



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 11:06 pm GMT

PDB ID : 6TBV
EMDB ID : EMD-10453
Title : Cryo-EM structure of an Escherichia coli ribosome-SpeFL complex stalled in response to L-ornithine (Replicate 2)
Authors : Herrero del Valle, A.; Innis, C.A.
Deposited on : 2019-11-04
Resolution : 2.70 Å(reported)
Based on initial model : 4YBB

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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

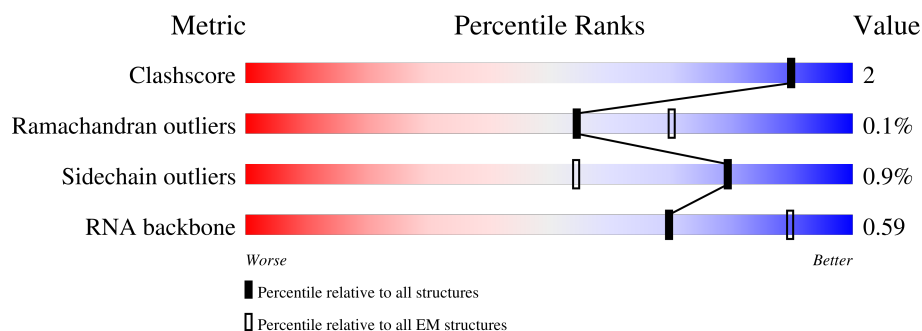
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



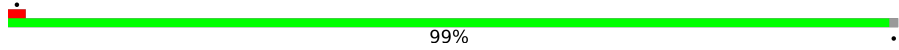
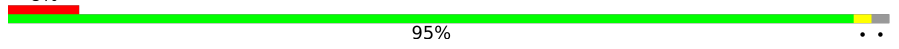
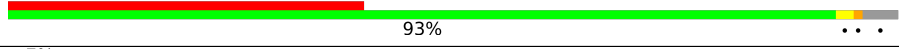
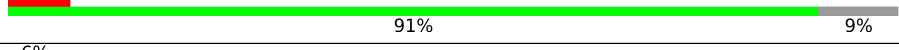
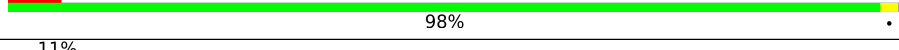
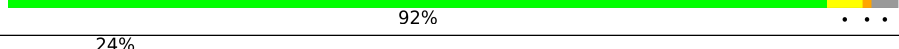
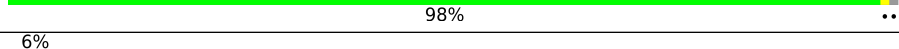
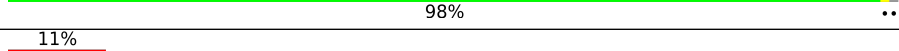
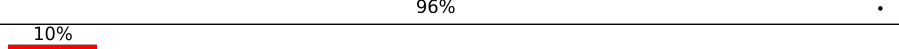
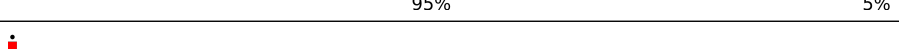
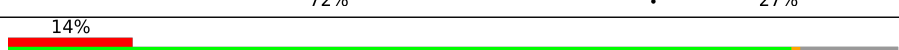



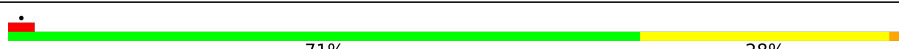
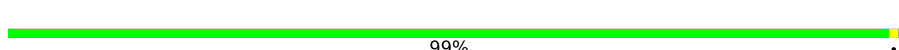
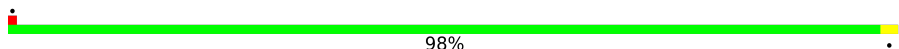
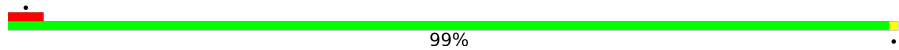
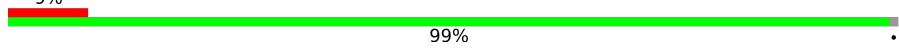
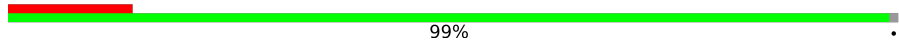
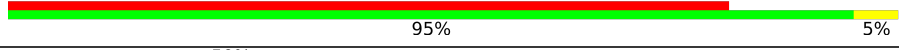
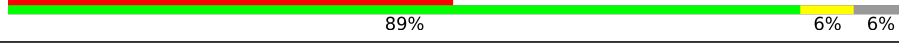
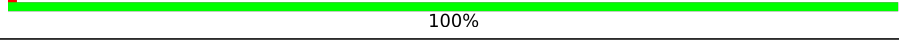
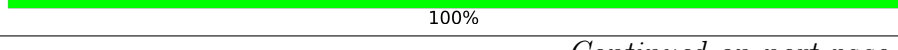

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	16S1	1534	<div> <div>6%</div> <div>65%</div> <div>30%</div> <div>5%</div> </div>
2	S021	241	<div> <div>34%</div> <div>90%</div> <div>7%</div> </div>
3	S031	233	<div> <div>7%</div> <div>88%</div> <div>12%</div> </div>
4	S041	206	<div> <div>20%</div> <div>97%</div> </div>
5	S051	167	<div> <div>9%</div> <div>92%</div> <div>7%</div> </div>
6	S061	135	<div> <div>9%</div> <div>79%</div> <div>21%</div> </div>
7	S071	179	<div> <div>27%</div> <div>82%</div> <div>16%</div> </div>

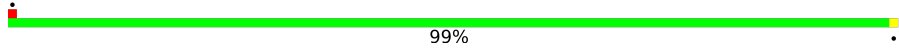
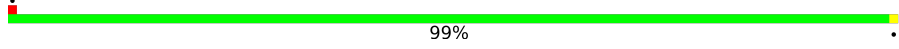
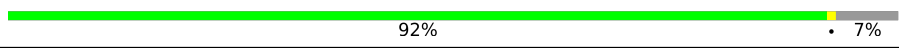
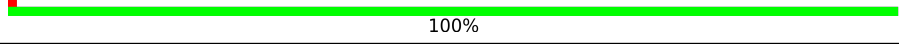
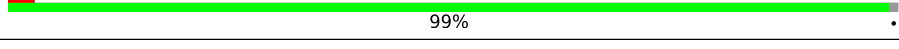
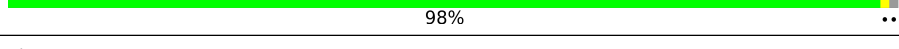
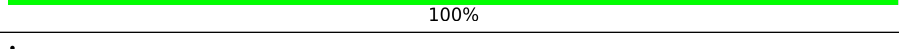
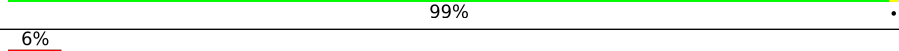
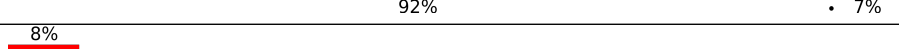
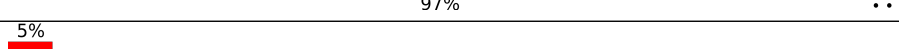
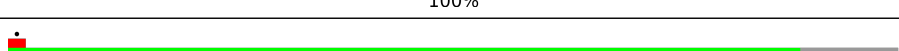


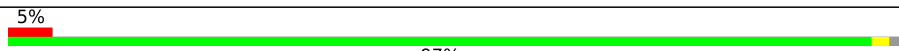
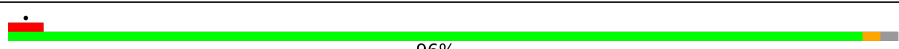

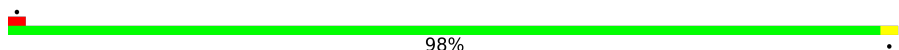
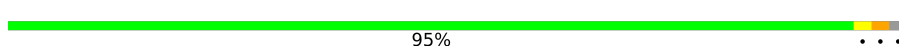
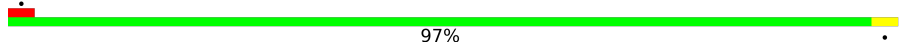

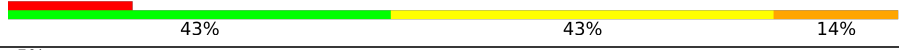


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Mol	Chain	Length	Quality of chain
8	S081	130	
9	S091	130	
10	S101	103	
11	S111	129	
12	S121	124	
13	S131	118	
14	S141	102	
15	S151	89	
16	S161	82	
17	S171	84	
18	S181	75	
19	S191	92	
20	S201	87	
21	S211	71	
22	23S1	2897	
23	05S1	120	
24	L021	273	
25	L031	209	
26	L041	201	
27	L051	179	
28	L061	177	
29	L091	149	
30	L311	70	
31	L131	142	
32	L141	123	

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Mol	Chain	Length	Quality of chain
33	L151	144	
34	L161	136	
35	L171	127	
36	L181	117	
37	L191	115	
38	L201	118	
39	L211	103	
40	L221	110	
41	L231	100	
42	L241	104	
43	L251	94	
44	L271	85	
45	L281	78	
46	L291	63	
47	L301	59	
48	L321	57	
49	L331	55	
50	L341	46	
51	L351	65	
52	L361	38	
53	SPE1	34	
54	MRN1	7	
55	PTR1	76	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 146672 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	16S1	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S021	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S031	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S041	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S051	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S061	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S071	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S081	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S091	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S101	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S111	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S121	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S131	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S141	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S141	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S151	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S161	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S171	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S181	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S191	82	Total	C	N	O	S	0	0
			656	419	125	110	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S201	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S211	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	23S1	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	05S1	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L021	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L031	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L041	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L051	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L061	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L091	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L311	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L131	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L141	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L151	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L161	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L171	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L181	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L191	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	L201	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L211	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L221	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	L231	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L241	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	L251	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L271	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L281	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L291	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L301	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L321	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L331	51	Total	C	N	O		0	0
			414	266	76	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L341	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	L351	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	L361	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called SpeFL.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SPE1	34	Total	C	N	O	S	0	0
			300	187	62	48	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SPE1	5	SER	ASN	conflict	UNP A0A4S4NWS2
SPE1	7	THR	LEU	conflict	UNP A0A4S4NWS2

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	MRN1	7	Total	C	N	O	P	0	0
			146	65	23	51	7		

- Molecule 55 is a RNA chain called P-site Arg-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	PTR1	76	Total	C	N	O	P	S	0	0
			1627	727	294	528	76	2		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	16S1	87	Total	Mg	0
			87	87	
56	23S1	250	Total	Mg	0
			250	250	
56	L231	1	Total	Mg	0
			1	1	
56	PTR1	1	Total	Mg	0
			1	1	

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	16S1	39	Total	K	0
			39	39	
57	23S1	105	Total	K	0
			105	105	
57	05S1	1	Total	K	0
			1	1	
57	L031	1	Total	K	0
			1	1	
57	L161	1	Total	K	0
			1	1	

- Molecule 58 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
58	16S1	148	Total	X	0
			148	148	
58	S021	1	Total	X	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
58	S031	1	Total 1	X 1	0
58	S111	2	Total 2	X 2	0
58	S131	1	Total 1	X 1	0
58	S171	1	Total 1	X 1	0
58	23S1	919	Total 919	X 919	0
58	05S1	9	Total 9	X 9	0
58	L021	20	Total 20	X 20	0
58	L031	14	Total 14	X 14	0
58	L041	10	Total 10	X 10	0
58	L131	5	Total 5	X 5	0
58	L141	7	Total 7	X 7	0
58	L151	4	Total 4	X 4	0
58	L161	3	Total 3	X 3	0
58	L171	5	Total 5	X 5	0
58	L181	1	Total 1	X 1	0
58	L191	4	Total 4	X 4	0
58	L201	7	Total 7	X 7	0
58	L211	1	Total 1	X 1	0
58	L221	8	Total 8	X 8	0
58	L231	1	Total 1	X 1	0
58	L241	2	Total 2	X 2	0

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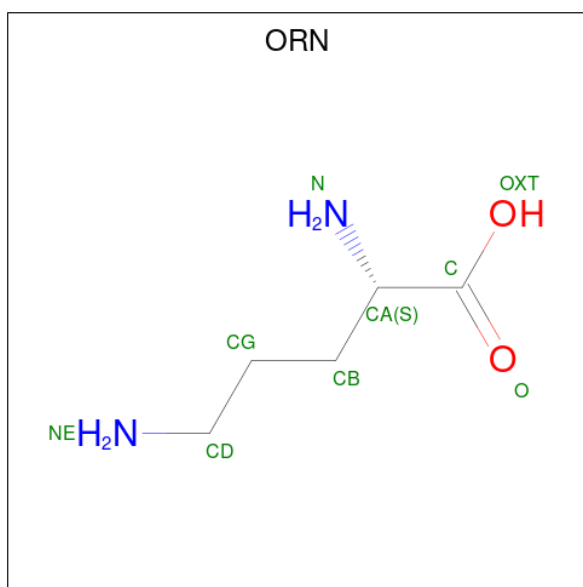
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Mol	Chain	Residues	Atoms		AltConf
58	L251	1	Total 1	X 1	0
58	L271	1	Total 1	X 1	0
58	L281	1	Total 1	X 1	0
58	L321	2	Total 2	X 2	0
58	L331	1	Total 1	X 1	0
58	L341	7	Total 7	X 7	0
58	L351	4	Total 4	X 4	0
58	SPE1	6	Total 6	X 6	0
58	MRN1	1	Total 1	X 1	0
58	PTR1	3	Total 3	X 3	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	S021	1	Total 1	Zn 1	0
59	L311	1	Total 1	Zn 1	0
59	L361	1	Total 1	Zn 1	0

- Molecule 60 is L-ornithine (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				AltConf
60	23S1	1	Total	C	N	O	0
			9	5	2	2	

- Molecule 61 is water.

