wwPDB EM Validation Summary Report

Sep 16, 2026 – 11:17 PM EDT

PDB ID	:	7S1J / pdb_00007s1j
EMDB ID	:	EMD-24803
Title	:	Wild-type Escherichia coli ribosome with antibiotic radezolid
Authors	:	Young, I.D.; Stojkovic, V.; Tsai, K.; Lee, D.J.; Fraser, J.S.; Galonic Fujimori, D.
Deposited on	:	2021-09-02
Resolution	:	2.47 Å(reported)

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

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

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

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

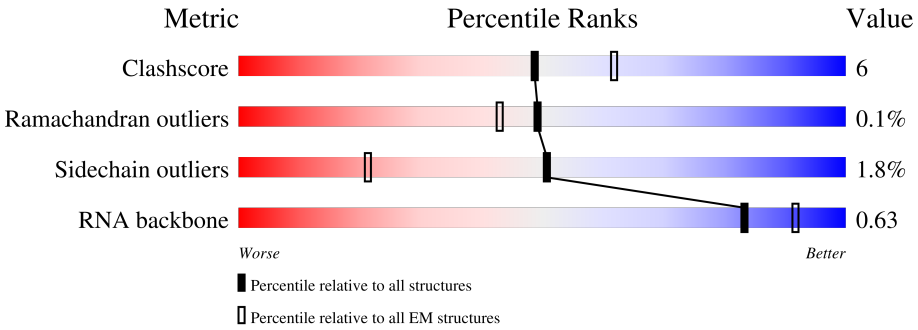
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

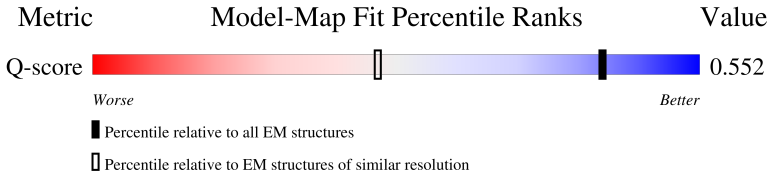
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.47 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6086 (1.98 - 2.97)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	92	9% 59% 26% 14%
2	2	87	75% 22%
3	3	71	24% 73% 25%

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Mol	Chain	Length	Quality of chain
4	C	1540	77% 20%
5	D	241	6% 64% 25% 10%
6	E	233	69% 20% 12%
7	F	206	75% 23%
8	G	167	71% 17% 10%
9	H	135	56% 19% 26%
10	I	2904	78% 18%
11	J	120	79% 18%
12	K	273	78% 21%
13	L	209	84% 16%
14	M	201	79% 20%
15	N	179	59% 39%
16	O	177	88% 12%
17	P	149	5% 80% 20%
18	Q	70	61% 23% 14%
19	R	142	85% 15%
20	S	123	82% 17%
21	T	144	79% 19%
22	U	136	81% 18%
23	V	127	81% 13% 6%
24	W	117	70% 28%
25	X	115	77% 22%
26	Y	118	90% 9%
27	Z	103	84% 15%
28	a	110	84% 15%

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Mol	Chain	Length	Quality of chain
29	b	100	
30	c	104	
31	d	94	
32	e	85	
33	f	78	
34	g	63	
35	h	59	
36	i	57	
37	j	55	
38	k	46	
39	l	65	
40	m	38	
41	n	179	
42	o	130	
43	p	130	
44	q	103	
45	r	129	
46	t	124	
47	u	118	
48	v	101	
49	w	89	
50	x	82	
51	y	84	
52	z	75	

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 238134 atoms, of which 95754 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S19.

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

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

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

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

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

- Molecule 4 is a RNA chain called 16S rRNA.

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

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	D	218	3437	1081	1733	305	311	7	0	0

- Molecule 6 is a protein called 30S ribosomal protein S3.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	205	Total	C	H	N	O	S	0	0
			3351	1026	1708	315	298	4		

- Molecule 8 is a protein called 30S ribosomal protein S5.

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

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	2898	Total	C	H	N	O	P	2	0
			93612	27787	31341	11455	20129	2900		

- Molecule 11 is a RNA chain called 5S rRNA.

