0	0	0	0
56	I	113	0	0	0	0
56	K	1	0	0	0	0
56	L	1	0	0	0	0
56	V	1	0	0	0	0
57	I	32	22	0	0	0
58	Q	1	0	0	0	0
58	m	1	0	0	0	0
59	C	3	6	0	0	0
59	I	32	64	0	0	0
59	k	1	2	0	0	0
All	All	144153	96700	96529	864	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 864 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)
12:I:2344:U:O4	39:j:22:THR:OG1	1.92	0.87
33:d:51:GLN:OE1	33:d:57:TYR:OH	1.94	0.85
9:F:13:ARG:NH1	9:F:37:ALA:O	2.10	0.84
45:p:34:SER:OG	45:p:37:GLN:OE1	1.95	0.84
6:C:1057:G:O2'	8:E:188:GLU:OE2	1.96	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	1	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
2	2	83/87 (95%)	79 (95%)	4 (5%)	0	100	100
3	3	68/71 (96%)	68 (100%)	0	0	100	100
7	D	216/241 (90%)	209 (97%)	6 (3%)	1 (0%)	24	40
8	E	204/233 (88%)	199 (98%)	5 (2%)	0	100	100
9	F	203/206 (98%)	196 (97%)	6 (3%)	1 (0%)	24	40
10	G	148/167 (89%)	142 (96%)	6 (4%)	0	100	100
11	H	98/135 (73%)	96 (98%)	2 (2%)	0	100	100
14	K	271/273 (99%)	260 (96%)	11 (4%)	0	100	100
15	L	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
16	M	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
17	N	175/179 (98%)	172 (98%)	3 (2%)	0	100	100
18	O	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
19	P	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
20	Q	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
21	R	140/142 (99%)	139 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	S	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
23	T	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
24	U	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
25	V	118/127 (93%)	118 (100%)	0	0	100	100
26	W	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
27	X	112/115 (97%)	112 (100%)	0	0	100	100
28	Y	115/118 (98%)	115 (100%)	0	0	100	100
29	Z	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
30	a	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
31	b	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
32	c	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
33	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
34	e	73/85 (86%)	73 (100%)	0	0	100	100
35	f	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
36	g	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
37	h	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
38	i	54/57 (95%)	54 (100%)	0	0	100	100
39	j	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
40	k	44/46 (96%)	44 (100%)	0	0	100	100
41	l	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
42	m	36/38 (95%)	36 (100%)	0	0	100	100
43	n	149/179 (83%)	148 (99%)	1 (1%)	0	100	100
44	o	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
45	p	125/130 (96%)	120 (96%)	4 (3%)	1 (1%)	16	28
46	q	96/103 (93%)	89 (93%)	6 (6%)	1 (1%)	12	22
47	r	115/129 (89%)	113 (98%)	2 (2%)	0	100	100
48	s	3/5 (60%)	3 (100%)	0	0	100	100
49	t	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
50	u	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
51	v	92/101 (91%)	90 (98%)	2 (2%)	0	100	100
52	w	86/89 (97%)	86 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	x	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
54	y	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
55	z	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
All	All	5558/5918 (94%)	5429 (98%)	125 (2%)	4 (0%)	49	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	F	28	ILE
45	p	55	VAL
46	q	57	VAL
7	D	14	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	70/79 (89%)	70 (100%)	0	100	100
2	2	65/66 (98%)	63 (97%)	2 (3%)	35	60
3	3	60/61 (98%)	60 (100%)	0	100	100
7	D	180/199 (90%)	177 (98%)	3 (2%)	53	75
8	E	170/190 (90%)	169 (99%)	1 (1%)	78	90
9	F	172/173 (99%)	171 (99%)	1 (1%)	78	90
10	G	113/126 (90%)	111 (98%)	2 (2%)	51	74
11	H	87/116 (75%)	87 (100%)	0	100	100
14	K	218/218 (100%)	218 (100%)	0	100	100
15	L	164/164 (100%)	163 (99%)	1 (1%)	78	90
16	M	165/165 (100%)	161 (98%)	4 (2%)	43	67
17	N	148/150 (99%)	145 (98%)	3 (2%)	48	72
18	O	137/138 (99%)	135 (98%)	2 (2%)	57	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	P	114/114 (100%)	112 (98%)	2 (2%)	51 74
20	Q	55/62 (89%)	54 (98%)	1 (2%)	51 74
21	R	116/116 (100%)	116 (100%)	0	100 100
22	S	103/104 (99%)	102 (99%)	1 (1%)	68 84
23	T	103/103 (100%)	103 (100%)	0	100 100
24	U	108/108 (100%)	108 (100%)	0	100 100
25	V	100/103 (97%)	99 (99%)	1 (1%)	68 84
26	W	86/87 (99%)	86 (100%)	0	100 100
27	X	99/100 (99%)	98 (99%)	1 (1%)	68 84
28	Y	89/90 (99%)	89 (100%)	0	100 100
29	Z	84/84 (100%)	83 (99%)	1 (1%)	63 81
30	a	93/93 (100%)	91 (98%)	2 (2%)	45 70
31	b	80/84 (95%)	79 (99%)	1 (1%)	61 80
32	c	83/85 (98%)	82 (99%)	1 (1%)	63 81
33	d	78/78 (100%)	78 (100%)	0	100 100
34	e	57/63 (90%)	57 (100%)	0	100 100
35	f	67/68 (98%)	67 (100%)	0	100 100
36	g	54/55 (98%)	54 (100%)	0	100 100
37	h	48/49 (98%)	47 (98%)	1 (2%)	47 71
38	i	47/48 (98%)	47 (100%)	0	100 100
39	j	45/49 (92%)	44 (98%)	1 (2%)	45 70
40	k	38/38 (100%)	38 (100%)	0	100 100
41	l	51/52 (98%)	51 (100%)	0	100 100
42	m	34/34 (100%)	34 (100%)	0	100 100
43	n	124/147 (84%)	123 (99%)	1 (1%)	73 87
44	o	104/105 (99%)	103 (99%)	1 (1%)	68 84
45	p	105/107 (98%)	104 (99%)	1 (1%)	68 84
46	q	86/90 (96%)	85 (99%)	1 (1%)	63 81
47	r	90/99 (91%)	89 (99%)	1 (1%)	65 83
48	s	4/4 (100%)	4 (100%)	0	100 100
49	t	103/104 (99%)	102 (99%)	1 (1%)	68 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	u	93/96 (97%)	92 (99%)	1 (1%)	65 83
51	v	79/84 (94%)	78 (99%)	1 (1%)	61 80
52	w	75/77 (97%)	75 (100%)	0	100 100
53	x	65/65 (100%)	64 (98%)	1 (2%)	57 78
54	y	74/78 (95%)	74 (100%)	0	100 100
55	z	48/65 (74%)	48 (100%)	0	100 100
All	All	4631/4833 (96%)	4590 (99%)	41 (1%)	68 86