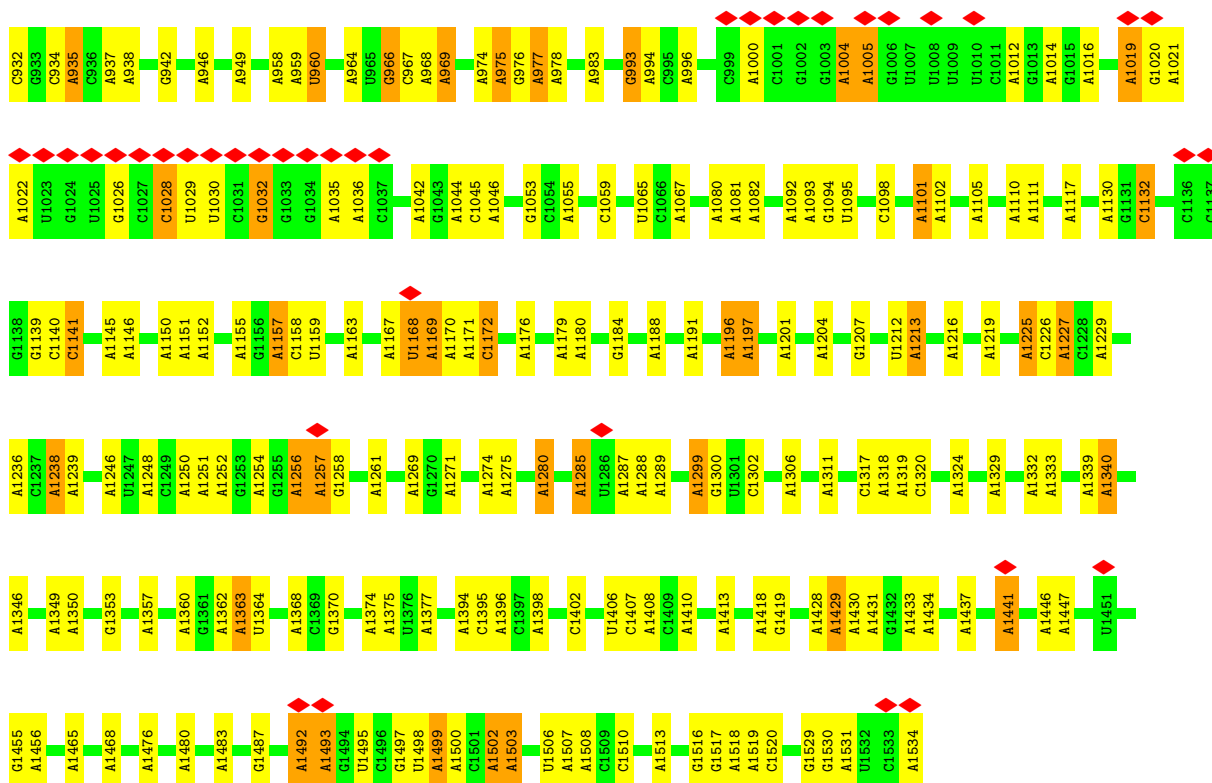
Mol	Chain	Residues	Atoms		AltConf
61	16S1	165	Total	O	0
			165	165	
61	S111	1	Total	O	0
			1	1	
61	S131	2	Total	O	0
			2	2	
61	S141	3	Total	O	0
			3	3	
61	S171	1	Total	O	0
			1	1	
61	23S1	616	Total	O	0
			616	616	
61	L021	6	Total	O	0
			6	6	
61	L031	2	Total	O	0
			2	2	
61	L151	2	Total	O	0
			2	2	
61	L171	2	Total	O	0
			2	2	

3 Residue-property plots

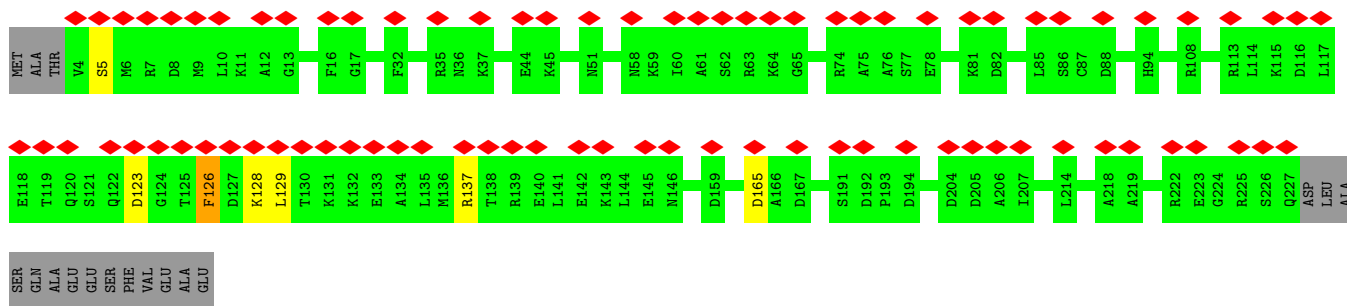
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

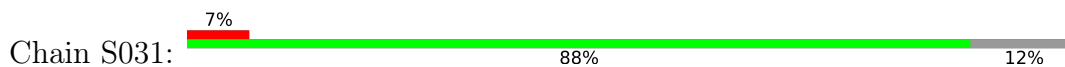




- Molecule 2: 30S ribosomal protein S2

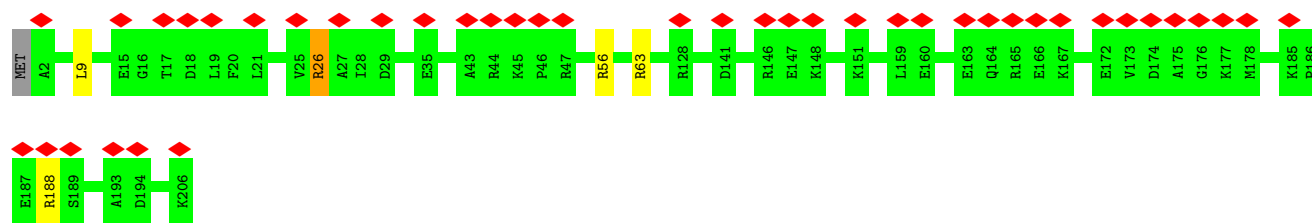


- Molecule 3: 30S ribosomal protein S3

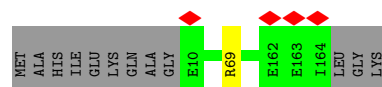


- Molecule 4: 30S ribosomal protein S4

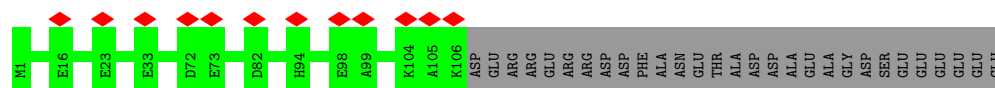
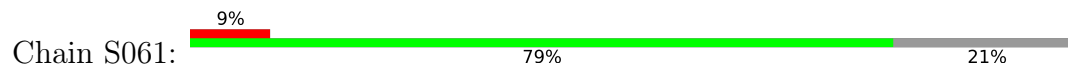




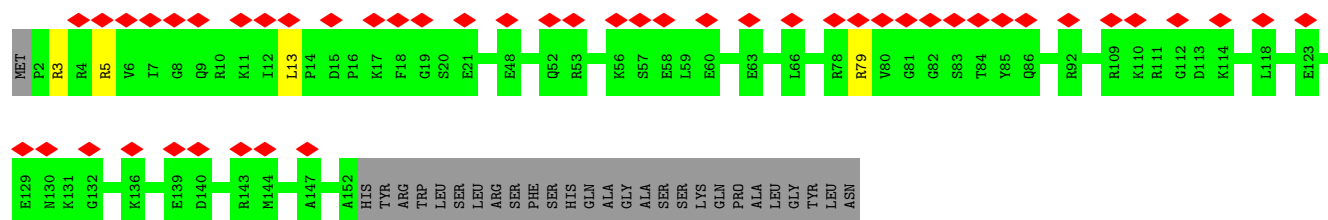
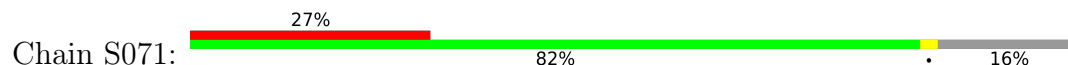
- Molecule 5: 30S ribosomal protein S5



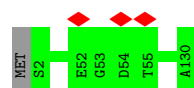
- Molecule 6: 30S ribosomal protein S6



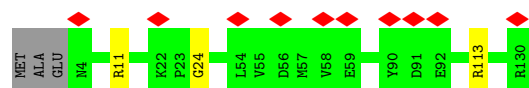
- Molecule 7: 30S ribosomal protein S7



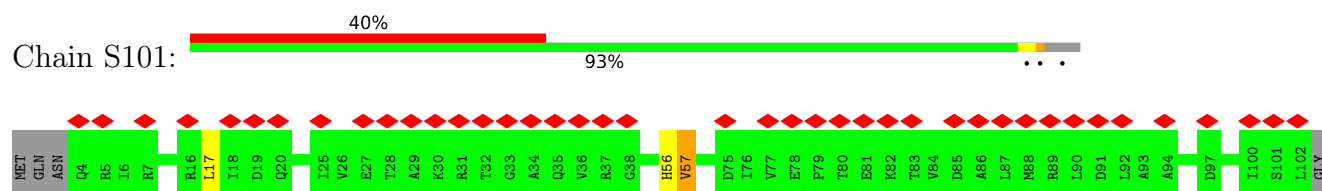
- Molecule 8: 30S ribosomal protein S8



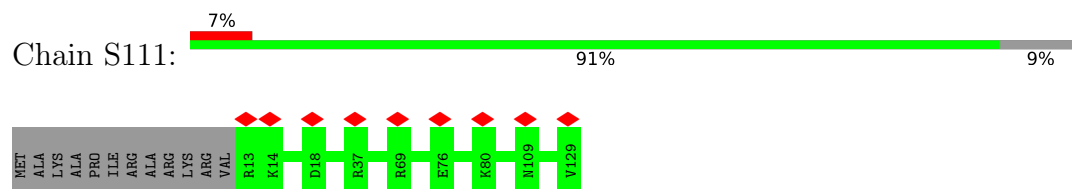
- Molecule 9: 30S ribosomal protein S9



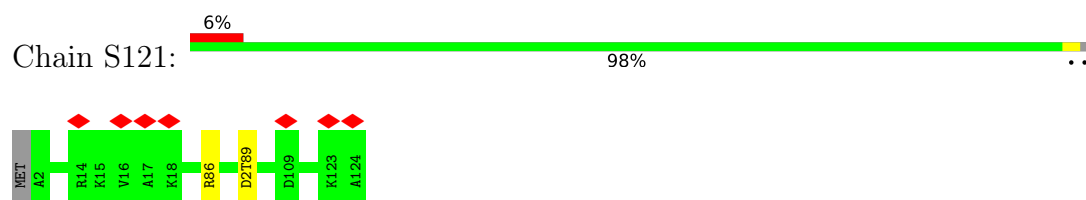
- Molecule 10: 30S ribosomal protein S10



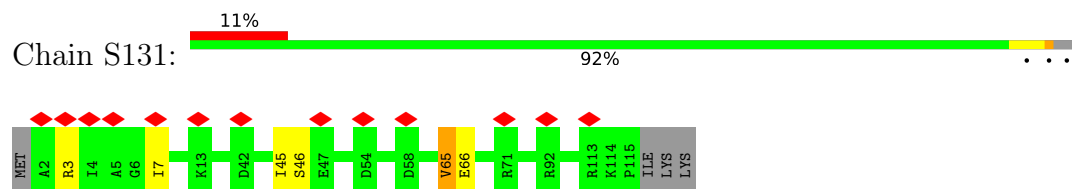
- Molecule 11: 30S ribosomal protein S11



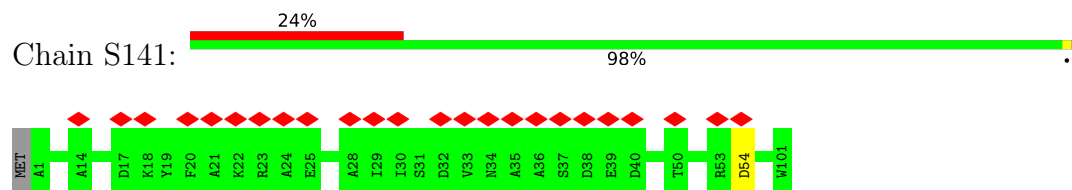
- Molecule 12: 30S ribosomal protein S12



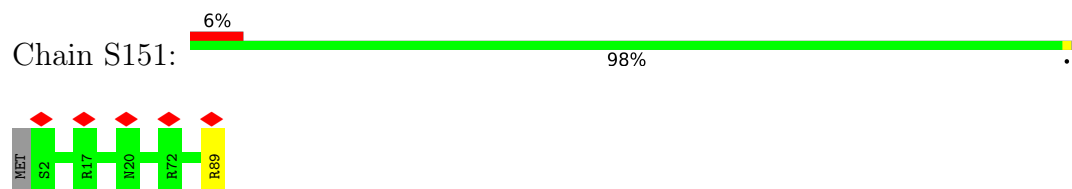
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

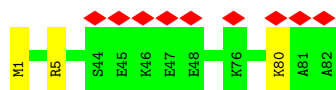


- Molecule 15: 30S ribosomal protein S15

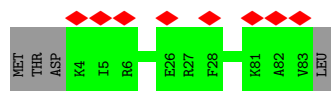


- Molecule 16: 30S ribosomal protein S16

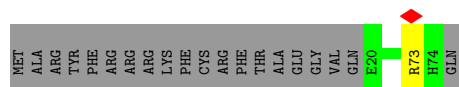
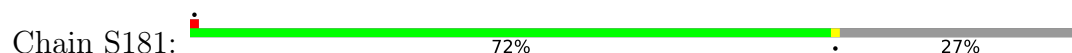




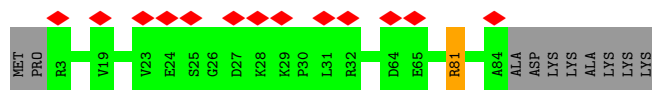
- Molecule 17: 30S ribosomal protein S17



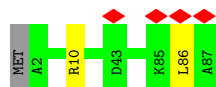
- Molecule 18: 30S ribosomal protein S18



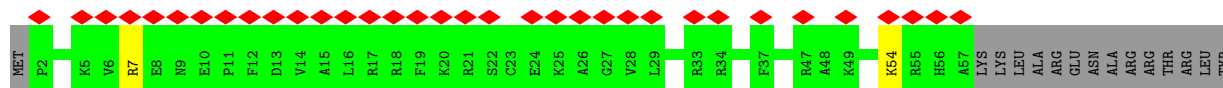
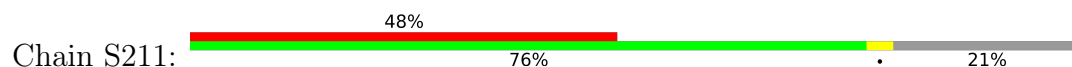
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