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

- Molecule 12 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	K	271	Total	C	H	N	O	S	2	0
			4237	1288	2155	423	364	7		

- Molecule 13 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	209	Total	C	H	N	O	S	0	0
			3183	979	1618	288	294	4		

- Molecule 14 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	M	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 15 is a protein called 50S ribosomal protein L5.

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

- Molecule 16 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	O	176	Total	C	H	N	O	S	0	0
			2695	832	1372	243	246	2		

- Molecule 17 is a protein called 50S ribosomal protein L9.

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

- Molecule 18 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Q	60	Total	C	H	N	O	S	0	0
			963	299	483	90	85	6		

- Molecule 19 is a protein called 50S ribosomal protein L13.

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

- Molecule 20 is a protein called 50S ribosomal protein L14.

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

- Molecule 21 is a protein called 50S ribosomal protein L15.

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

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	U	136	Total	C	H	N	O	S	0	0
			2230	686	1155	205	178	6		

- Molecule 23 is a protein called 50S ribosomal protein L17.

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

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	116	Total	C	H	N	O	0	0
			1816	552	924	178	162		

- Molecule 25 is a protein called 50S ribosomal protein L19.

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

- Molecule 26 is a protein called 50S ribosomal protein L20.

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

- Molecule 27 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Z	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 28 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	a	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	b	93	Total	C	H	N	O	S	0	0
			1545	466	807	139	131	2		

- Molecule 30 is a protein called 50S ribosomal protein L24.

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

- Molecule 31 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	d	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 32 is a protein called 50S ribosomal protein L27.

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

- Molecule 33 is a protein called 50S ribosomal protein L28.

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

- Molecule 34 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	g	62	Total	C	H	N	O	S	0	0
			1034	308	533	98	94	1		

- Molecule 35 is a protein called 50S ribosomal protein L30.

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

- Molecule 36 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

- Molecule 37 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	50	Total	C	H	N	O	0	0
			850	263	441	75	71		

- Molecule 38 is a protein called 50S ribosomal protein L34.

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

- Molecule 39 is a protein called 50S ribosomal protein L35.

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

- Molecule 40 is a protein called 50S ribosomal protein L36.

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

- Molecule 41 is a protein called 30S ribosomal protein S7.

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

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

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

- Molecule 45 is a protein called 30S ribosomal protein S11.

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

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	u	115	Total	C	H	N	O	S	0	0
			1844	552	953	179	157	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

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

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	w	88	Total	C	H	N	O	S	0	0
			1439	437	729	143	129	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

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

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	y	80	Total	C	H	N	O	S	0	0
			1340	411	692	121	113	3		

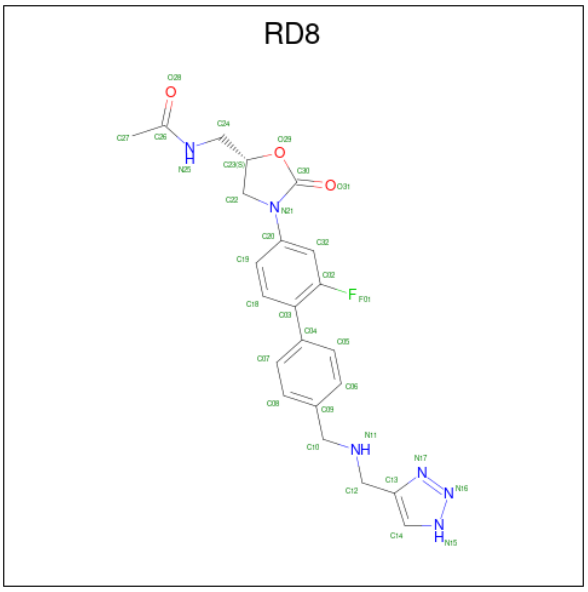
- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	55	Total	C	H	N	O	0	0
			934	288	479	86	81		