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	b	89	GLU
46	q	5	ARG
32	c	29	LEU
43	n	72	THR
49	t	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
43	n	148	ASN
55	z	54	GLN
44	o	67	GLN
47	r	64	GLN
16	M	9	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	I	2896/2904 (99%)	352 (12%)	30 (1%)
13	J	117/120 (97%)	11 (9%)	0
4	4	5/15 (33%)	0	0
5	A	75/76 (98%)	17 (22%)	3 (4%)
6	C	1539/1540 (99%)	175 (11%)	9 (0%)
All	All	4632/4655 (99%)	555 (11%)	42 (0%)

5 of 555 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	3	C
5	A	5	G
5	A	11	C
5	A	17	A
5	A	18	G

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	I	1846	G
12	I	2425	A
12	I	1847	A
12	I	2158	A
12	I	2506	U

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

25 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	$\#\|Z\| > 2$
12	H2U	I	2449	12	18,21,22	0.43	0	19,30,33	0.68	0
12	2MA	I	2503	56,12	22,25,26	1.36	3 (13%)	32,37,40	2.06	8 (25%)
12	2MG	I	1835	12	23,26,27	0.76	0	33,38,41	2.17	10 (30%)
12	3TD	I	1915	12	19,22,23	1.09	2 (10%)	23,32,35	1.88	2 (8%)
12	6MZ	I	1618	12	22,25,26	1.09	1 (4%)	29,36,39	2.19	9 (31%)
12	OMU	I	2552	12	19,22,23	0.95	2 (10%)	25,31,34	1.95	6 (24%)
12	PSU	I	2580	56,12	18,21,22	0.97	0	21,30,33	2.00	5 (23%)
12	PSU	I	1917	12	18,21,22	0.90	0	21,30,33	2.00	4 (19%)
12	PSU	I	746	56,12	18,21,22	0.97	1 (5%)	21,30,33	1.89	4 (19%)
12	G7M	I	2069	12	23,26,27	0.54	0	34,39,42	0.91	2 (5%)
12	OMG	I	2251	5,12	23,26,27	0.73	0	32,38,41	1.96	10 (31%)
12	PSU	I	2504	56,12	18,21,22	0.90	0	21,30,33	1.99	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	PSU	I	1911	12	18,21,22	0.90	0	21,30,33	1.98	4 (19%)
12	2MG	I	2445	12	23,26,27	0.77	0	33,38,41	2.19	11 (33%)
12	5MC	I	1962	12	19,22,23	1.22	2 (10%)	26,32,35	1.10	3 (11%)
24	4D4	U	81	24	9,11,12	2.13	2 (22%)	7,13,15	1.96	3 (42%)
12	PSU	I	2604	12	18,21,22	0.92	1 (5%)	21,30,33	1.98	4 (19%)
12	5MU	I	1939	12	19,22,23	1.04	2 (10%)	27,32,35	2.10	6 (22%)
12	5MU	I	747	12	19,22,23	1.02	2 (10%)	27,32,35	2.13	6 (22%)
12	6MZ	I	2030	12	22,25,26	1.11	1 (4%)	29,36,39	2.24	9 (31%)
12	PSU	I	2605	12	18,21,22	0.92	1 (5%)	21,30,33	1.96	4 (19%)
12	OMC	I	2498	56,12	19,22,23	0.89	1 (5%)	25,31,34	0.96	1 (4%)
12	PSU	I	955	12	18,21,22	0.93	0	21,30,33	1.98	4 (19%)
12	PSU	I	2457	12	18,21,22	0.93	0	21,30,33	2.01	4 (19%)
12	1MG	I	745	12	23,26,27	0.91	2 (8%)	33,39,42	1.77	6 (18%)

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
12	H2U	I	2449	12	-	0/7/38/39	0/2/2/2
12	2MA	I	2503	56,12	-	2/7/25/26	0/3/3/3
12	2MG	I	1835	12	-	0/9/27/28	0/3/3/3
12	3TD	I	1915	12	-	2/7/25/26	0/2/2/2
12	6MZ	I	1618	12	-	2/9/27/28	0/3/3/3
12	OMU	I	2552	12	-	0/9/27/28	0/2/2/2
12	PSU	I	2580	56,12	-	0/7/25/26	0/2/2/2
12	PSU	I	1917	12	-	0/7/25/26	0/2/2/2
12	PSU	I	746	56,12	-	1/7/25/26	0/2/2/2
12	G7M	I	2069	12	-	0/7/25/26	0/3/3/3
12	OMG	I	2251	5,12	-	0/9/27/28	0/3/3/3
12	PSU	I	2504	56,12	-	2/7/25/26	0/2/2/2
12	PSU	I	1911	12	-	0/7/25/26	0/2/2/2
12	2MG	I	2445	12	-	1/9/27/28	0/3/3/3
12	5MC	I	1962	12	-	0/7/25/26	0/2/2/2
24	4D4	U	81	24	-	1/11/12/14	-
12	PSU	I	2604	12	-	0/7/25/26	0/2/2/2
12	5MU	I	1939	12	-	0/7/25/26	0/2/2/2
12	5MU	I	747	12	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	6MZ	I	2030	12	-	2/9/27/28	0/3/3/3
12	PSU	I	2605	12	-	2/7/25/26	0/2/2/2
12	OMC	I	2498	56,12	-	1/9/27/28	0/2/2/2
12	PSU	I	955	12	-	0/7/25/26	0/2/2/2
12	PSU	I	2457	12	-	0/7/25/26	0/2/2/2
12	1MG	I	745	12	-	0/7/25/26	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	81	4D4	CZ-NE	5.32	1.43	1.33
12	I	1962	5MC	C5-C4	-3.93	1.41	1.44
12	I	2503	2MA	C6-N1	3.88	1.40	1.35
12	I	2030	6MZ	C6-N6	3.85	1.38	1.34
12	I	1618	6MZ	C6-N6	3.82	1.38	1.34