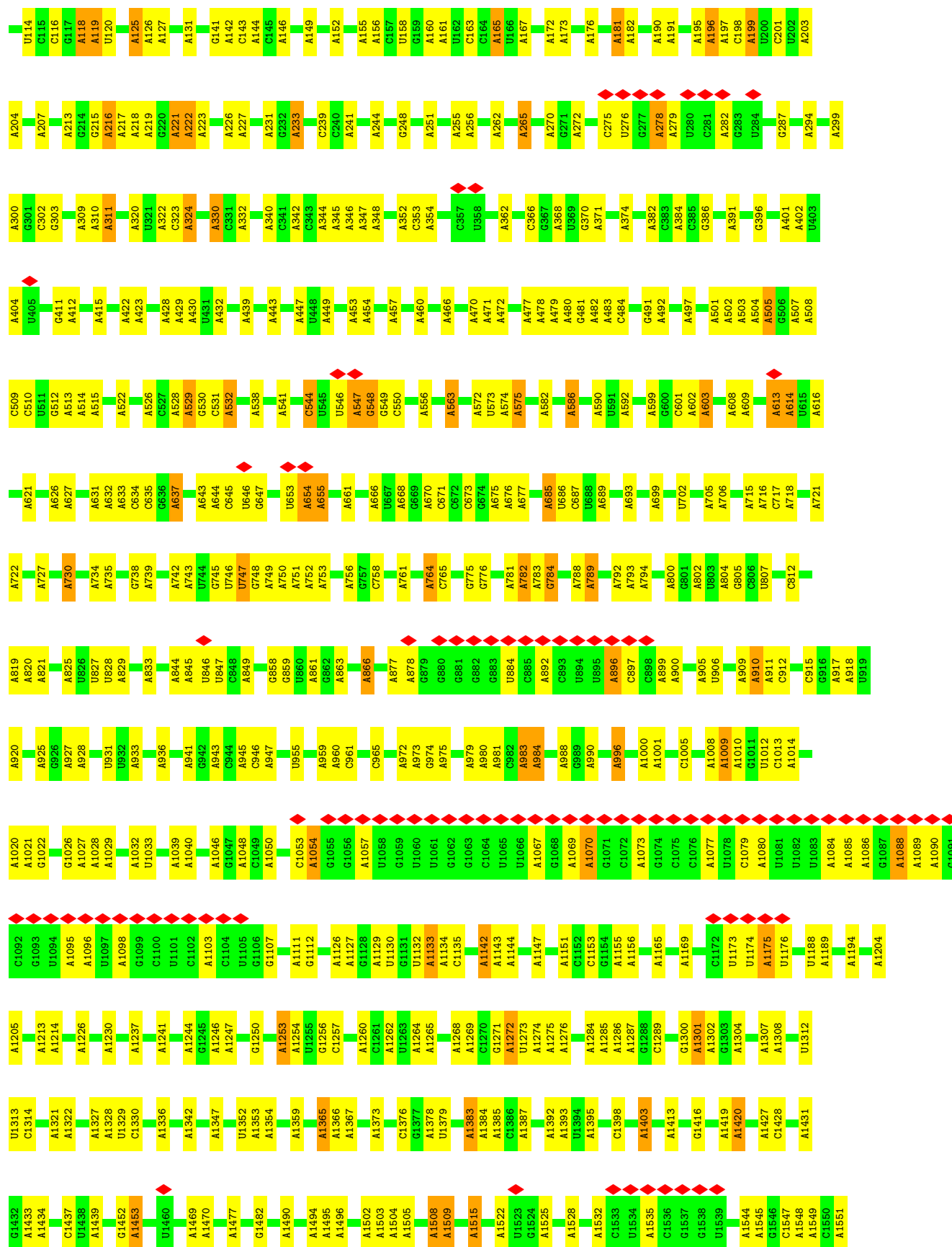


- Molecule 21: 30S ribosomal protein S21

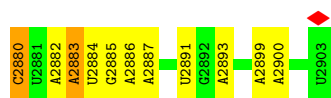


- Molecule 22: 23S rRNA





A1552	A1553	A1566	A1569	A1570	A1571	A1572	U1578	A1579	A1580	A1583	U1584	C1585	A1586	A1590	A1591	C1592	A1593	A1596	A1597	A1598	A1603	C1606	C1607	A1608	A1609	A1610	A1614	C1615	A1616	C1617	A1618	A1626	A1630	G1631	A1632	G1633	A1634	A1635	U1636	A1637	A1640	A1641	C1644	U1647	U1648																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
G1649	A1650	G1651	G1653	A1654	A1655	C1656	A1664	A1665	A1668	A1669	U1670	U1671	G1672	G1673	G1674	C1675	A1676	A1677	A1678	A1679	A1688	G1699	A1700	A1701	A1705	A1711	U1712	A1713	A1717	A1722	U1729	C1730	G1731	A1735	G1738	A1739	A1744	A1745	A1746	A1749	U1754	A1755																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
G1756	A1757	U1758	A1759	A1762	G1763	C1764	A1772	A1773	C1774	U1775	U1779	A1780	U1781	U1782	A1783	A1784	A1785	A1786	C1788	A1789	G1790	A1791	A1794	C1800	A1801	A1802	A1803	A1804	A1805	A1808	A1809	A1810	G1811	A1815	C1816	A1819	U1820	A1821	A1829	G1835	A1847	A1848	A1853	A1854	A1858																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
A1866	C1870	A1871	A1872	A1873	A1876	A1877	A1885	A1889	A1890	A1899	A1900	A1901	G1906	U1911	A1912	A1913	C1914	3TD1915	A1916	U1917	A1918	A1919	C1920	A1927	A1928	G1929	G1930	U1931	A1932	A1936	A1937	A1938	U1939	A1952	A1953	G1954	U1955	A1960	C1961	C1962	A1966	G1967	G1968	A1969	U1970	U1971																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G1972	A1977	A1978	A1981	A1987	U1991	G1992	U1993	C1997	A1998	A2003	A2004	A2005	C2006	A2009	A2013	A2014	A2015	A2019	A2020	C2023	G2027	A2030	A2031	G2032	A2033	A2037	A2042	C2043	C2044	A2051	A2052	G2053	A2054	C2055	C2056	G2057	A2058	A2059	A2060	G2061	A2062	C2063	G2069																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
A2070	A2071	C2072	A2077	A2080	U2081	A2082	A2088	C2089	A2090	G2093	A2094	A2095	C2096	A2097	U2098	U2099	G2100	A2101	G2102	C2103	C2104	U2105	U2106	G2107	A2108	U2109	G2110	G2111	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	C2150	U2151	G2152	C2153	A2154	U2155	G2156	G2157	A2158	C2159	G2160	C2161	G2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	U2183	A2184	U2185	G2186	U2187	U2188	U2189	G2190	A2191	U2192	U2195	C2196	A2198																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
A2199	G2204	A2205	A2211	A2212	A2225	C2226	A2227	G2238	A2241	G2242	U2243	A2247	G2251	G2252	A2266	A2267	A2268	G2269	A2273	A2274	A2278	A2281	G2282	C2283	A2284	C2285	G2286	A2287	A2288	A2297	A2298	U2305	C2306	G2307	G2308	A2309	A2311	A2314	A2317	U2321	U2322	A2324	A2325	A2326	U2327	A2328	A2330	A2331	A2334	A2337	U2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393	A2394	A2395	A2396	A2397	A2398	A2399	A2400	A2401	A2402	A2403	A2404	A2405	A2406	A2407	A2408	A2409	A2410	A2411	A2412	A2413	A2414	A2415	A2416	A2417	A2418	A2419	A2420	A2421	A2422	A2423	A2424	A2425	A2426	A2427	A2428	A2429	A2430	A2431	A2432	A2433	A2434	A2435	A2436	A2437	A2438	A2439	A2440	A2441	A2442	A2443	A2444	A2445	A2446	A2447	A2448	A2449	A2450	A2451	A2452	A2453	A2454	A2455	A2456	A2457	A2458	A2459	A2460	A2461	A2462	A2463	A2464	A2465	A2466	A2467	A2468	A2469	A2470	A2471	A2472	A2473	A2474	A2475	A2476	A2477	A2478	A2479	A2480	A2481	A2482	A2483	A2484	A2485	A2486	A2487	A2488	A2489	A2490	A2491	A2492	A2493	A2494	A2495	A2496	A2497	A2498	A2499	A2500	A2501	A2502	A2503	A2504	A2505	A2506	A2507	A2508	A2509	A2510	A2511	A2512	A2513	A2514	A2515	A2516	A2517	A2518	A2519	A2520	A2521	A2522	A2523	A2524	A2525	A2526	A2527	A2528	A2529	A2530	A2531	A2532	A2533	A2534	A2535	A2536	A2537	A2538	A2539	A2540	A2541	A2542	A2543	A2544	A2545	A2546	A2547	A2548	A2549	A2550	A2551	A2552	A2553	A2554	A2555	A2556	A2557	A2558	A2559	A2560	A2561	A2562	A2563	A2564	A2565	A2566	A2567	A2568	A2569	A2570	A2571	A2572	A2573	A2574	A2575	A2576	A2577	A2578	A2579	A2580	A2581	A2582	A2583	A2584	A2585	A2586	A2587	A2588	A2589	A2590	A2591	A2592	A2593	A2594	A2595	A2596	A2597	A2598	A2599	A2600	A2601	A2602	A2603	A2604	A2605	A2606	A2607	A2608	A2609	A2610	A2611	A2612	A2613	A2614	A2615	A2616	A2617	A2618	A2619	A2620	A2621	A2622	A2623	A2624	A2625	A2626	A2627	A2628	A2629	A2630	A2631	A2632	A2633	A2634	A2635	A2636	A2637	A2638	A2639	A2640	A2641	A2642	A2643	A2644	A2645	A2646	A2647	A2648	A2649	A2650	A2651	A2652	A2653	A2654	A2655	A2656	A2657	A2658	A2659	A2660	A2661	A2662	A2663	A2664	A2665	A2666	A2667	A2668	A2669	A2670	A2671	A2672	A2673	A2674	A2675	A2676	A2677	A2678	A2679	A2680	A2681	A2682	A2683	A2684	A2685	A2686	A2687	A2688	A2689	A2690	A2691	A2692	A2693	A2694	A2695	A2696	A2697	A2698	A2699	A2700	A2701	A2702	A2703	A2704	A2705	A2706	A2707	A2708	A2709	A2710	A2711	A2712	A2713	A2714	A2715	A2716	A2717	A2718	A2719	A2720	A2721	A2722	A2723	A2724	A2725	A2726	A2727	A2728	A2729	A2730	A2731	A2732	A2733	A2734	A2735	A2736	A2737	A2738	A2739	A2740	A2741	A2742	A2743	A2744	A2745	A2746	A2747	A2748	A2749	A2750	A2751	A2752	A2753	A2754	A2755	A2756	A2757	A2758	A2759	A2760	A2761	A2762	A2763	A2764	A2765	A2766	A2767	A2768	A2769	A2770	A2771	A2772	A2773	A2774	A2775	A2776	A2777	A2778	A2779	A2780	A2781	A2782	A2783	A2784	A2785	A2786	A2787	A2788	A2789	A2790	A2791	A2792	A2793	A2794	A2795	A2796	A2797	A2798	A2799	A2800	A2801	A2802	A2803	A2804	A2805	A2806	A2807	A2808	A2809	A2810	A2811	A2812	A2813	A2814	A2815	A2816	A2817	A2818	A2819	A2820	A2821	A2822	A2823	A2824	A2825	A2826	A2827	A2828	A2829	A2830	A2831	A2832	A2833	A2834	A2835	A2836	A2837	A2838	A2839	A2840	A2841	A2842	A2843	A2844	A2845	A2846	A2847	A2848	A2849	A2850	A2851	A2852	A2853	A2854	A2855	A2856	A2857	A2858	A2859	A2860	A2861	A2862	A2863	A2864	A2865	A2866	A2867	A2868	A2869	A2870	A2871	A2872	A2873	A2874	A2875	A2876	A2877	A2878	A2879	A2880	A2881	A2882	A2883	A2884	A2885	A2886	A2887	A2888	A2889	A2890	A2891	A2892	A2893	A2894	A2895	A2896	A2897	A2898	A2899	A2900	A2901	A2902	A2903	A2904	A2905	A2906	A2907	A2908	A2909	A2910	A2911	A2912	A2913	A2914	A2915	A2916	A2917	A2918	A2919	A2920	A2921	A2922	A2923	A2924	A2925	A2926	A2927	A2928	A2929	A2930	A2931	A2932	A2933	A2934	A2935	A2936	A2937	A2938	A2939	A2940	A2941	A2942	A2943	A2944	A2945	A2946	A2947	A2948	A2949	A2950	A2951	A2952	A2953	A2954	A2955	A2956	A2957	A2958	A2959	A2960	A2961	A2962	A2963	A2964	A2965	A2966	A2967	A2968	A2969	A2970	A2971	A2972	A2973	A2974	A2975	A2976	A2977	A2978	A2979	A2980	A2981	A2982	A2983	A2984	A2985	A2986	A2987	A2988	A2989	A2990	A2991	A2992	A2993	A2994	A2995	A2996	A2997	A2998	A2999	A3000	A3001	A3002	A3003	A3004	A3005	A3006	A3007	A3008	A3009	A3010	A3011	A3012	A3013	A3014	A3015	A3016	A3017	A3018	A3019	A3020	A3021	A3022	A3023	A3024	A3025	A3026	A3027	A3028	A3029	A3030	A3031	A3032	A3033	A3034	A3035	A3036	A3037	A3038	A3039	A3040	A3041	A3042	A3043	A3044	A3045	A3046	A3047	A3048	A3049	A3050	A3051	A3052	A3053	A3054	A3055	A3056	A3057	A3058	A3059	A3060	A3061	A3062	A3063	A3064	A3065	A3066	A3067	A3068	A3069	A3070	A3071	A3072	A3073	A3074	A3075	A3076	A3077	A3078	A3079	A3080	A3081	A3082	A3083	A3084	A3085	A3086	A3087	A3088	A3089	A3090	A3091	A3092	A3093	A3094	A3095	A3096	A3097	A3098	A3099	A3100	A3101	A3102	A3103	A3104	A3105	A3106	A3107	A3108	A3109	A3110	A3111	A3112	A3113	A3114	A3115	A3116	A3117	A3118	A3119	A3120	A3121	A3122	A3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• Molecule 23: 5S rRNA