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	C	84	Total	Mg	0
			84	84	
53	I	111	Total	Mg	0
			111	111	
53	K	1	Total	Mg	0
			1	1	
53	L	1	Total	Mg	0
			1	1	
53	T	1	Total	Mg	0
			1	1	
53	v	1	Total	Mg	0
			1	1	

- Molecule 54 is Radezolid (CCD ID: RD8) (formula: $C_{22}H_{23}FN_6O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

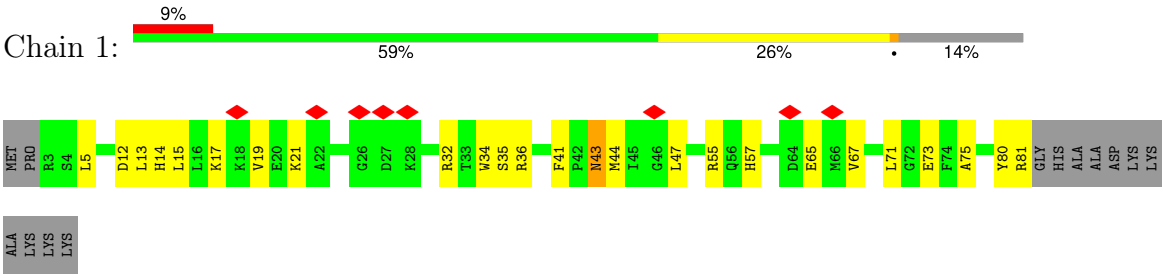
- Molecule 56 is water.

Mol	Chain	Residues	Atoms			AltConf
56	C	3	Total	H	O	0
			9	6	3	
56	I	31	Total	H	O	0
			93	62	31	
56	c	1	Total	H	O	0
			3	2	1	

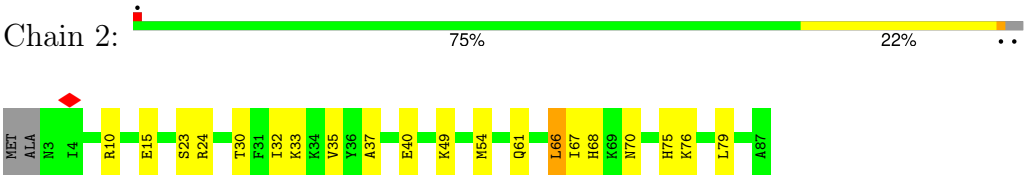
3 Residue-property plots (i)