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	2445	2MG	C2-N3-C4	7.30	121.13	112.00
12	I	1835	2MG	C2-N3-C4	7.29	121.11	112.00
12	I	1915	3TD	N1-C2-N3	6.61	120.94	116.13
12	I	2503	2MA	C5-C4-N3	-6.11	120.74	127.18
12	I	2457	PSU	N1-C2-N3	5.64	121.12	115.17

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	1618	6MZ	O4'-C4'-C5'-O5'
12	I	1915	3TD	O4'-C4'-C5'-O5'
12	I	2504	PSU	O4'-C4'-C5'-O5'
12	I	2605	PSU	O4'-C4'-C5'-O5'
12	I	1618	6MZ	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	I	2445	2MG	1	0
12	I	2030	6MZ	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 212 ligands modelled in this entry, 211 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	RD8	I	3114	56	35,35,35	1.32	4 (11%)	45,48,48	1.77	10 (22%)

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
57	RD8	I	3114	56	-	0/19/31/31	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	I	3114	RD8	C30-N21	3.72	1.40	1.36
57	I	3114	RD8	O29-C23	-3.18	1.41	1.46
57	I	3114	RD8	C24-C23	3.16	1.55	1.51
57	I	3114	RD8	C13-N17	-2.54	1.31	1.36

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	I	3114	RD8	C13-N17-N16	-5.58	103.00	109.01
57	I	3114	RD8	C23-O29-C30	4.55	113.74	110.10
57	I	3114	RD8	C22-N21-C30	-4.02	108.20	111.17
57	I	3114	RD8	C23-C22-N21	3.01	104.69	101.85
57	I	3114	RD8	C22-C23-C24	2.79	116.54	113.38

There are no chirality outliers.

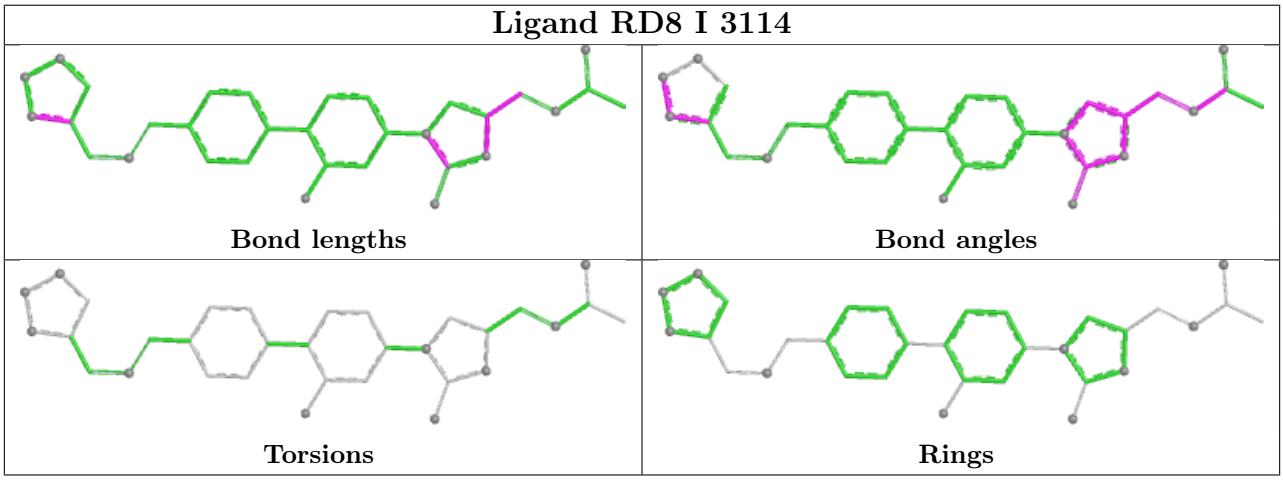
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand RD8 I 3114



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.

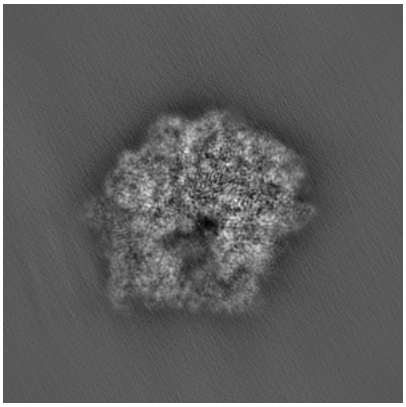
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24802. These allow visual inspection of the internal detail of the map and identification of artifacts.

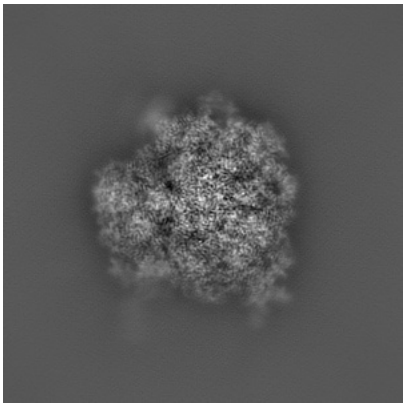
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

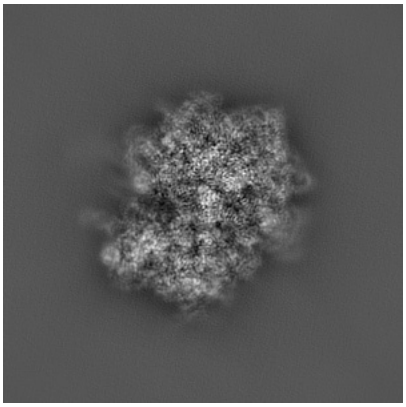
6.1.1 Primary map



X



Y

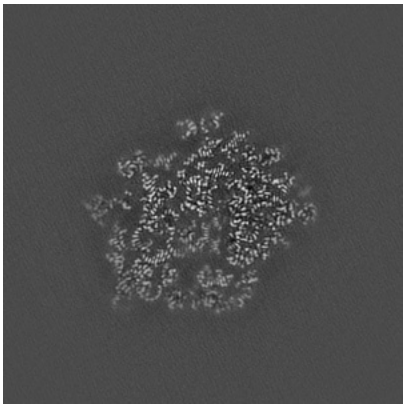


Z

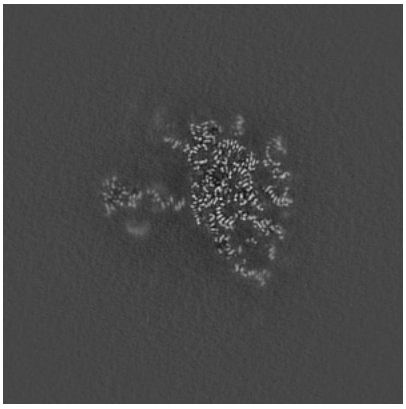
The images above show the map projected in three orthogonal directions.