Chain 05S1: 71% 28%



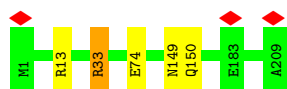
• Molecule 24: 50S ribosomal protein L2

Chain L021: 99%



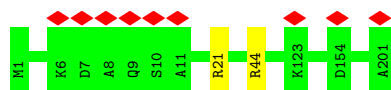
• Molecule 25: 50S ribosomal protein L3

Chain L031: 98%



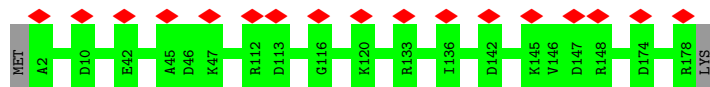
• Molecule 26: 50S ribosomal protein L4

Chain L041: 99%



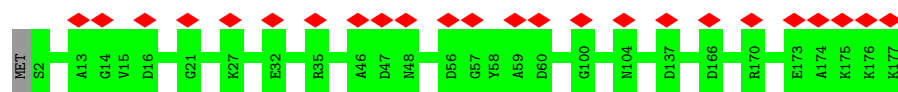
• Molecule 27: 50S ribosomal protein L5

Chain L051: 9% 99%

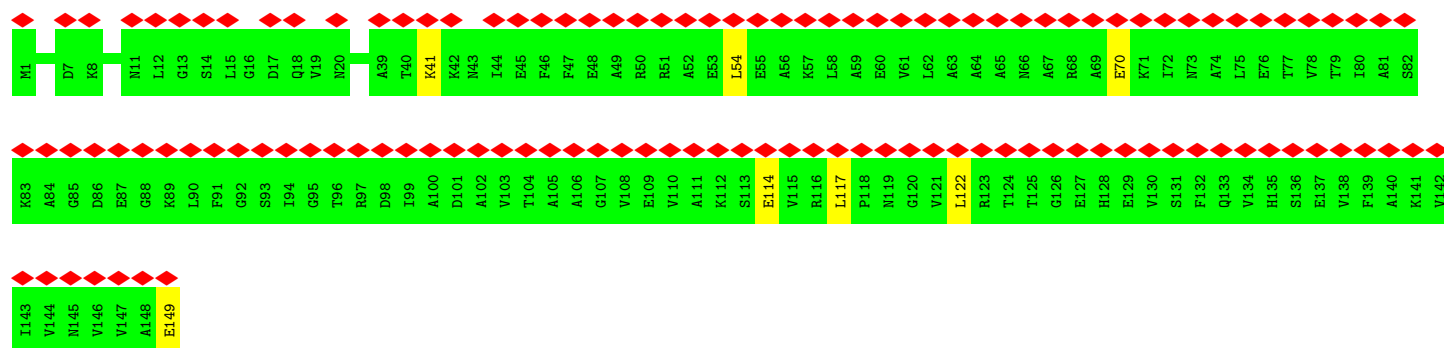
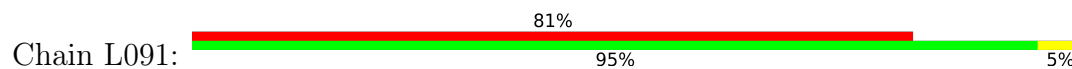


• Molecule 28: 50S ribosomal protein L6

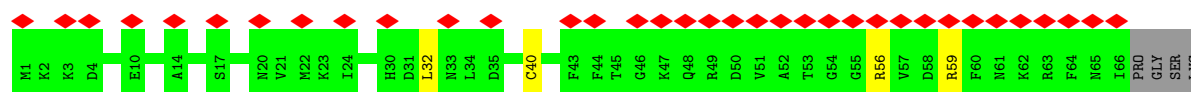
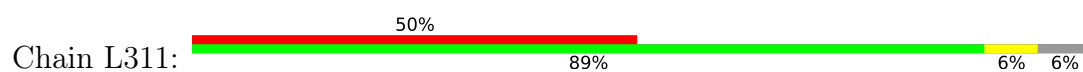
Chain L061: 14% 99%



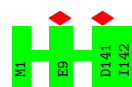
- Molecule 29: 50S ribosomal protein L9



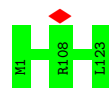
- Molecule 30: 50S ribosomal protein L31



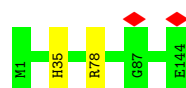
- Molecule 31: 50S ribosomal protein L13



- Molecule 32: 50S ribosomal protein L14

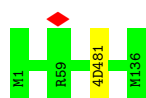


- Molecule 33: 50S ribosomal protein L15



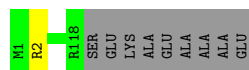
- Molecule 34: 50S ribosomal protein L16

Chain L161:  99%



- Molecule 35: 50S ribosomal protein L17

Chain L171:  92% 7%



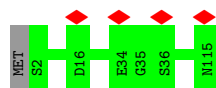
- Molecule 36: 50S ribosomal protein L18

Chain L181:  100%



- Molecule 37: 50S ribosomal protein L19

Chain L191:  99%



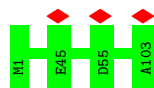
- Molecule 38: 50S ribosomal protein L20

Chain L201:  98%



- Molecule 39: 50S ribosomal protein L21

Chain L211:  100%

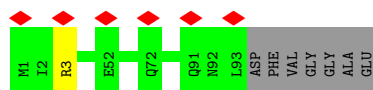


- Molecule 40: 50S ribosomal protein L22

Chain L221:  99%



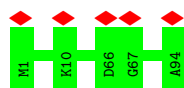
- Molecule 41: 50S ribosomal protein L23



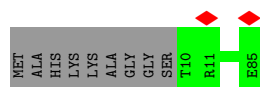
- Molecule 42: 50S ribosomal protein L24



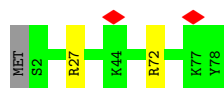
- Molecule 43: 50S ribosomal protein L25



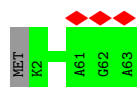
- Molecule 44: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L28

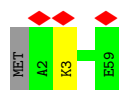


- Molecule 46: 50S ribosomal protein L29

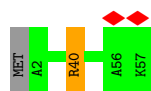


- Molecule 47: 50S ribosomal protein L30

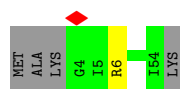




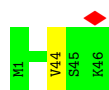
- Molecule 48: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L33



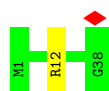
- Molecule 50: 50S ribosomal protein L34



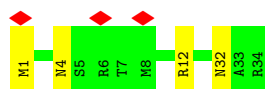
- Molecule 51: 50S ribosomal protein L35



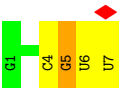
- Molecule 52: 50S ribosomal protein L36



- Molecule 53: SpeFL



- Molecule 54: mRNA



• Molecule 55: P-site Arg-tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	137494	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 ($e^-/\text{\AA}^2$)	29.6	Depositor
Minimum defocus (nm)	-600	Depositor
Maximum defocus (nm)	-1500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	29.219	Depositor
Minimum map value	-11.851	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	384.12003, 384.12003, 384.12003	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5335, 0.5335, 0.5335	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, MG, ORN, OMU, 5MC, 5MU, 4OC, OMC, MEQ, K, 4D4, UNX, 4SU, 6MZ, D2T, 2MG, 2MA, ZN, PSU, RSP, UR3, OMG, 3TD, MA6, G7M, FME

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	16S1	1.46	1103/36593 (3.0%)	3.48	4366/57081 (7.6%)
2	S021	0.68	0/1784	0.72	5/2403 (0.2%)
3	S031	0.78	0/1651	0.58	1/2225 (0.0%)
4	S041	0.83	0/1665	0.61	2/2227 (0.1%)
5	S051	0.72	0/1157	0.60	0/1557
6	S061	0.71	0/881	0.57	0/1189
7	S071	0.85	0/1195	0.65	1/1602 (0.1%)
8	S081	0.67	0/989	0.56	0/1326
9	S091	0.99	0/1034	0.83	0/1375
10	S101	0.88	0/805	0.70	1/1089 (0.1%)
11	S111	0.80	0/893	0.63	0/1205
12	S121	0.89	0/960	0.62	0/1286
13	S131	0.95	1/892 (0.1%)	0.78	1/1193 (0.1%)
14	S141	0.91	0/811	0.62	0/1081
15	S151	0.87	0/722	0.51	0/964
16	S161	0.87	0/659	0.68	0/884
17	S171	0.76	0/657	0.56	0/881
18	S181	0.87	0/462	0.56	0/621
19	S191	0.77	0/672	0.59	0/904
20	S201	0.72	0/676	0.53	1/895 (0.1%)
21	S211	1.01	0/472	0.53	0/627
22	23S1	1.53	2027/69120 (2.9%)	3.56	8534/107824 (7.9%)
23	05S1	1.32	71/2872 (2.5%)	3.09	276/4478 (6.2%)
24	L021	0.84	0/2121	0.60	1/2852 (0.0%)
25	L031	0.73	2/1576 (0.1%)	0.75	4/2119 (0.2%)
26	L041	0.70	0/1571	0.54	0/2113
27	L051	0.78	0/1434	0.63	0/1926
28	L061	0.65	0/1343	0.56	0/1816
29	L091	0.76	1/1121 (0.1%)	0.88	4/1515 (0.3%)
30	L311	0.77	0/531	0.87	3/709 (0.4%)
31	L131	0.72	0/1152	0.50	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	L141	0.81	0/955	0.58	0/1279
33	L151	0.81	0/1062	0.55	0/1413
34	L161	0.79	0/1081	0.54	0/1443
35	L171	0.94	0/958	0.60	0/1281
36	L181	0.83	0/910	0.52	0/1219
37	L191	0.84	0/929	0.52	0/1242
38	L201	0.90	0/960	0.50	0/1278
39	L211	0.73	0/829	0.54	0/1107
40	L221	0.78	0/864	0.54	0/1156
41	L231	0.72	0/744	0.61	0/994
42	L241	0.68	0/787	0.60	1/1051 (0.1%)
43	L251	0.66	0/766	0.53	0/1025
44	L271	0.83	0/587	0.49	0/776
45	L281	0.96	0/635	0.55	0/848
46	L291	0.77	0/502	0.48	0/667
47	L301	0.82	0/453	0.56	0/605
48	L321	0.89	0/450	0.69	1/599 (0.2%)
49	L331	0.67	0/421	0.68	1/561 (0.2%)
50	L341	1.14	0/380	0.69	1/498 (0.2%)
51	L351	0.77	0/513	0.64	1/676 (0.1%)
52	L361	0.91	0/303	0.52	0/397
53	SPE1	0.91	0/299	0.71	0/399
54	MRN1	0.61	0/161	1.28	1/248 (0.4%)
55	PTR1	1.65	56/1672 (3.3%)	3.19	173/2598 (6.7%)
All	All	1.34	3261/155692 (2.1%)	3.04	13379/232878 (5.7%)

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
2	S021	0	3
9	S091	0	1
10	S101	0	2
13	S131	0	3
19	S191	0	1
21	S211	0	1
29	L091	0	2
33	L151	0	1
47	L301	0	1
51	L351	0	1
All	All	0	16

The worst 5 of 3261 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	20	U	C5-C6	23.07	1.54	1.34
55	PTR1	17	U	C5-C6	22.09	1.54	1.34
22	23S1	2449	U	C5-C6	20.84	1.52	1.34
55	PTR1	17	U	N1-C6	10.44	1.47	1.38
55	PTR1	20	U	N1-C6	10.04	1.47	1.38

The worst 5 of 13379 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2189	U	O5'-P-OP1	-28.80	76.14	110.70
22	23S1	2872	A	N1-C6-N6	-26.88	102.47	118.60
22	23S1	2887	A	C2-N3-C4	26.20	123.70	110.60
22	23S1	504	A	N1-C2-N3	-25.31	116.65	129.30
22	23S1	1434	A	N1-C6-N6	-24.56	103.86	118.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S021	123	ASP	Peptide
2	S021	126	PHE	Sidechain
2	S021	5	SER	Peptide
9	S091	24	GLY	Peptide
10	S101	56	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16S1	32930	0	0	0	0
2	S021	1753	0	0	0	0
3	S031	1624	0	0	0	0
4	S041	1643	0	0	0	0
5	S051	1144	0	0	0	0
6	S061	862	0	0	0	0
7	S071	1181	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	S081	979	0	0	0	0
9	S091	1022	0	0	0	0
10	S101	795	0	0	0	0
11	S111	877	0	0	0	0
12	S121	957	0	0	0	0
13	S131	883	0	0	0	0
14	S141	799	0	0	0	0
15	S151	714	0	0	0	0
16	S161	649	0	0	0	0
17	S171	648	0	0	0	0
18	S181	455	0	0	0	0
19	S191	656	0	0	0	0
20	S201	670	0	0	0	0
21	S211	465	0	0	0	0
22	23S1	62209	0	0	0	0
23	05S1	2569	0	0	0	0
24	L021	2082	0	0	0	0
25	L031	1566	0	0	0	0
26	L041	1552	0	0	0	0
27	L051	1410	0	0	0	0
28	L061	1323	0	0	0	0
29	L091	1110	0	0	0	0
30	L311	522	0	0	0	0
31	L131	1129	0	0	0	0
32	L141	946	0	0	0	0
33	L151	1053	0	0	0	0
34	L161	1075	0	0	0	0
35	L171	945	0	0	0	0
36	L181	900	0	0	0	0
37	L191	917	0	0	0	0
38	L201	947	0	0	0	0
39	L211	816	0	0	0	0
40	L221	857	0	0	0	0
41	L231	738	0	0	0	0
42	L241	779	0	0	0	0
43	L251	753	0	0	0	0
44	L271	580	0	0	0	0
45	L281	625	0	0	0	0
46	L291	501	0	0	0	0
47	L301	449	0	0	0	0
48	L321	444	0	0	0	0
49	L331	414	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	L341	377	0	0	0	0
51	L351	504	0	0	0	0
52	L361	302	0	0	0	0
53	SPE1	300	0	0	0	0
54	MRN1	146	0	0	0	0
55	PTR1	1627	0	0	0	0
56	16S1	87	0	0	0	0
56	23S1	250	0	0	0	0
56	L231	1	0	0	0	0
56	PTR1	1	0	0	0	0
57	05S1	1	0	0	0	0
57	16S1	39	0	0	0	0
57	23S1	105	0	0	0	0
57	L031	1	0	0	0	0
57	L161	1	0	0	0	0
58	05S1	9	0	0	0	0
58	16S1	148	0	0	0	0
58	23S1	919	0	0	0	0
58	L021	20	0	0	0	0
58	L031	14	0	0	0	0
58	L041	10	0	0	0	0
58	L131	5	0	0	0	0
58	L141	7	0	0	0	0
58	L151	4	0	0	0	0
58	L161	3	0	0	0	0
58	L171	5	0	0	0	0
58	L181	1	0	0	0	0
58	L191	4	0	0	0	0
58	L201	7	0	0	0	0
58	L211	1	0	0	0	0
58	L221	8	0	0	0	0
58	L231	1	0	0	0	0
58	L241	2	0	0	0	0
58	L251	1	0	0	0	0
58	L271	1	0	0	0	0
58	L281	1	0	0	0	0
58	L321	2	0	0	0	0
58	L331	1	0	0	0	0
58	L341	7	0	0	0	0
58	L351	4	0	0	0	0
58	MRN1	1	0	0	0	0
58	PTR1	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	S021	1	0	0	0	0
58	S031	1	0	0	0	0
58	S111	2	0	0	0	0
58	S131	1	0	0	0	0
58	S171	1	0	0	0	0
58	SPE1	6	0	0	0	0
59	L311	1	0	0	0	0
59	L361	1	0	0	0	0
59	S021	1	0	0	0	0
60	23S1	9	0	0	0	0
61	16S1	165	0	0	0	0
61	23S1	616	0	0	0	0
61	L021	6	0	0	0	0
61	L031	2	0	0	0	0
61	L151	2	0	0	0	0
61	L171	2	0	0	0	0
61	S111	1	0	0	0	0
61	S131	2	0	0	0	0
61	S141	3	0	0	0	0
61	S171	1	0	0	0	0
All	All	146672	0	0	0	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 2.