6.2 Central slices

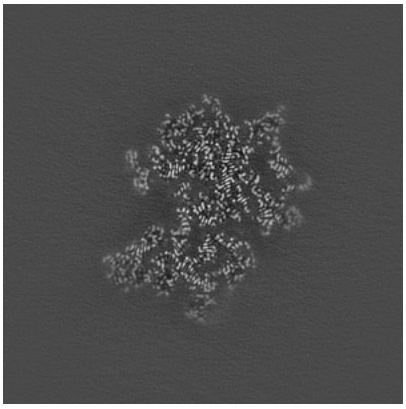
6.2.1 Primary map



X Index: 256



Y Index: 256

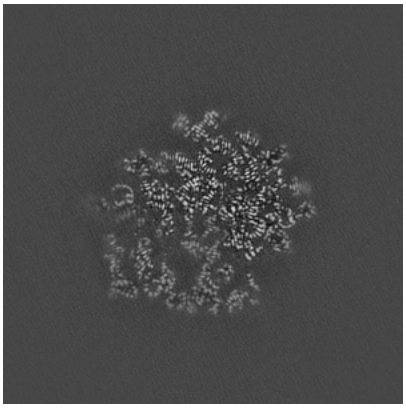


Z Index: 256

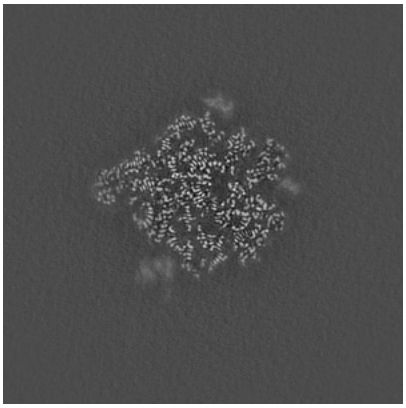
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

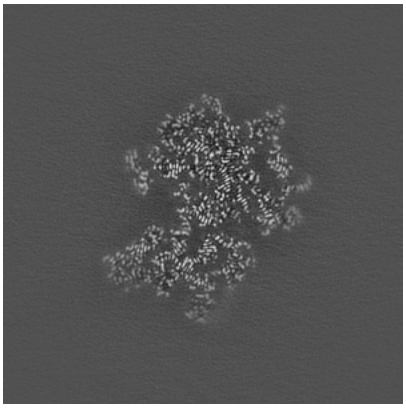
6.3.1 Primary map



X Index: 264



Y Index: 293

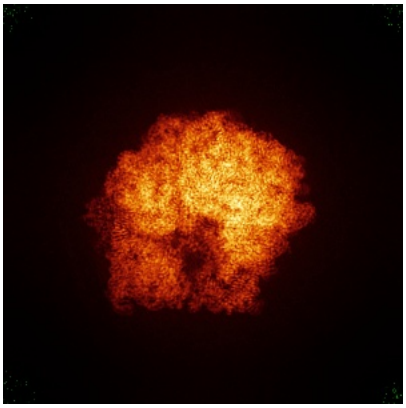


Z Index: 255

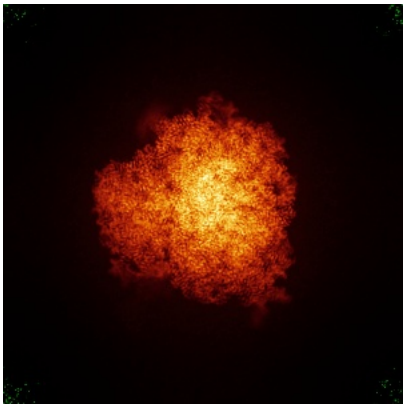
The images above show the largest variance slices of the map in three orthogonal directions.

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

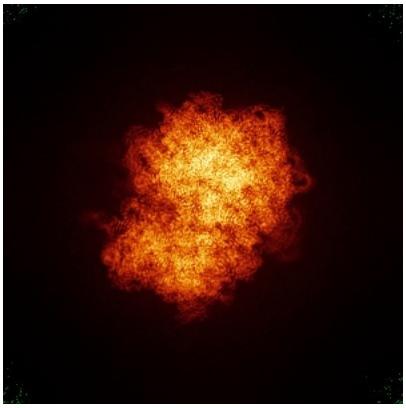
6.4.1 Primary map



X



Y

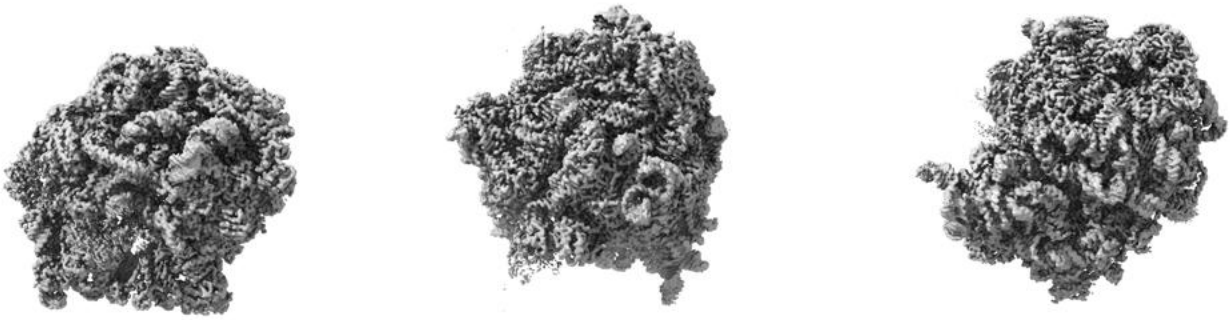


Z

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 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