There are no clashes within the asymmetric unit.

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	
2	S021	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	S031	204/233 (88%)	194 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S041	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	S051	153/167 (92%)	146 (95%)	7 (5%)	0	100	100
6	S061	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	S071	149/179 (83%)	140 (94%)	9 (6%)	0	100	100
8	S081	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
9	S091	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
10	S101	97/103 (94%)	92 (95%)	4 (4%)	1 (1%)	15	37
11	S111	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
12	S121	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
13	S131	112/118 (95%)	101 (90%)	10 (9%)	1 (1%)	17	40
14	S141	99/102 (97%)	87 (88%)	11 (11%)	1 (1%)	15	37
15	S151	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	S161	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	S171	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
18	S181	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
19	S191	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
20	S201	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	S211	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
24	L021	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
25	L031	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	29	54
26	L041	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
27	L051	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
28	L061	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
29	L091	147/149 (99%)	129 (88%)	18 (12%)	0	100	100
30	L311	64/70 (91%)	59 (92%)	5 (8%)	0	100	100
31	L131	140/142 (99%)	140 (100%)	0	0	100	100
32	L141	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	L151	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
34	L161	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
35	L171	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
36	L181	115/117 (98%)	113 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	L191	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
38	L201	115/118 (98%)	115 (100%)	0	0	100	100
39	L211	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
40	L221	108/110 (98%)	108 (100%)	0	0	100	100
41	L231	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
42	L241	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
43	L251	92/94 (98%)	92 (100%)	0	0	100	100
44	L271	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
45	L281	75/78 (96%)	75 (100%)	0	0	100	100
46	L291	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
47	L301	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	L321	54/57 (95%)	54 (100%)	0	0	100	100
49	L331	49/55 (89%)	49 (100%)	0	0	100	100
50	L341	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
51	L351	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	9	24
52	L361	36/38 (95%)	36 (100%)	0	0	100	100
53	SPE1	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5607/5948 (94%)	5397 (96%)	205 (4%)	5 (0%)	54	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	S101	57	VAL
25	L031	149	ASN
51	L351	32	ILE
13	S131	66	GLU
14	S141	54	ASP

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	
2	S021	186/199 (94%)	185 (100%)	1 (0%)	88	96
3	S031	170/190 (90%)	170 (100%)	0	100	100
4	S041	172/173 (99%)	168 (98%)	4 (2%)	50	78
5	S051	118/126 (94%)	117 (99%)	1 (1%)	81	93
6	S061	92/116 (79%)	92 (100%)	0	100	100
7	S071	124/147 (84%)	121 (98%)	3 (2%)	49	77
8	S081	104/105 (99%)	104 (100%)	0	100	100
9	S091	105/107 (98%)	103 (98%)	2 (2%)	57	82
10	S101	87/90 (97%)	87 (100%)	0	100	100
11	S111	90/99 (91%)	90 (100%)	0	100	100
12	S121	102/103 (99%)	101 (99%)	1 (1%)	76	91
13	S131	92/96 (96%)	91 (99%)	1 (1%)	73	90
14	S141	79/84 (94%)	79 (100%)	0	100	100
15	S151	76/77 (99%)	75 (99%)	1 (1%)	69	87
16	S161	65/65 (100%)	62 (95%)	3 (5%)	27	54
17	S171	74/78 (95%)	74 (100%)	0	100	100
18	S181	48/65 (74%)	47 (98%)	1 (2%)	53	80
19	S191	71/79 (90%)	70 (99%)	1 (1%)	67	86
20	S201	65/66 (98%)	64 (98%)	1 (2%)	65	86
21	S211	48/61 (79%)	47 (98%)	1 (2%)	53	80
24	L021	216/218 (99%)	215 (100%)	1 (0%)	88	96
25	L031	163/163 (100%)	162 (99%)	1 (1%)	86	95
26	L041	165/165 (100%)	163 (99%)	2 (1%)	71	88
27	L051	148/150 (99%)	148 (100%)	0	100	100
28	L061	137/138 (99%)	137 (100%)	0	100	100
29	L091	114/114 (100%)	113 (99%)	1 (1%)	78	92
30	L311	59/62 (95%)	57 (97%)	2 (3%)	37	66
31	L131	116/116 (100%)	116 (100%)	0	100	100
32	L141	104/104 (100%)	104 (100%)	0	100	100
33	L151	103/103 (100%)	102 (99%)	1 (1%)	76	91
34	L161	108/108 (100%)	108 (100%)	0	100	100
35	L171	98/103 (95%)	97 (99%)	1 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	L181	87/87 (100%)	87 (100%)	0	100	100
37	L191	99/100 (99%)	99 (100%)	0	100	100
38	L201	89/90 (99%)	88 (99%)	1 (1%)	73	90
39	L211	84/84 (100%)	84 (100%)	0	100	100
40	L221	93/93 (100%)	92 (99%)	1 (1%)	73	90
41	L231	80/84 (95%)	79 (99%)	1 (1%)	69	87
42	L241	83/85 (98%)	83 (100%)	0	100	100
43	L251	78/78 (100%)	78 (100%)	0	100	100
44	L271	57/63 (90%)	57 (100%)	0	100	100
45	L281	67/68 (98%)	65 (97%)	2 (3%)	41	70
46	L291	54/55 (98%)	54 (100%)	0	100	100
47	L301	48/49 (98%)	48 (100%)	0	100	100
48	L321	47/48 (98%)	46 (98%)	1 (2%)	53	80
49	L331	45/49 (92%)	45 (100%)	0	100	100
50	L341	38/38 (100%)	38 (100%)	0	100	100
51	L351	51/52 (98%)	51 (100%)	0	100	100
52	L361	34/34 (100%)	33 (97%)	1 (3%)	42	71
53	SPE1	31/31 (100%)	28 (90%)	3 (10%)	8	19
All	All	4664/4858 (96%)	4624 (99%)	40 (1%)	79	92

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	L151	78	ARG
48	L321	40	ARG
35	L171	2	ARG
41	L231	3	ARG
53	SPE1	4	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16S1	1530/1534 (99%)	173 (11%)	1 (0%)
22	23S1	2890/2897 (99%)	296 (10%)	18 (0%)
23	05S1	119/120 (99%)	7 (5%)	0
54	MRN1	6/7 (85%)	3 (50%)	1 (16%)
55	PTR1	73/76 (96%)	11 (15%)	1 (1%)
All	All	4618/4634 (99%)	490 (10%)	21 (0%)

5 of 490 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16S1	7	A
1	16S1	9	G
1	16S1	22	G
1	16S1	32	A
1	16S1	39	G

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	23S1	2189	U
22	23S1	2756	U
55	PTR1	19	A
22	23S1	2873	A
22	23S1	2518	A

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

44 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
22	2MA	23S1	2503	57,22,56	17,25,26	2.38	5 (29%)	17,37,40	1.36	2 (11%)
1	UR3	16S1	1498	1	19,22,23	2.98	8 (42%)	26,32,35	1.39	2 (7%)
22	OMG	23S1	2251	57,22,55	18,26,27	2.46	8 (44%)	19,38,41	1.99	7 (36%)
22	5MU	23S1	1939	57,22	19,22,23	0.73	0	28,32,35	1.25	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	23S1	1917	22	18,21,22	4.13	7 (38%)	22,30,33	1.67	4 (18%)
1	PSU	16S1	516	56,1	18,21,22	4.07	8 (44%)	22,30,33	1.70	4 (18%)
1	G7M	16S1	527	57,1	20,26,27	2.40	6 (30%)	17,39,42	1.18	2 (11%)
1	5MC	16S1	1407	1	18,22,23	3.38	7 (38%)	26,32,35	1.03	3 (11%)
22	6MZ	23S1	2030	22	18,25,26	2.88	5 (27%)	16,36,39	2.80	4 (25%)
1	2MG	16S1	1516	1	18,26,27	2.33	7 (38%)	16,38,41	1.51	4 (25%)
55	2MG	PTR1	37	55	18,26,27	2.40	7 (38%)	16,38,41	1.41	4 (25%)
55	G7M	PTR1	46	55	20,26,27	2.56	6 (30%)	17,39,42	1.23	3 (17%)
22	OMU	23S1	2552	22,56	19,22,23	2.80	7 (36%)	26,31,34	1.83	5 (19%)
22	PSU	23S1	955	22	18,21,22	4.02	7 (38%)	22,30,33	1.94	5 (22%)
22	5MU	23S1	747	22	19,22,23	0.78	0	28,32,35	1.21	2 (7%)
22	6MZ	23S1	1618	22	18,25,26	2.96	4 (22%)	16,36,39	2.10	3 (18%)
22	G7M	23S1	2069	57,22	20,26,27	2.25	6 (30%)	17,39,42	1.27	3 (17%)
22	PSU	23S1	2580	57,22	18,21,22	4.10	7 (38%)	22,30,33	2.04	6 (27%)
1	5MC	16S1	967	1	18,22,23	3.42	7 (38%)	26,32,35	1.04	2 (7%)
1	MA6	16S1	1518	1	19,26,27	1.22	1 (5%)	18,38,41	3.21	2 (11%)
1	MA6	16S1	1519	1	19,26,27	1.24	1 (5%)	18,38,41	3.43	2 (11%)
55	PSU	PTR1	55	55	18,21,22	4.27	7 (38%)	22,30,33	1.76	5 (22%)
55	4SU	PTR1	8	55	18,21,22	3.47	8 (44%)	26,30,33	1.65	4 (15%)
22	PSU	23S1	2504	57,22	18,21,22	4.16	7 (38%)	22,30,33	1.74	4 (18%)
22	5MC	23S1	1962	57,22	18,22,23	3.29	7 (38%)	26,32,35	1.03	2 (7%)
55	5MU	PTR1	54	55	19,22,23	1.01	2 (10%)	28,32,35	1.21	4 (14%)
22	OMC	23S1	2498	22,56	19,22,23	2.73	7 (36%)	26,31,34	1.01	1 (3%)
12	D2T	S121	89	12	7,9,10	1.02	0	6,11,13	2.29	2 (33%)
1	2MG	16S1	1207	57,1	18,26,27	2.40	7 (38%)	16,38,41	1.45	3 (18%)
22	PSU	23S1	2605	22	18,21,22	4.04	7 (38%)	22,30,33	1.87	5 (22%)
22	PSU	23S1	2457	22	18,21,22	4.07	7 (38%)	22,30,33	2.05	5 (22%)
22	2MG	23S1	1835	22	18,26,27	2.29	7 (38%)	16,38,41	1.47	4 (25%)
22	1MG	23S1	745	22	18,26,27	2.50	5 (27%)	19,39,42	1.52	4 (21%)
22	PSU	23S1	746	22,56	18,21,22	4.04	7 (38%)	22,30,33	1.91	5 (22%)
34	4D4	L161	81	34	9,11,12	2.55	3 (33%)	8,13,15	1.21	1 (12%)
22	2MG	23S1	2445	22	18,26,27	2.29	7 (38%)	16,38,41	1.49	3 (18%)
22	3TD	23S1	1915	22	18,22,23	4.10	8 (44%)	22,32,35	1.63	2 (9%)
1	4OC	16S1	1402	56,1	20,23,24	2.93	8 (40%)	26,32,35	1.09	2 (7%)
53	FME	SPE1	1	53	8,9,10	0.98	0	7,9,11	1.14	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	MEQ	L031	150	25	8,9,10	1.49	2 (25%)	5,10,12	1.81	2 (40%)
22	PSU	23S1	2604	22	18,21,22	4.00	7 (38%)	22,30,33	1.78	5 (22%)
55	RSP	PTR1	32	55	17,21,22	3.90	6 (35%)	22,30,33	1.15	2 (9%)
1	2MG	16S1	966	1	18,26,27	2.41	7 (38%)	16,38,41	1.49	4 (25%)
22	PSU	23S1	1911	22	18,21,22	4.18	7 (38%)	22,30,33	1.89	5 (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
22	2MA	23S1	2503	57,22,56	-	2/3/25/26	0/3/3/3
1	UR3	16S1	1498	1	-	0/7/25/26	0/2/2/2
22	OMG	23S1	2251	57,22,55	-	0/5/27/28	0/3/3/3
22	5MU	23S1	1939	57,22	-	2/7/25/26	0/2/2/2
22	PSU	23S1	1917	22	-	0/7/25/26	0/2/2/2
1	PSU	16S1	516	56,1	-	0/7/25/26	0/2/2/2
1	G7M	16S1	527	57,1	-	2/3/25/26	0/3/3/3
1	5MC	16S1	1407	1	-	0/7/25/26	0/2/2/2
22	6MZ	23S1	2030	22	-	2/5/27/28	0/3/3/3
1	2MG	16S1	1516	1	-	0/5/27/28	0/3/3/3
55	2MG	PTR1	37	55	-	1/5/27/28	0/3/3/3
55	G7M	PTR1	46	55	-	1/3/25/26	0/3/3/3
22	OMU	23S1	2552	22,56	-	1/9/27/28	0/2/2/2
22	PSU	23S1	955	22	-	0/7/25/26	0/2/2/2
22	5MU	23S1	747	22	-	0/7/25/26	0/2/2/2
22	6MZ	23S1	1618	22	-	0/5/27/28	0/3/3/3
22	G7M	23S1	2069	57,22	-	2/3/25/26	0/3/3/3
22	PSU	23S1	2580	57,22	-	0/7/25/26	0/2/2/2
1	5MC	16S1	967	1	-	0/7/25/26	0/2/2/2
1	MA6	16S1	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	16S1	1519	1	-	2/7/29/30	0/3/3/3
55	PSU	PTR1	55	55	-	0/7/25/26	0/2/2/2
55	4SU	PTR1	8	55	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2504	57,22	-	2/7/25/26	0/2/2/2
22	5MC	23S1	1962	57,22	-	0/7/25/26	0/2/2/2
55	5MU	PTR1	54	55	-	2/7/25/26	0/2/2/2
22	OMC	23S1	2498	22,56	-	0/9/27/28	0/2/2/2
12	D2T	S121	89	12	-	1/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	16S1	1207	57,1	-	0/5/27/28	0/3/3/3
22	PSU	23S1	2605	22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2457	22	-	0/7/25/26	0/2/2/2
22	2MG	23S1	1835	22	-	0/5/27/28	0/3/3/3
22	1MG	23S1	745	22	-	0/3/25/26	0/3/3/3
22	PSU	23S1	746	22,56	-	1/7/25/26	0/2/2/2
34	4D4	L161	81	34	-	3/11/12/14	-
22	2MG	23S1	2445	22	-	2/5/27/28	0/3/3/3
22	3TD	23S1	1915	22	-	0/7/25/26	0/2/2/2
1	4OC	16S1	1402	56,1	-	2/9/29/30	0/2/2/2
53	FME	SPE1	1	53	-	6/7/9/11	-
25	MEQ	L031	150	25	-	2/8/9/11	-
22	PSU	23S1	2604	22	-	0/7/25/26	0/2/2/2
55	RSP	PTR1	32	55	-	2/7/25/26	0/2/2/2
1	2MG	16S1	966	1	-	2/5/27/28	0/3/3/3
22	PSU	23S1	1911	22	-	0/7/25/26	0/2/2/2