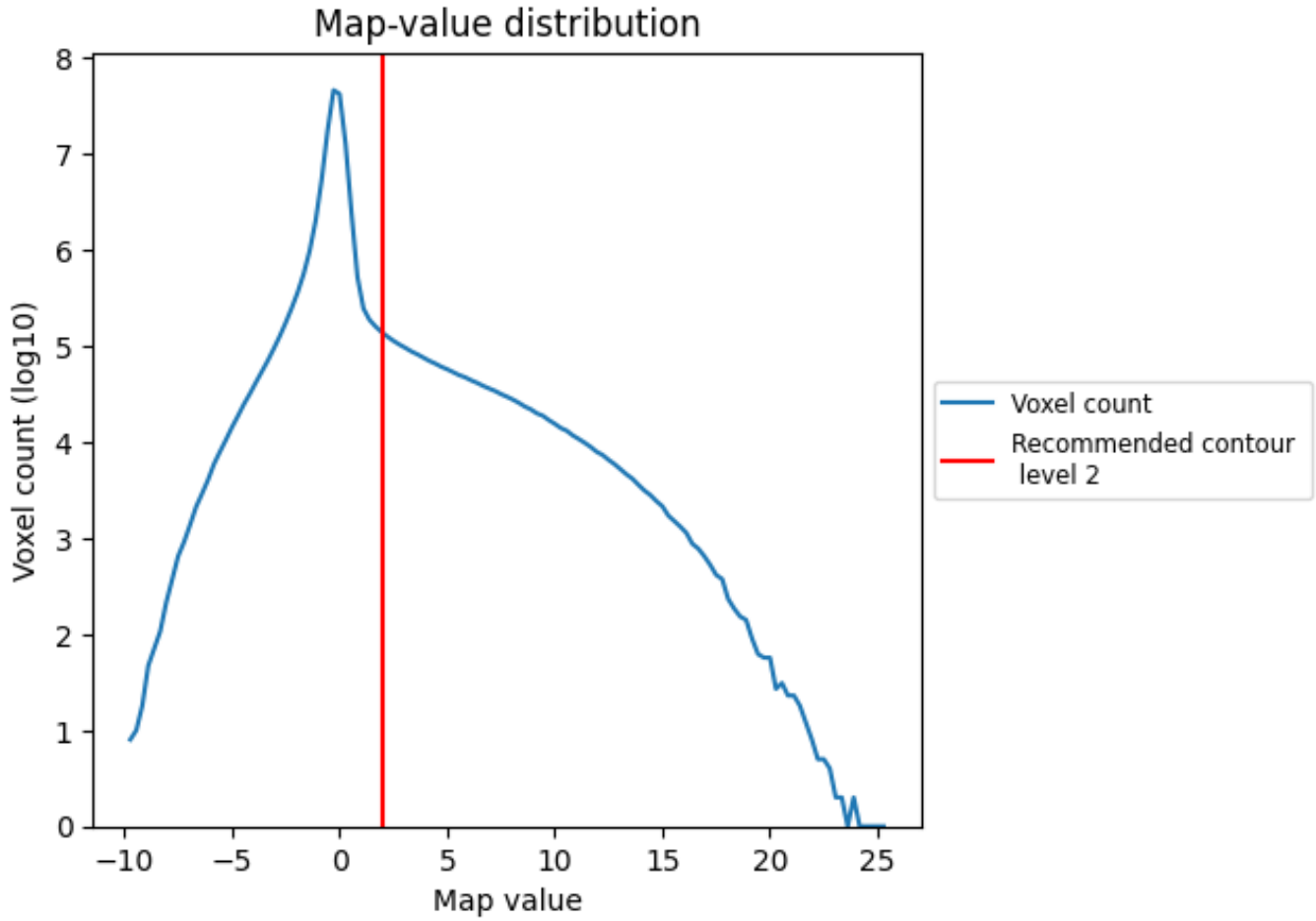
6.6 Mask visualisation (i)

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

7 Map analysis

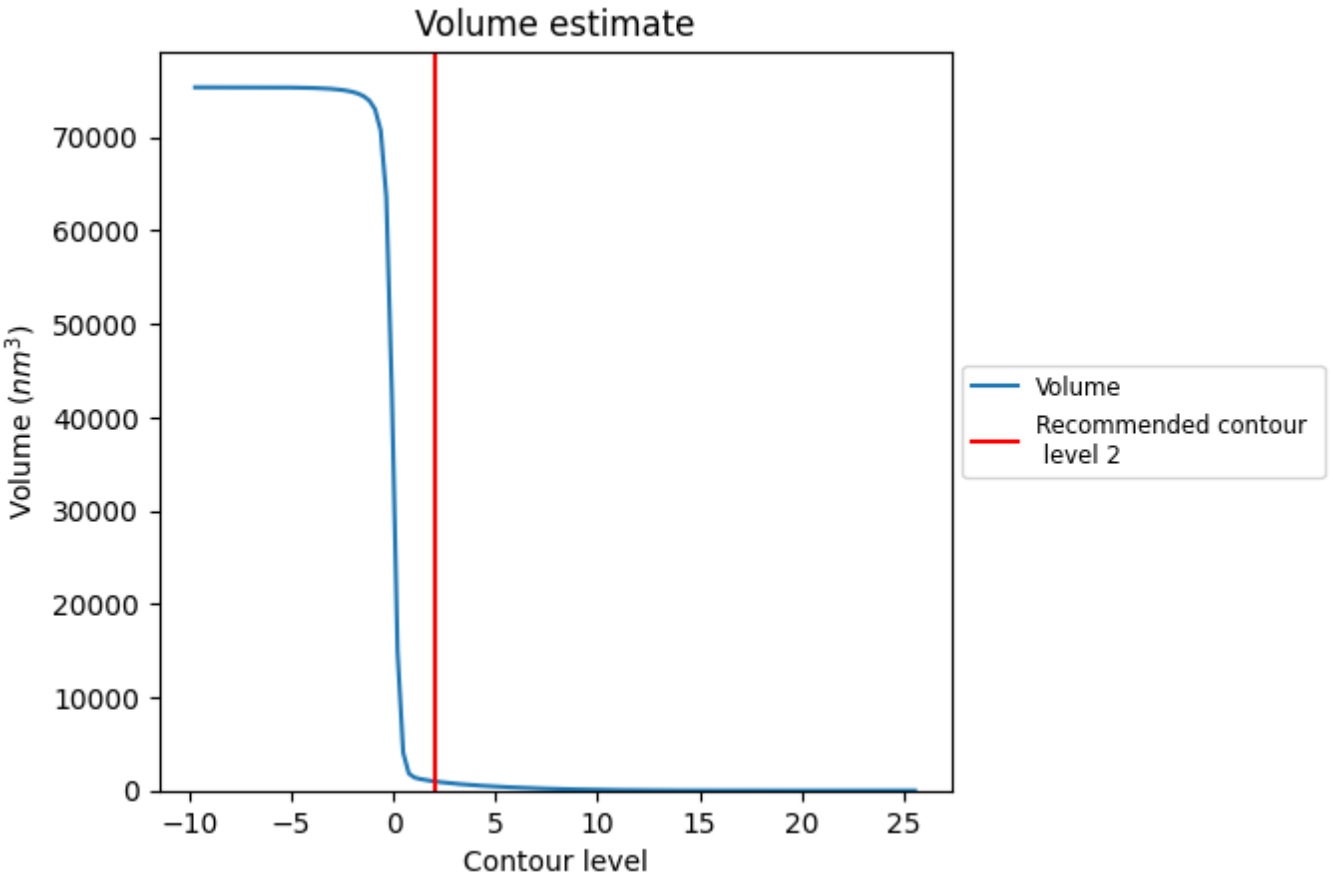
This section contains the results of statistical analysis of the map.

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.

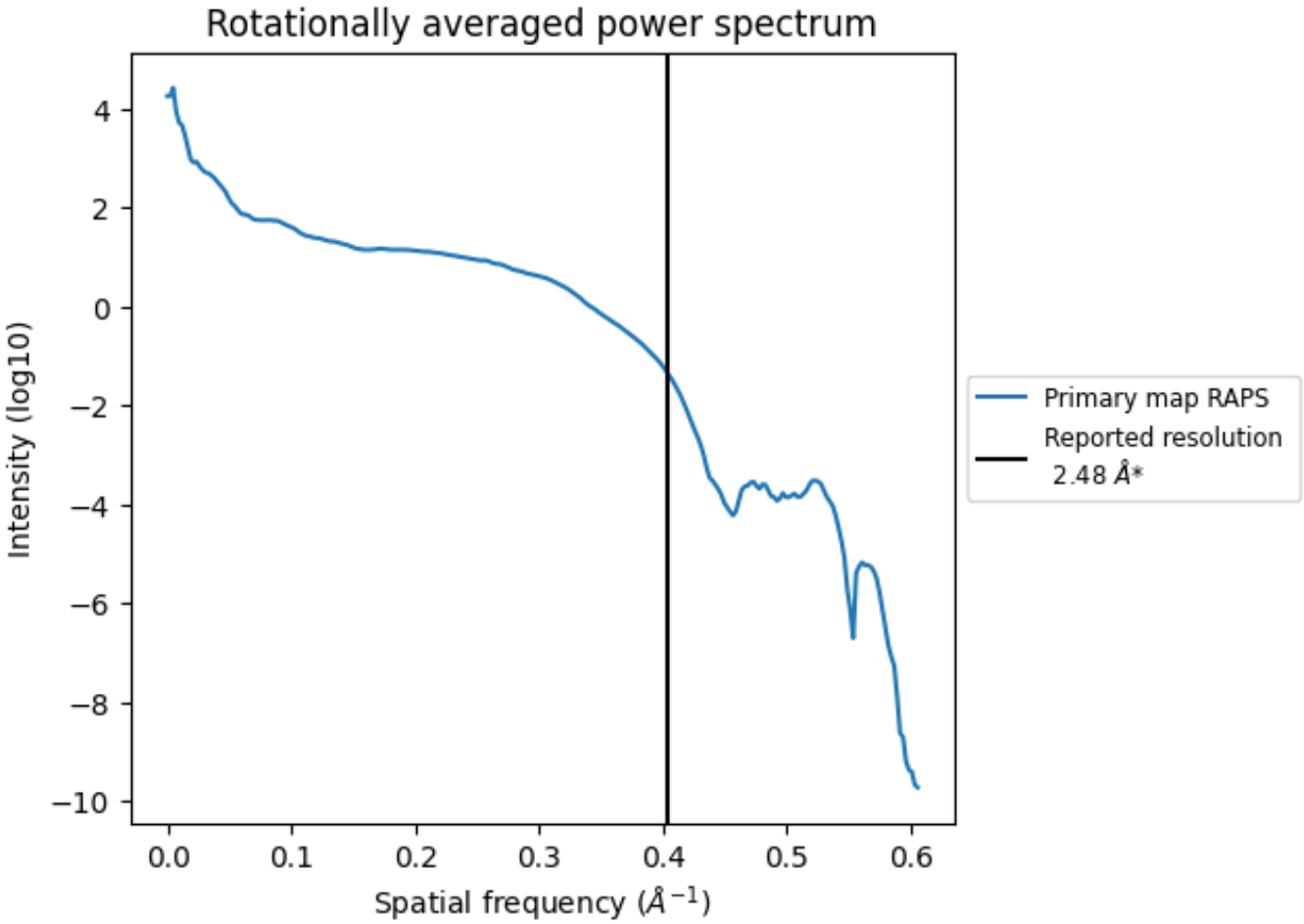
7.2 Volume estimate (i)



The volume at the recommended contour level is 988 nm^3; this corresponds to an approximate mass of 893 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)