The worst 5 of 247 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	32	RSP	C2-N3	11.95	1.49	1.36
22	23S1	1915	3TD	C6-C5	11.82	1.49	1.35
22	23S1	2504	PSU	C6-C5	11.47	1.48	1.35
22	23S1	1911	PSU	C6-C5	11.22	1.48	1.35
55	PTR1	55	PSU	C6-C5	11.21	1.48	1.35

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1519	MA6	N1-C6-N6	-12.83	103.56	117.06
1	16S1	1518	MA6	N1-C6-N6	-11.96	104.47	117.06
22	23S1	2030	6MZ	C9-N6-C6	-7.25	116.63	122.87
1	16S1	1518	MA6	N3-C2-N1	-6.07	119.19	128.68
1	16S1	1519	MA6	N3-C2-N1	-6.07	119.20	128.68

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16S1	527	G7M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	16S1	527	G7M	C3'-C4'-C5'-O5'
1	16S1	966	2MG	O4'-C4'-C5'-O5'
1	16S1	1519	MA6	O4'-C4'-C5'-O5'
25	L031	150	MEQ	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1691 ligands modelled in this entry, 489 are monoatomic and 1201 are unknown - 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	$\# Z > 2$
60	ORN	23S1	3001	-	7,8,8	0.78	0	8,9,9	0.71	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
60	ORN	23S1	3001	-	-	2/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	23S1	3001	ORN	N-CA-CB-CG
60	23S1	3001	ORN	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	23S1	2
55	PTR1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	23S1	885:C	O3'	892:A	P	13.18
1	PTR1	46:G7M	O3'	48:C	P	5.16
1	23S1	2099:U	O3'	2100:G	P	4.33

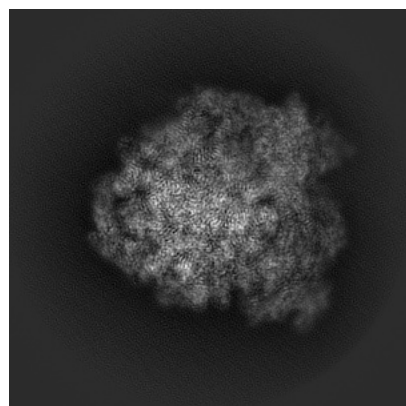
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10453. These allow visual inspection of the internal detail of the map and identification of artifacts.

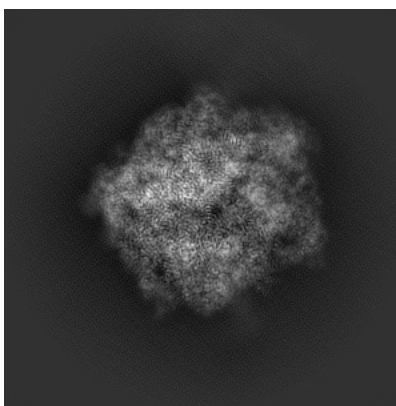
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

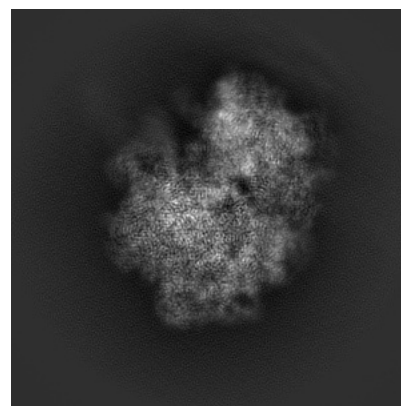
6.1.1 Primary map



X

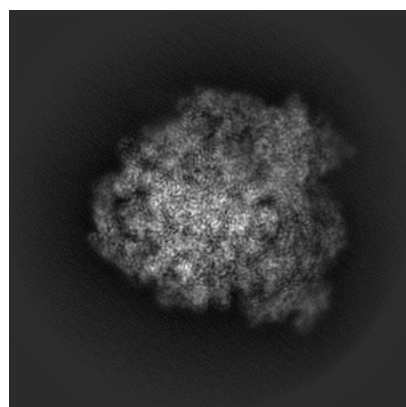


Y

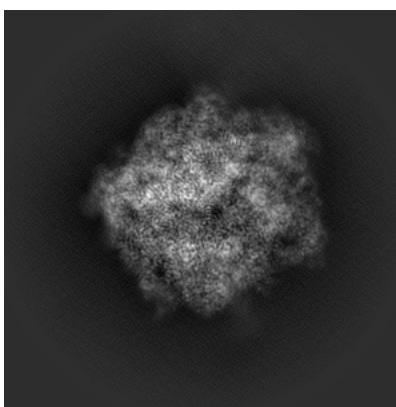


Z

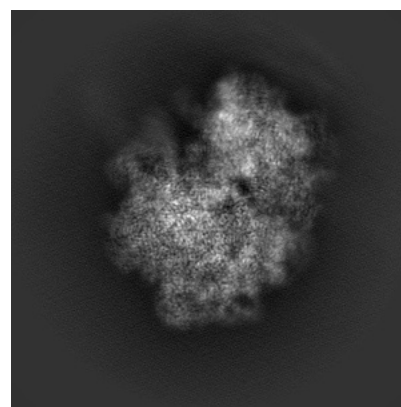
6.1.2 Raw map



X



Y

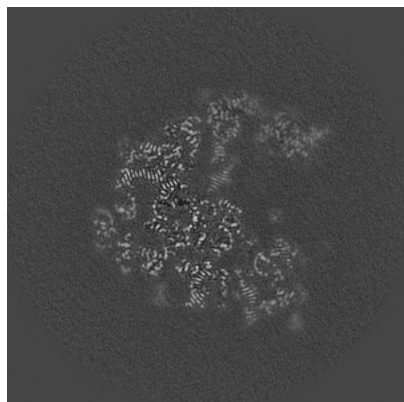


Z

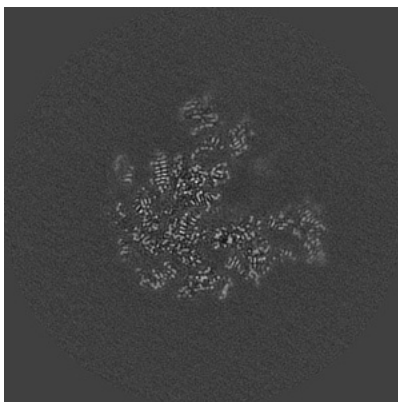
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

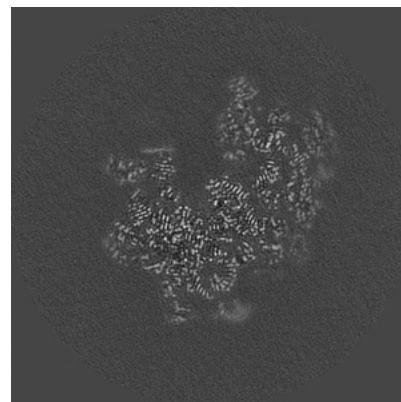
6.2.1 Primary map



X Index: 360

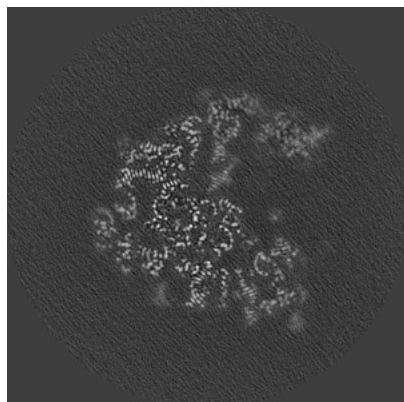


Y Index: 360

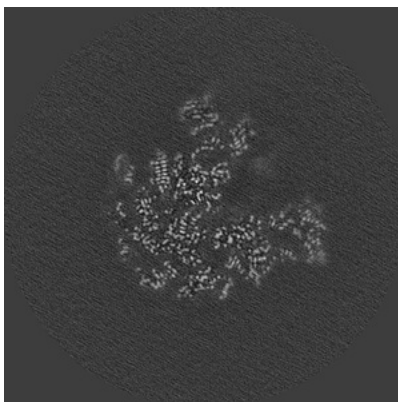


Z Index: 360

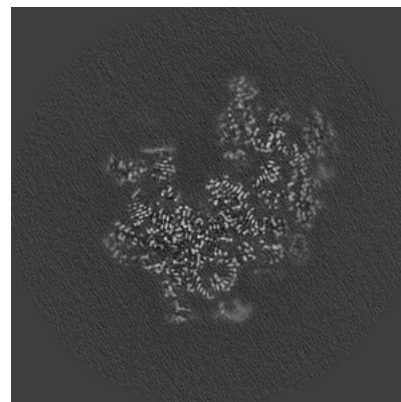
6.2.2 Raw map



X Index: 180



Y Index: 180

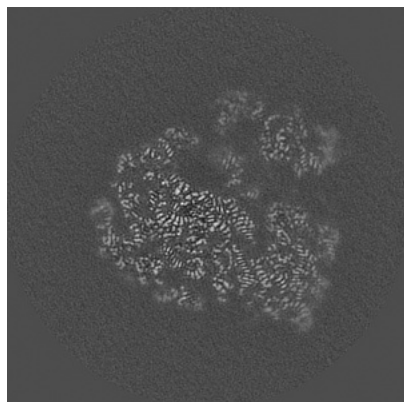


Z Index: 180

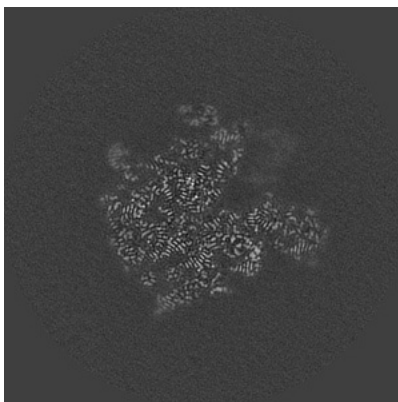
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