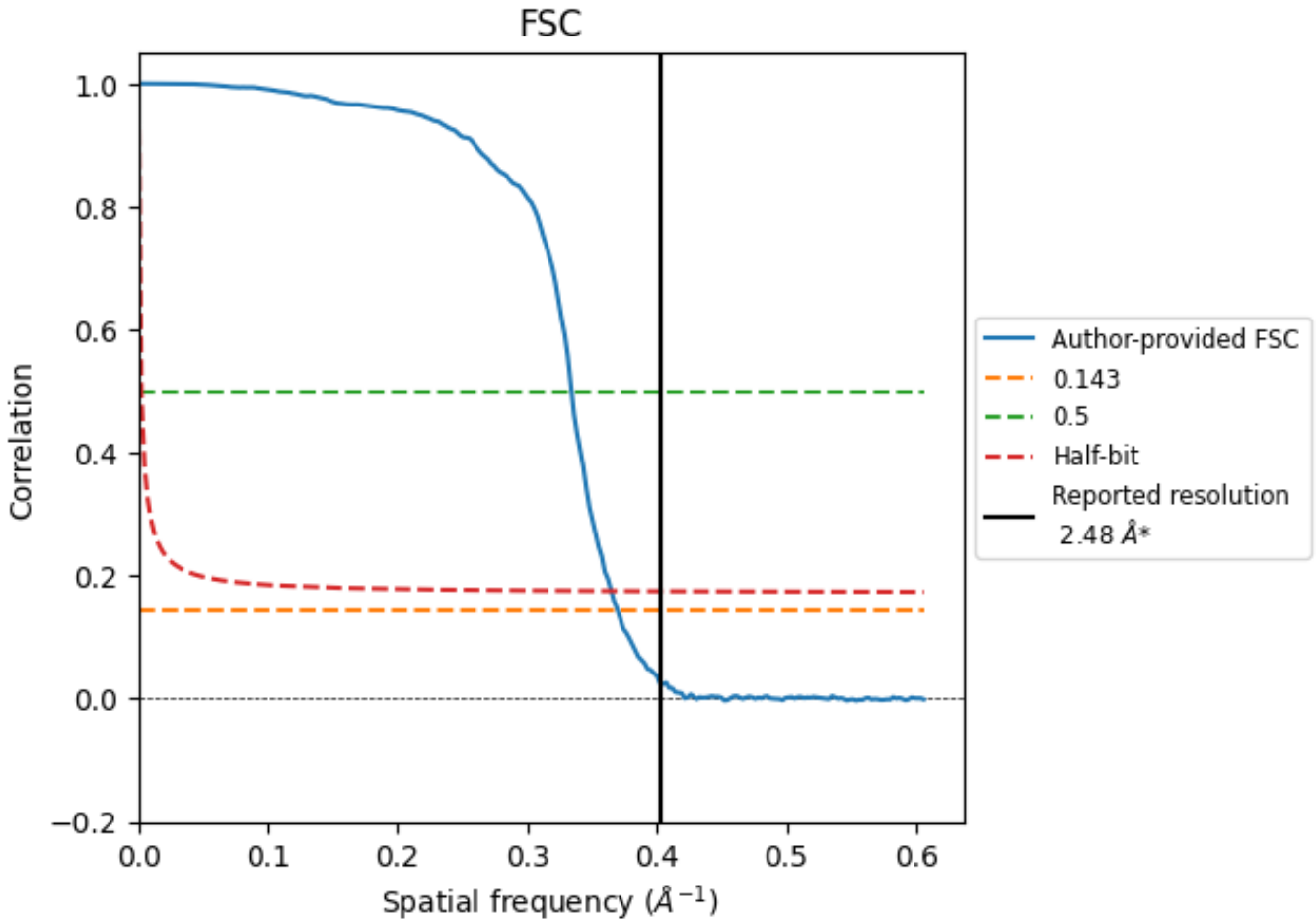


*Reported resolution corresponds to spatial frequency of 0.403 Å^{-1}

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 0.403 Å^{-1}

8.2 Resolution estimates (i)

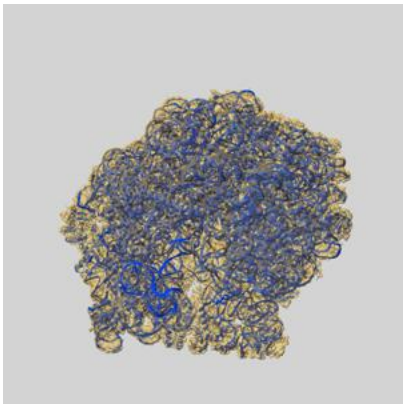
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.70	2.99	2.74
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

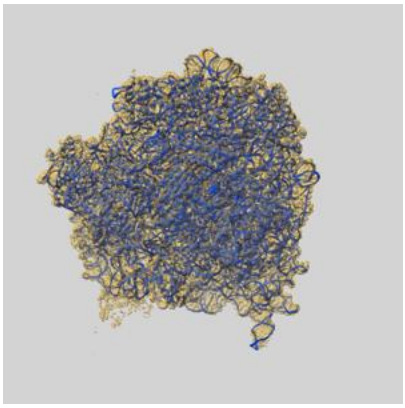
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24802 and PDB model 7S1I. Per-residue inclusion information can be found in section 3 on page 16.

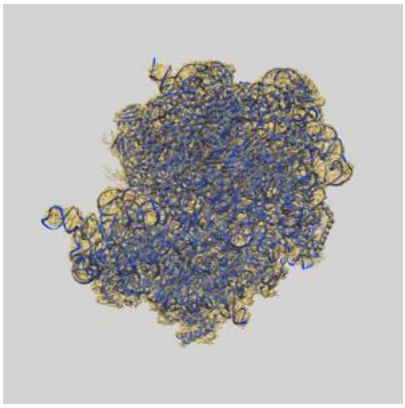
9.1 Map-model overlay



X



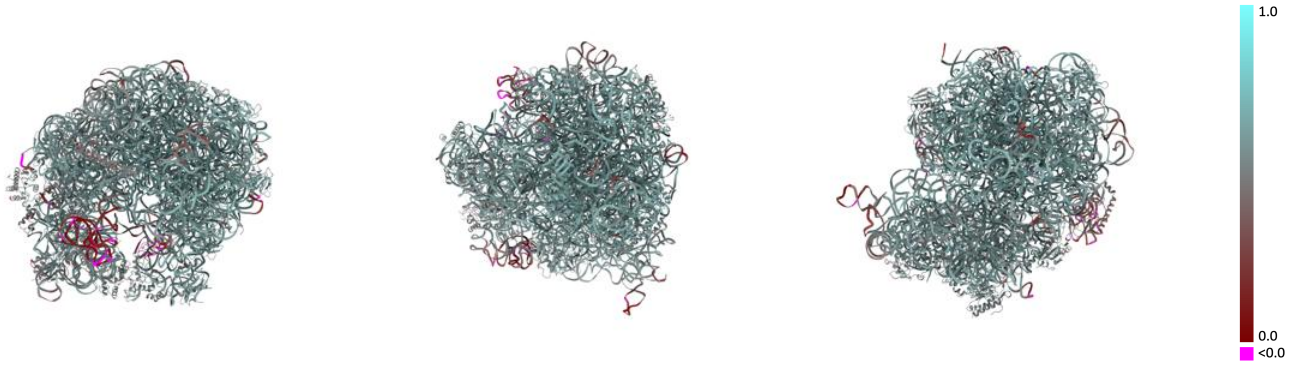
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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.