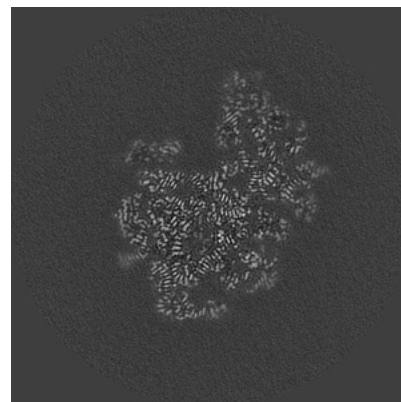
6.3.1 Primary map



X Index: 381

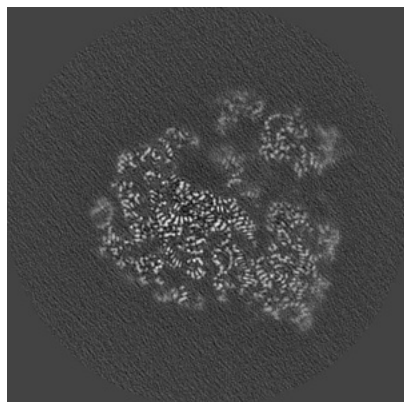


Y Index: 342

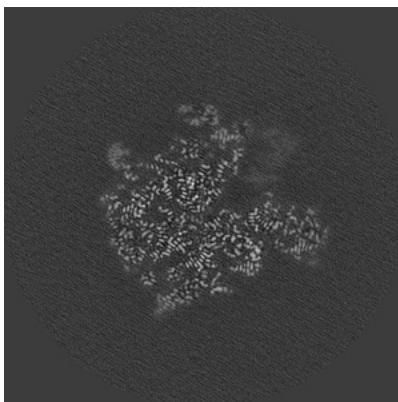


Z Index: 329

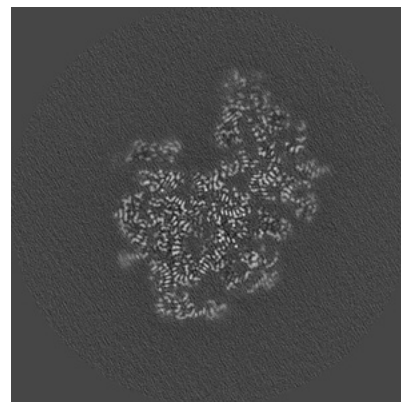
6.3.2 Raw map



X Index: 191



Y Index: 171

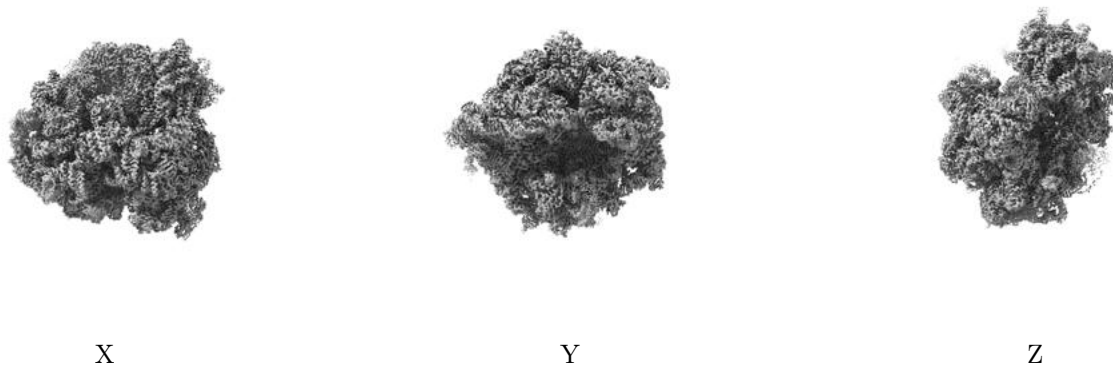


Z Index: 165

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

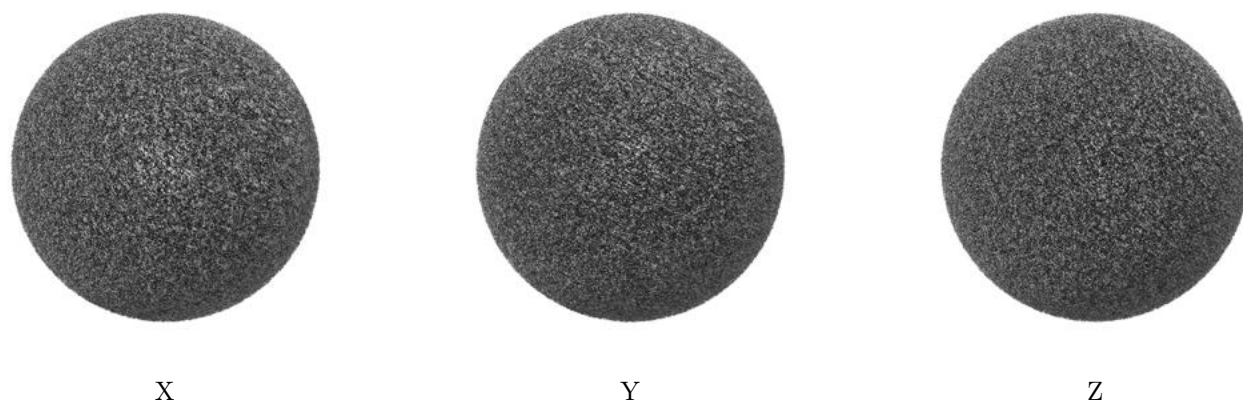
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

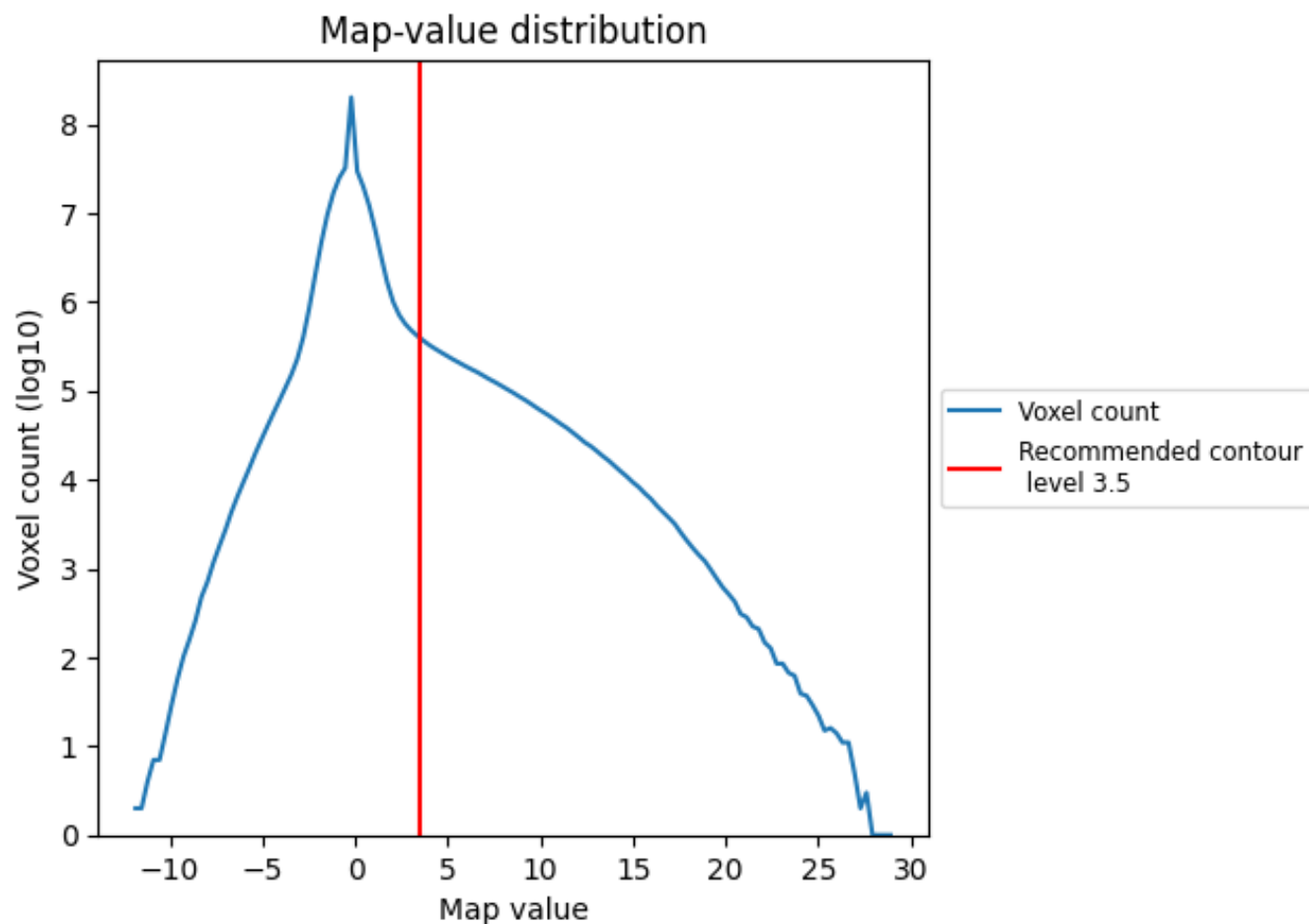
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

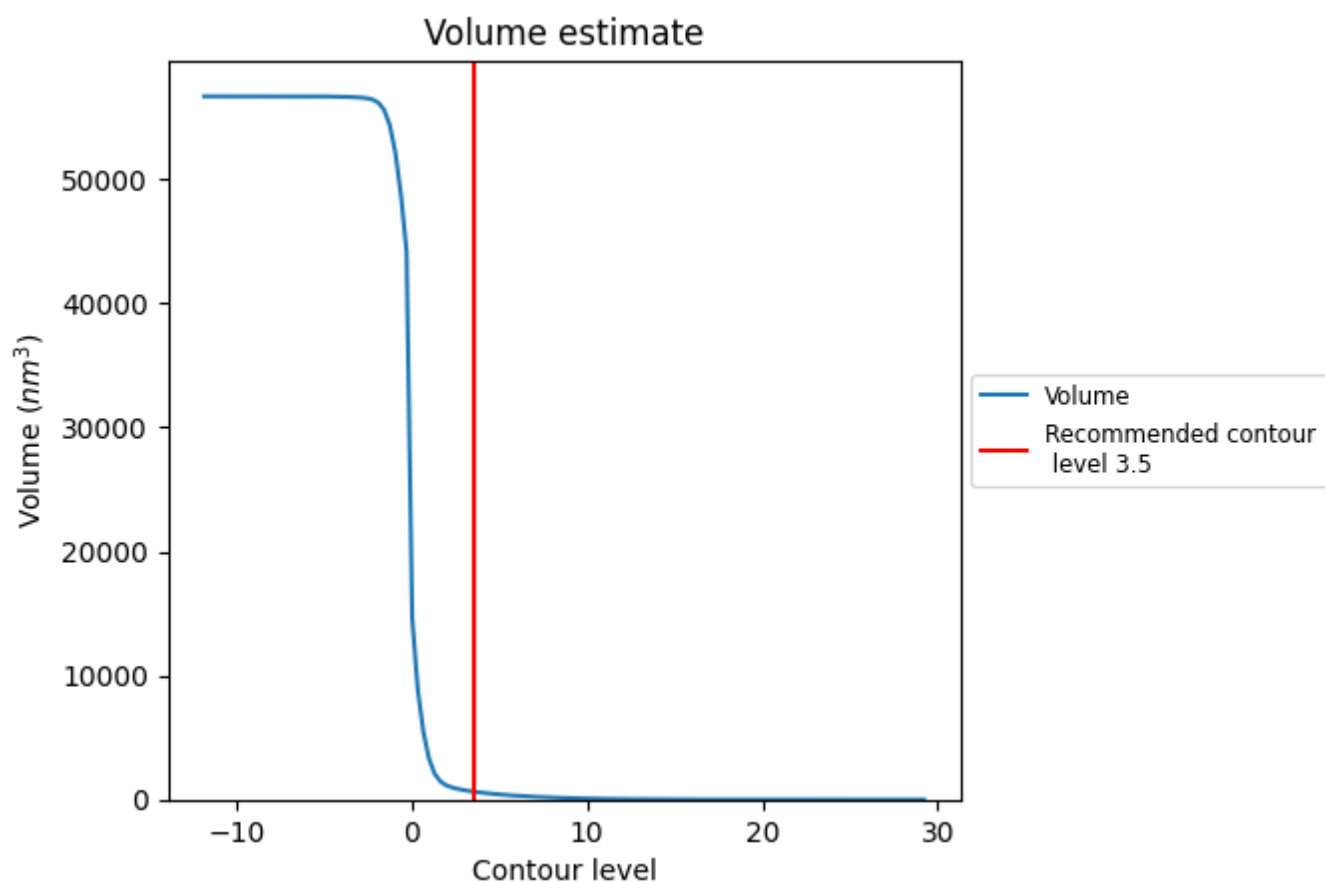
This section contains the results of statistical analysis of the map.

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.

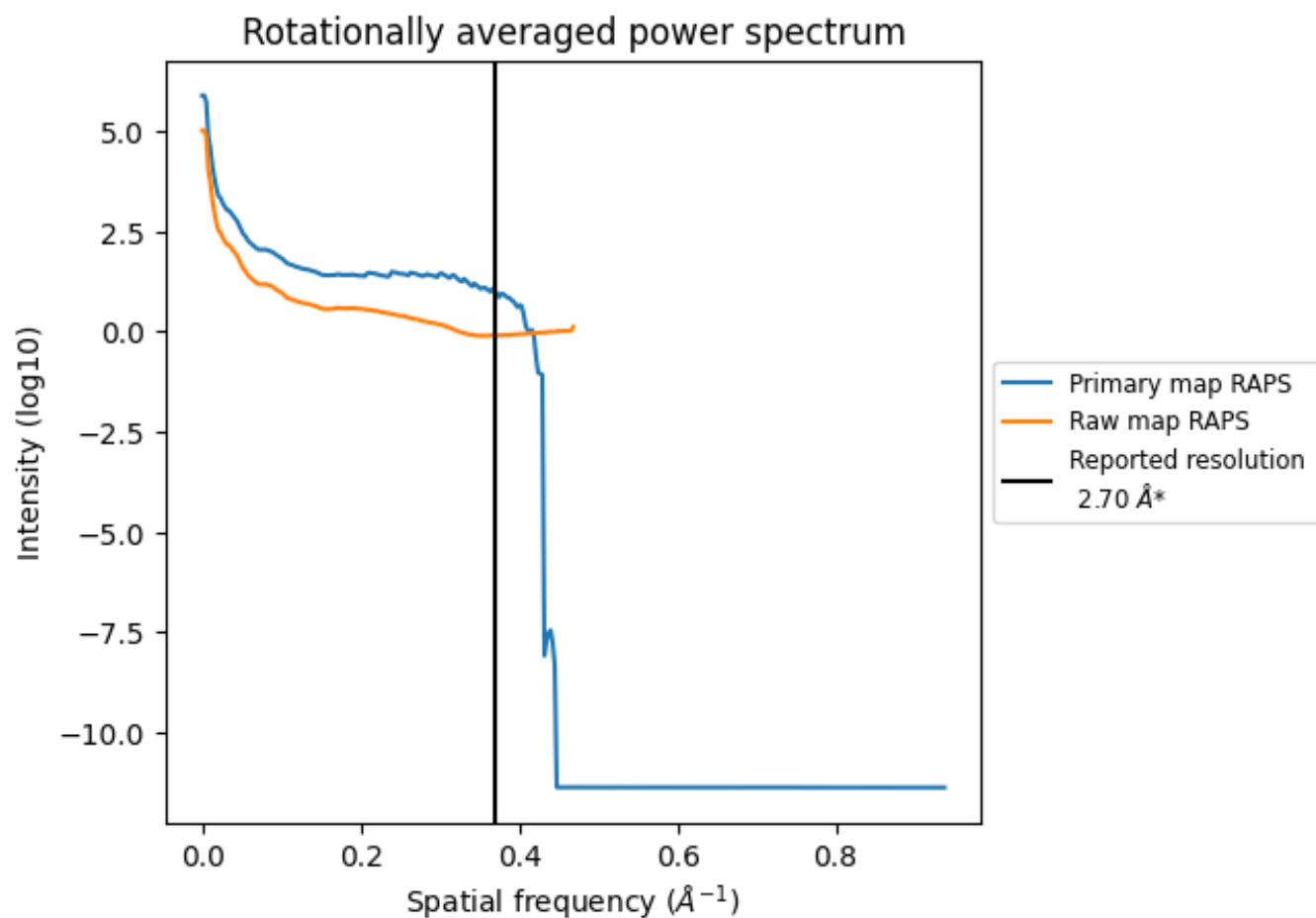
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 641 nm³; this corresponds to an approximate mass of 579 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 ⓘ

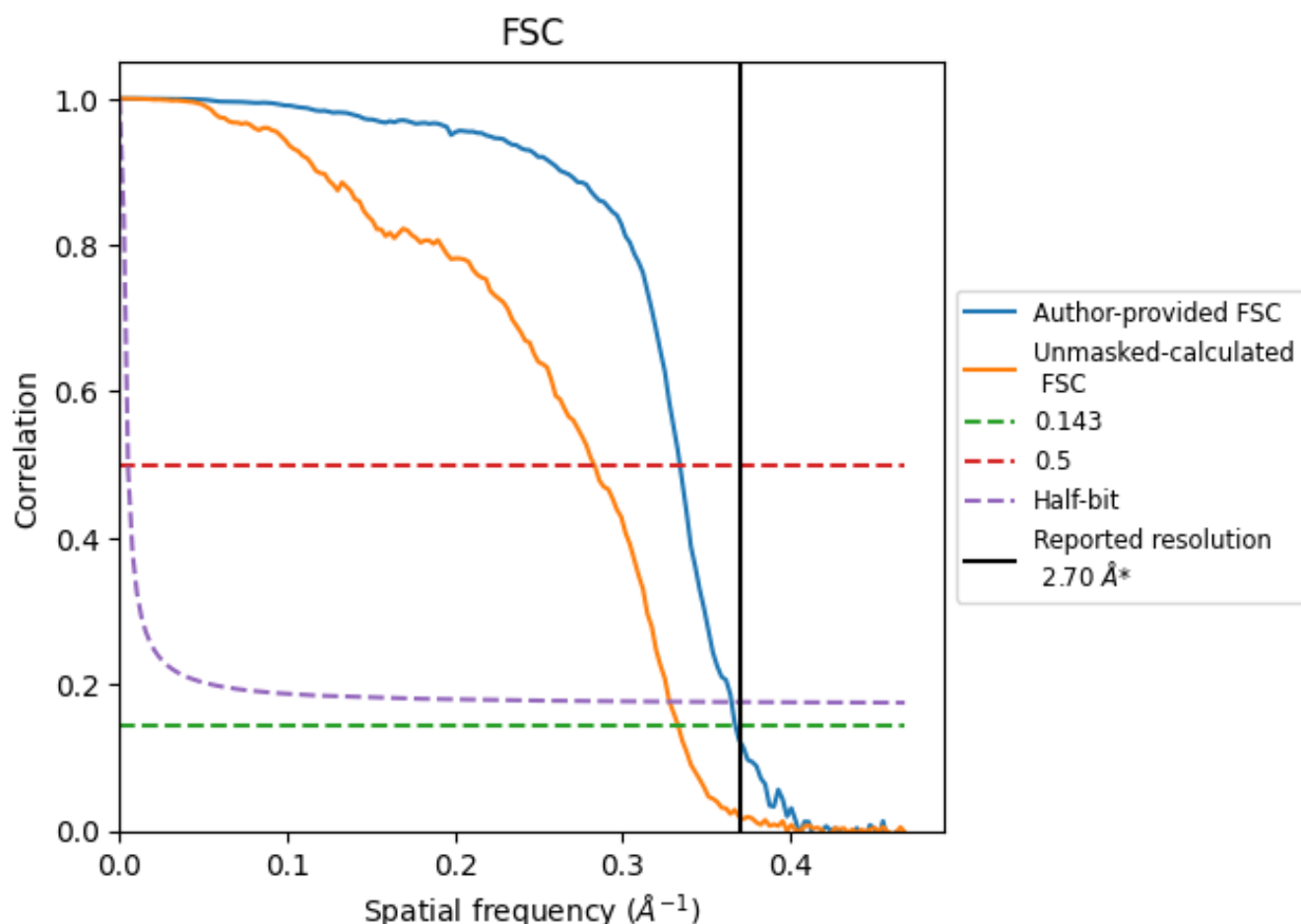


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

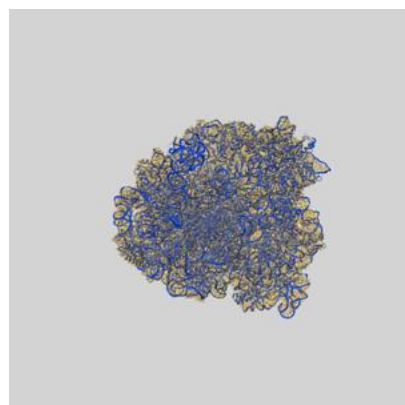
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	2.99	2.74
Unmasked-calculated*	3.00	3.53	3.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.7 by more than 10 %

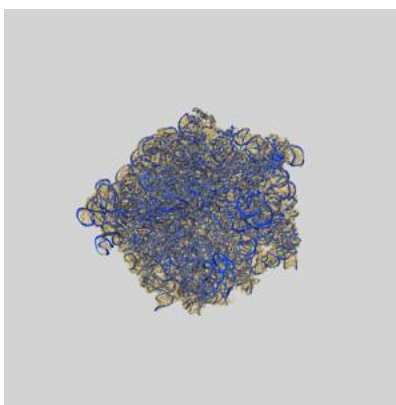
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10453 and PDB model 6TBV. Per-residue inclusion information can be found in section 3 on page 17.

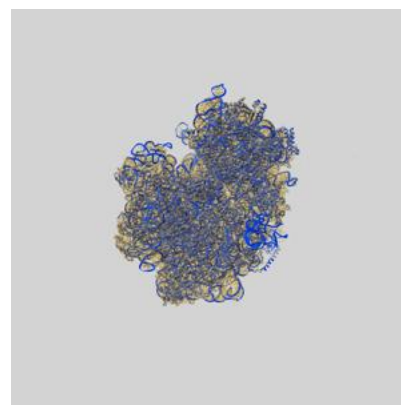
9.1 Map-model overlay [i](#)



X



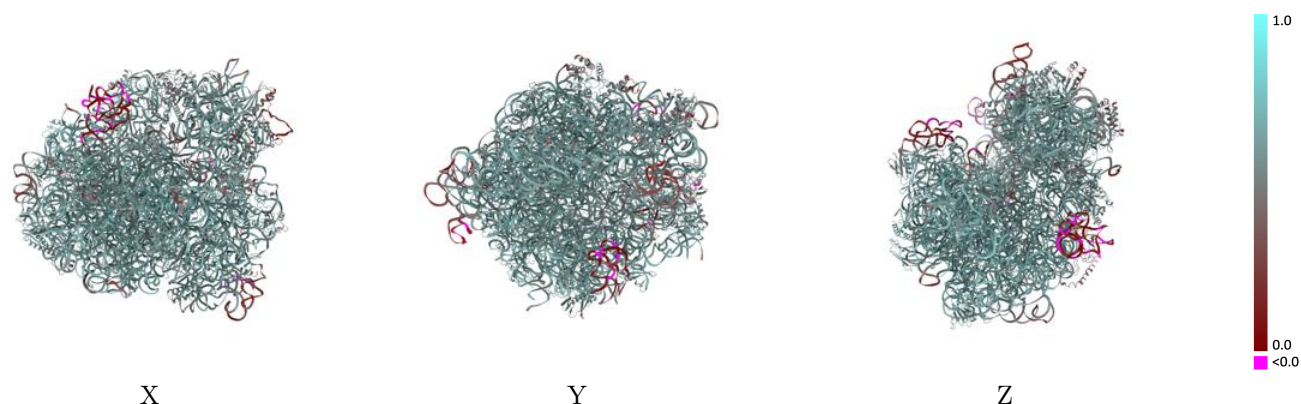
Y



Z

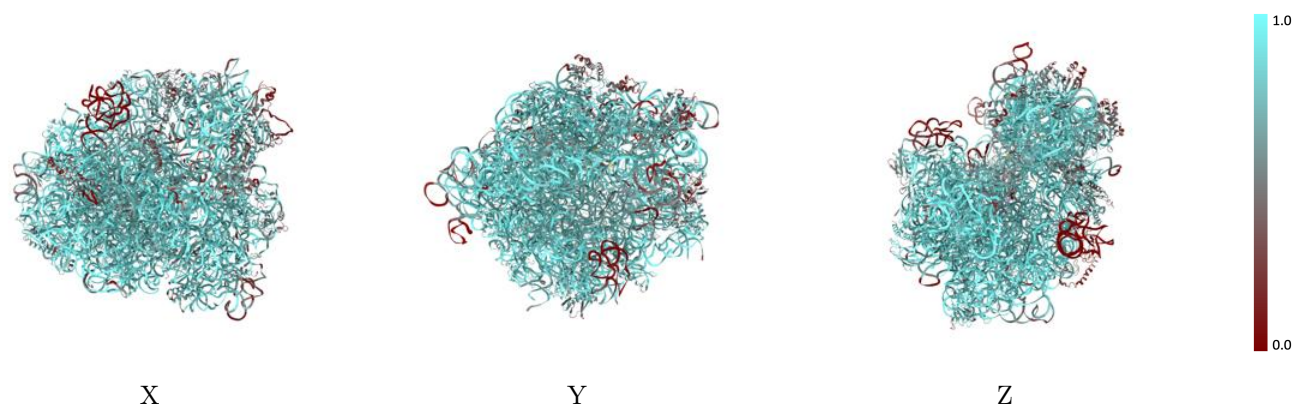
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



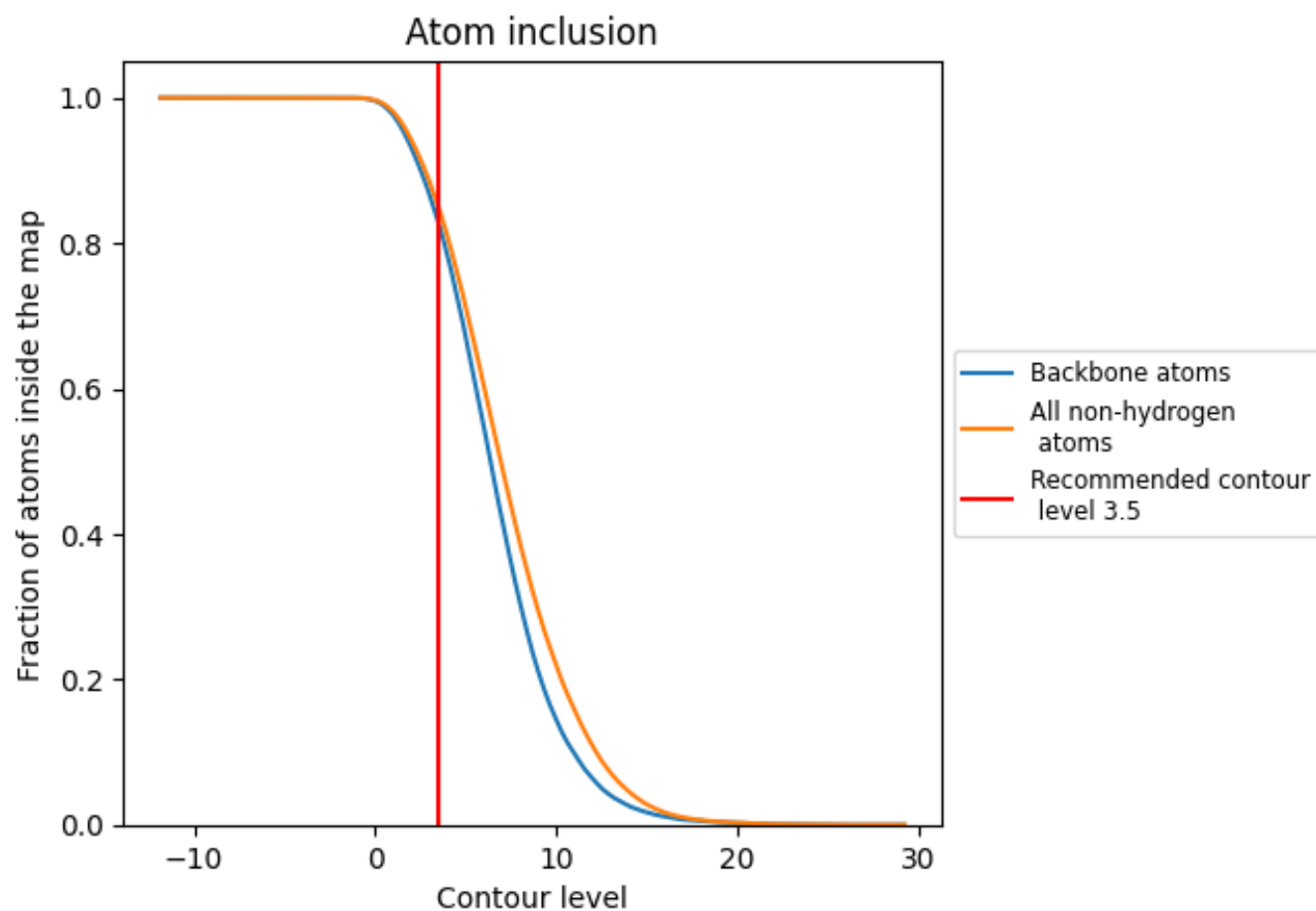
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 85% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8493	 0.6140
05S1	 0.9221	 0.6320
16S1	 0.8905	 0.6140
23S1	 0.9015	 0.6260
L021	 0.9155	 0.6720
L031	 0.8945	 0.6600
L041	 0.8131	 0.6300
L051	 0.6730	 0.5650
L061	 0.6715	 0.5680
L091	 0.2064	 0.4070
L131	 0.9050	 0.6570
L141	 0.8631	 0.6550
L151	 0.8765	 0.6480
L161	 0.8711	 0.6520
L171	 0.9474	 0.6710
L181	 0.8119	 0.6150
L191	 0.8554	 0.6480
L201	 0.9290	 0.6730
L211	 0.8358	 0.6420
L221	 0.8768	 0.6510
L231	 0.8066	 0.6170
L241	 0.7646	 0.5990
L251	 0.7957	 0.6140
L271	 0.8973	 0.6600
L281	 0.8754	 0.6470
L291	 0.7587	 0.6030
L301	 0.8581	 0.6290
L311	 0.3789	 0.4260
L321	 0.8651	 0.6430
L331	 0.7764	 0.6160
L341	 0.9254	 0.6700
L351	 0.9313	 0.6740
L361	 0.8874	 0.6470
MRN1	 0.7551	 0.5570
PTR1	 0.7376	 0.5520



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Chain	Atom inclusion	Q-score
S021	 0.5006	 0.5180
S031	 0.7239	 0.5910
S041	 0.6428	 0.5760
S051	 0.8280	 0.6170
S061	 0.6552	 0.5570
S071	 0.5210	 0.5130
S081	 0.8104	 0.6240
S091	 0.6793	 0.5560
S101	 0.5169	 0.5080
S111	 0.7298	 0.5890
S121	 0.7833	 0.6060
S131	 0.6714	 0.5320
S141	 0.6667	 0.5170
S151	 0.7754	 0.6000
S161	 0.7464	 0.5850
S171	 0.7030	 0.5720
S181	 0.8142	 0.6030
S191	 0.6500	 0.5530
S201	 0.7542	 0.5840
S211	 0.3851	 0.5110
SPE1	 0.7703	 0.6640