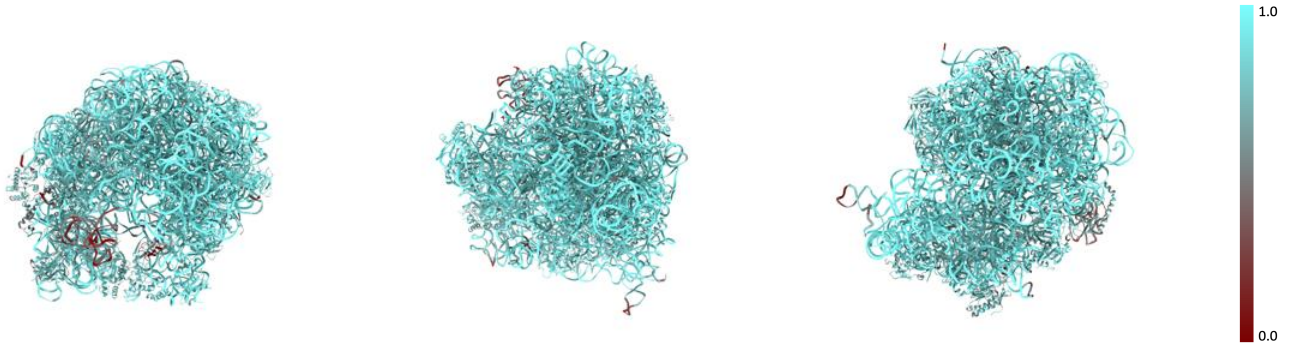
9.2 Q-score mapped to coordinate model (i)



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.

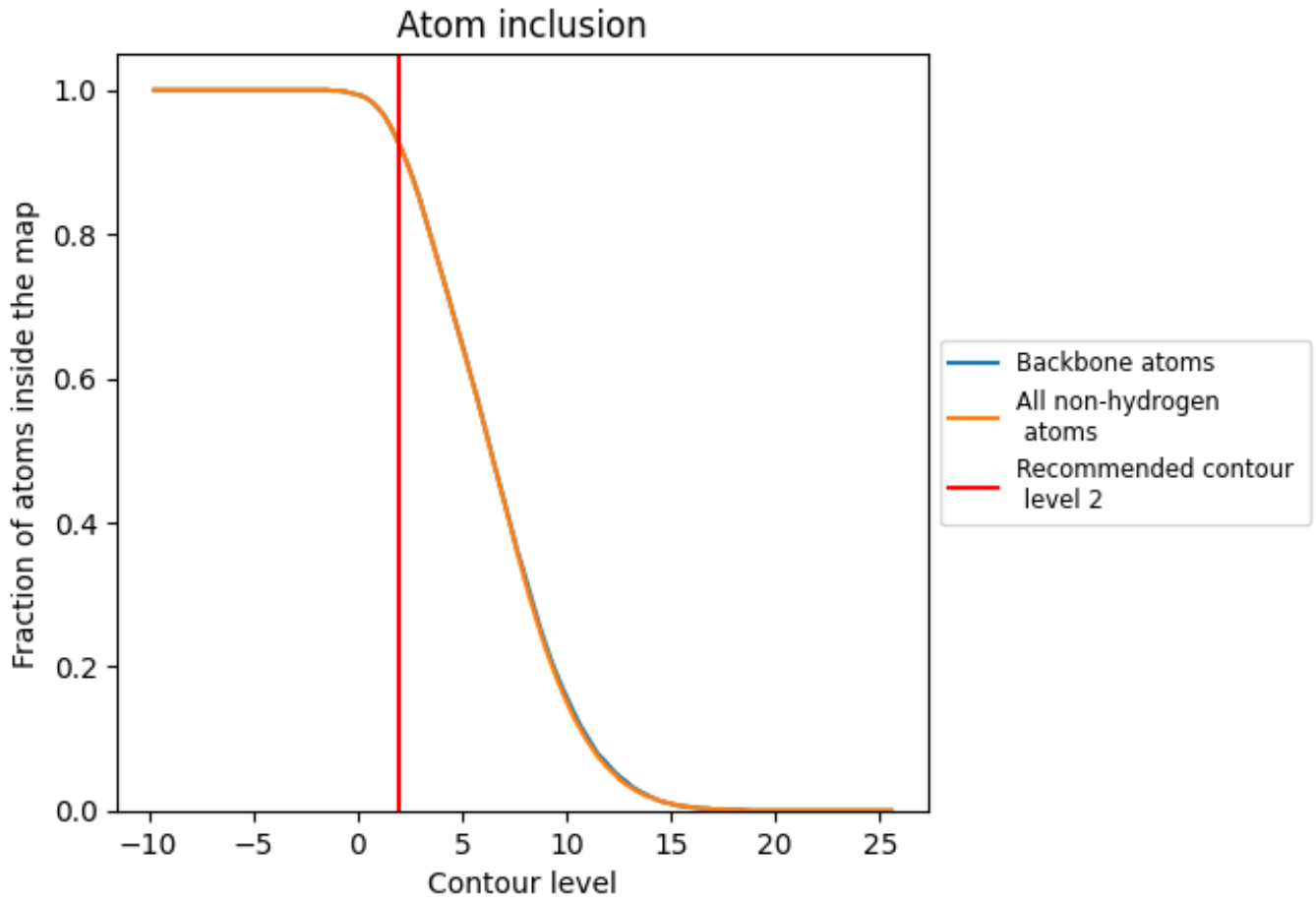
9.3 Atom inclusion mapped to coordinate model (i)



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 (2).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9250	0.5750
1	0.8440	0.5300
2	0.8450	0.5410
3	0.6540	0.4820
4	0.9040	0.5620
A	0.9200	0.5500
C	0.9610	0.5770
D	0.6860	0.4960
E	0.8270	0.5550
F	0.8040	0.5340
G	0.8860	0.5790
H	0.8930	0.5400
I	0.9560	0.5830
J	0.9800	0.5910
K	0.9420	0.6190
L	0.9300	0.6150
M	0.8820	0.5800
N	0.8480	0.5330
O	0.8470	0.5420
P	0.6840	0.4550
Q	0.8410	0.5310
R	0.9210	0.6120
S	0.9100	0.6100
T	0.9210	0.6030
U	0.9110	0.6050
V	0.9500	0.6220
W	0.8810	0.5640
X	0.9130	0.6100
Y	0.9580	0.6290
Z	0.9120	0.6040
a	0.8980	0.6120
b	0.8630	0.5700
c	0.8590	0.5690
d	0.8860	0.5940
e	0.9160	0.6220



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Chain	Atom inclusion	Q-score
f	0.9080	0.6110
g	0.8550	0.5460
h	0.8830	0.5930
i	0.9180	0.6140
j	0.1000	0.0700
k	0.9440	0.6370
l	0.9390	0.6340
m	0.8770	0.6020
n	0.7970	0.5140
o	0.8910	0.5930
p	0.7900	0.5080
q	0.6970	0.5120
r	0.8820	0.5590
s	0.7050	0.6360
t	0.8910	0.5820
u	0.8790	0.5520
v	0.8280	0.5370
w	0.9140	0.5720
x	0.8630	0.5610
y	0.8260	0.5520
z	0.9270	0.5810