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

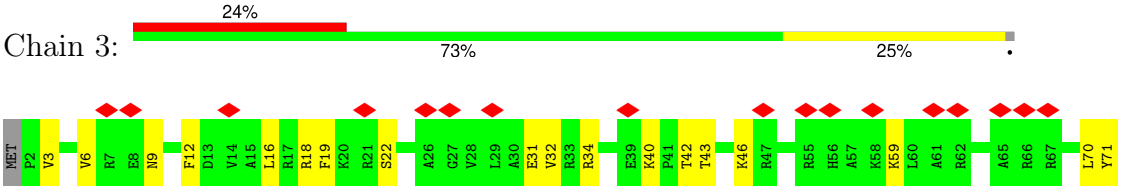
• Molecule 1: 30S ribosomal protein S19



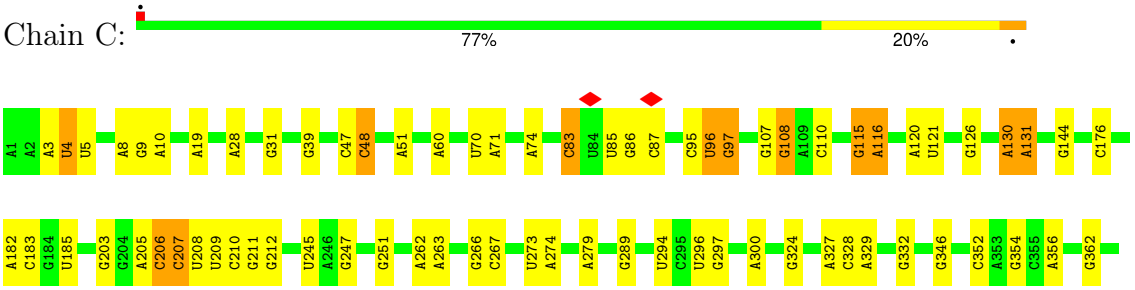
• Molecule 2: 30S ribosomal protein S20

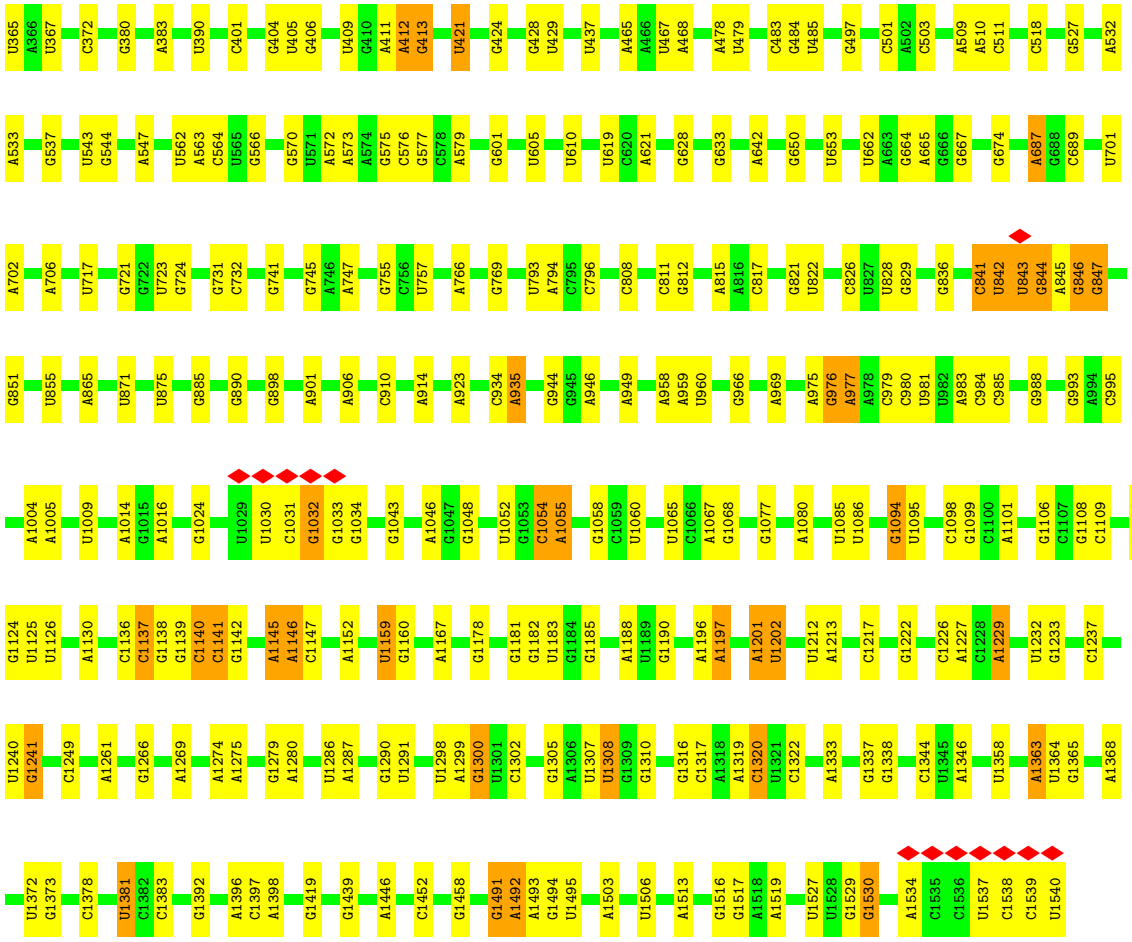


• Molecule 3: 30S ribosomal protein S21



• Molecule 4: 16S rRNA

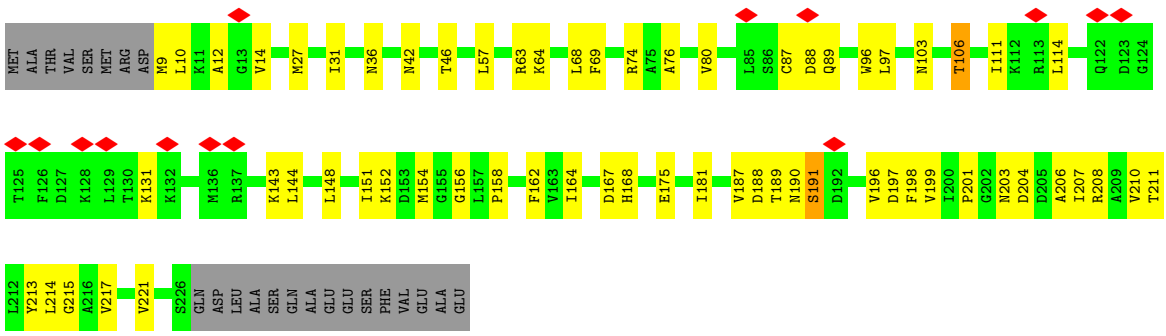




• Molecule 5: 30S ribosomal protein S2

Chain D:

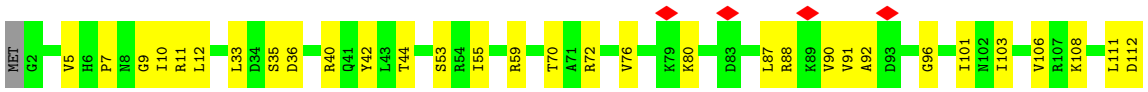


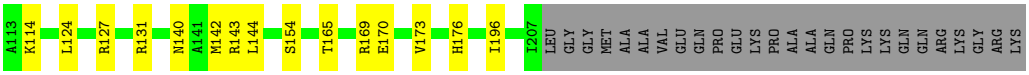


• Molecule 6: 30S ribosomal protein S3

Chain E:





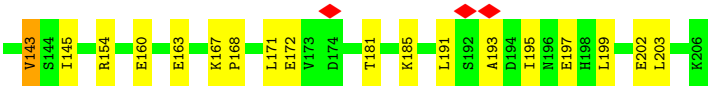


• Molecule 7: 30S ribosomal protein S4

Chain F:



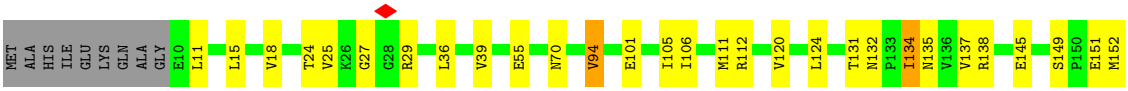




• Molecule 8: 30S ribosomal protein S5

Chain G:





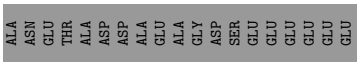


• Molecule 9: 30S ribosomal protein S6

Chain H:



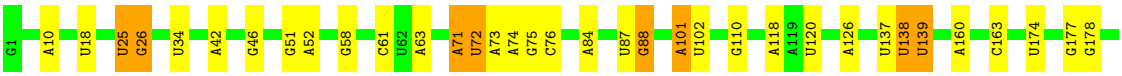


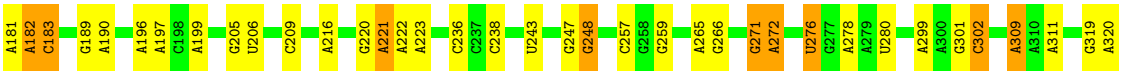


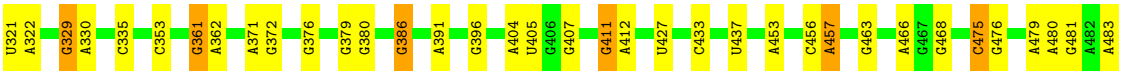
• Molecule 10: 23S rRNA

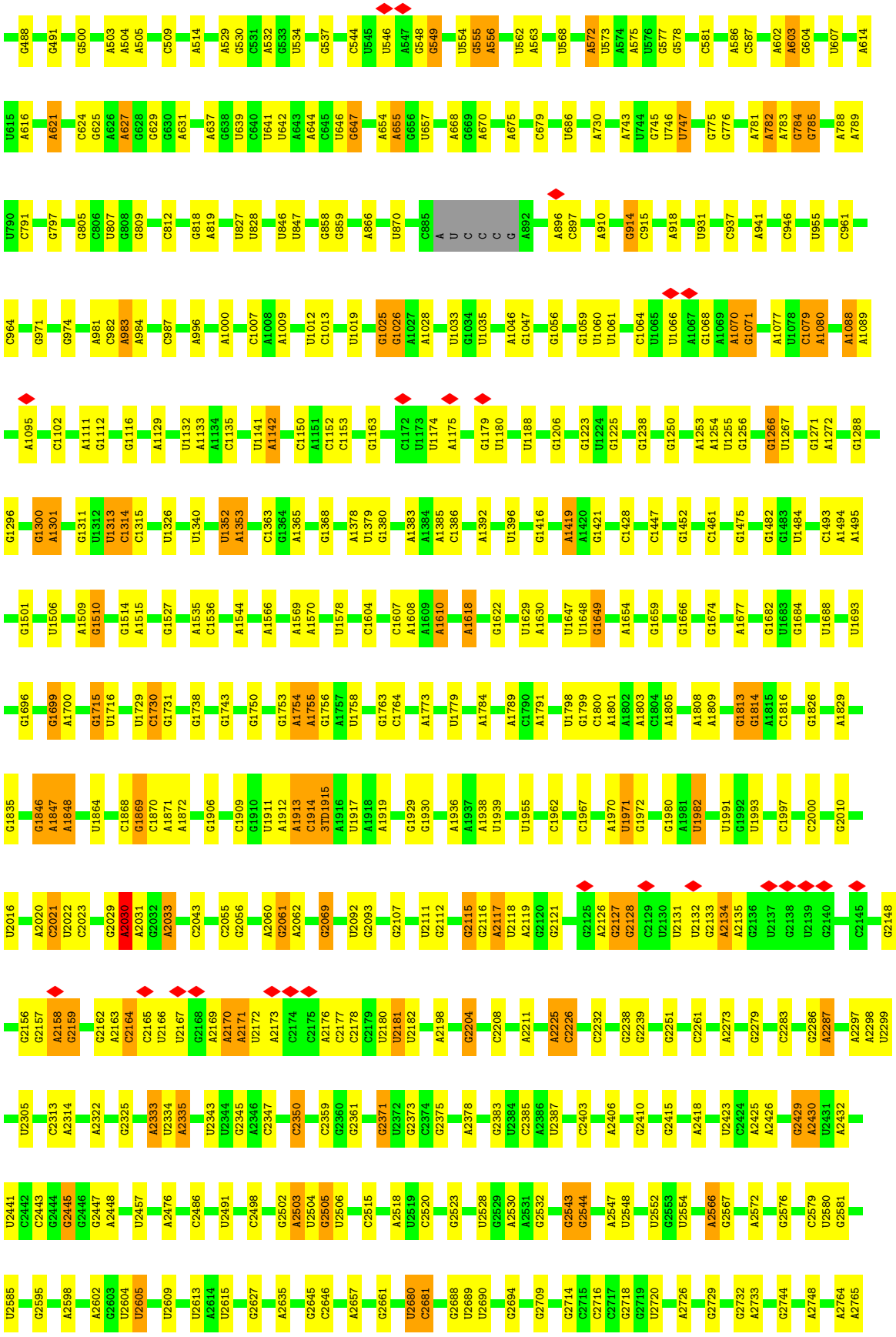
Chain I:







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U615 A616 A621 C624 G625 A626 A627 G628 G629 G630 A631 A637 G638 U639 C640 U641 U642 A643 A644 C645 U646 G647 A654 A655 G656 U657 A668 G669 A670 A675 C679 U686 A730 A743 U744 G745 U746 U747 G775 G776 A781 A782 A783 G784 G785 A788 A789
U790 C791 G797 G805 C806 U807 G808 G809 C812 G818 A819 U827 U828 U846 U847 G858 G859 A866 U870 C885 A U C C C G A892 A896 C897 A910 G914 C915 A918 U931 C937 A941 C946 U955 C961
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A1095 C1102 A1111 G1112 G1116 A1129 U1132 A1133 A1134 C1135 U1141 A1142 C1150 A1151 C1152 C1153 G1163 C1172 U1173 U1174 A1175 G1179 U1180 U1188 G1206 G1223 U1224 G1225 G1238 G1250 A1253 A1254 U1255 G1256 G1266 U1267 G1271 A1272 G1288
G1296 G1300 A1301 G1311 U1312 U1313 C1314 C1315 U1326 U1340 U1352 A1353 C1363 G1364 A1365 G1368 A1378 U1379 G1380 A1383 A1384 A1385 C1386 A1392 U1396 G1416 A1419 A1420 G1421 C1428 C1447 G1452 C1461 G1475 G1482 G1483 U1484 C1493 A1494 A1495
G1501 U1506 A1509 G1510 G1514 A1515 G1527 A1535 C1536 A1544 A1566 A1569 A1570 U1578 C1604 C1607 A1608 A1609 A1610 A1618 G1622 U1629 A1630 U1647 U1648 G1649 A1654 G1659 G1666 G1674 A1677 G1682 U1683 G1684 U1688 U1693
G1696 G1699 A1700 G1715 U1716 U1729 C1730 G1731 G1738 G1743 G1750 G1753 A1754 A1755 G1756 A1757 U1758 G1763 C1764 A1773 U1779 A1784 A1789 C1790 A1791 U1798 G1799 C1800 A1801 A1802 A1803 C1804 A1805 A1808 A1809 G1813 G1814 A1815 C1816 G1826 A1829
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U2016 A2020 C2021 U2022 C2023 G2029 A2030 A2031 G2032 A2033 C2043 C2055 G2056 A2060 G2061 A2062 G2069 U2092 G2093 G2107 U2111 G2112 G2115 G2116 A2117 U2118 A2119 G2120 G2121 C2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 C2145 G2148
G2156 G2157 A2158 G2159 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2198 G2204 C2208 A2211 A2225 C2226 C2232 G2238 G2239 G2251 C2261 A2273 G2279 C2283 G2286 A2287 A2297 A2298 U2299
U2305 C2313 A2314 A2322 G2325 A2333 U2334 A2335 U2343 U2344 G2345 A2346 C2347 C2350 C2359 G2360 G2361 G2371 U2372 G2373 C2374 G2375 A2378 G2383 U2384 C2385 A2386 U2387 C2403 A2406 G2410 G2415 A2418 U2423 C2424 A2425 A2426 G2429 A2430 U2431 A2432
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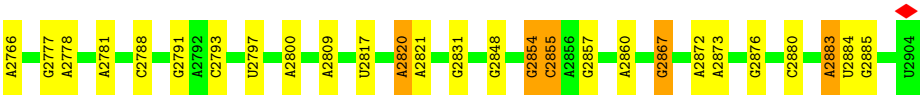
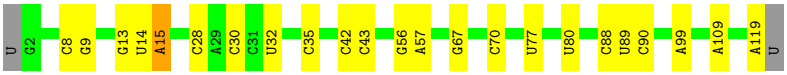


• Molecule 11: 5S rRNA

Chain J:

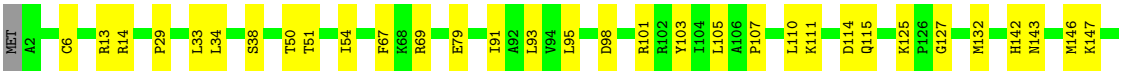




• Molecule 12: 50S ribosomal protein L2

Chain K:



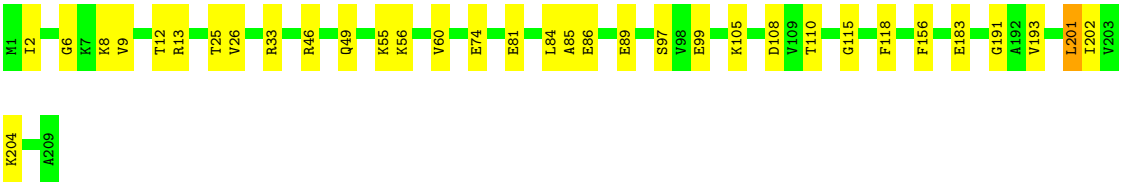




• Molecule 13: 50S ribosomal protein L3

Chain L:

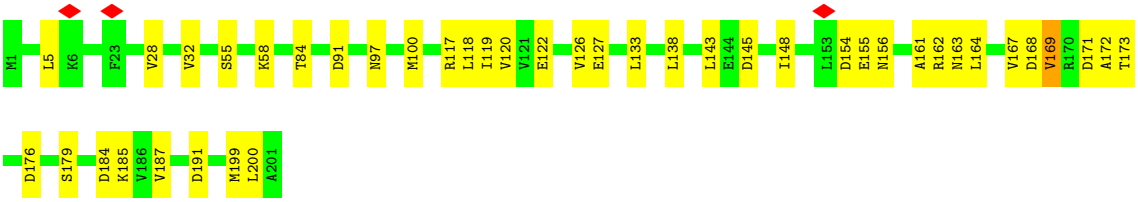




• Molecule 14: 50S ribosomal protein L4

Chain M:

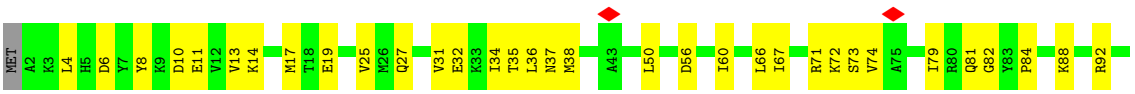


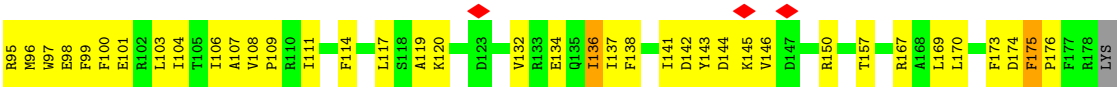


• Molecule 15: 50S ribosomal protein L5

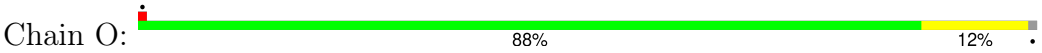
Chain N:

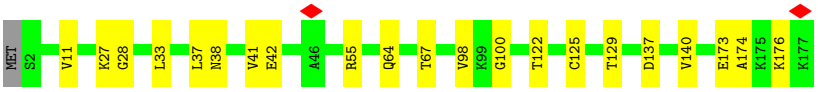




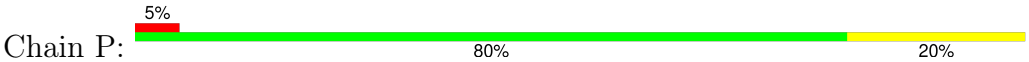


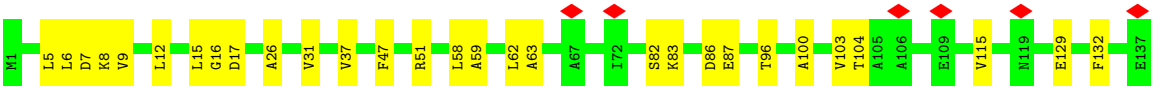
• Molecule 16: 50S ribosomal protein L6





• Molecule 17: 50S ribosomal protein L9

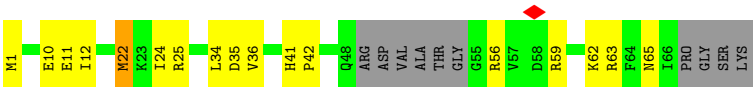




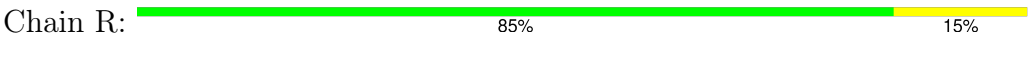


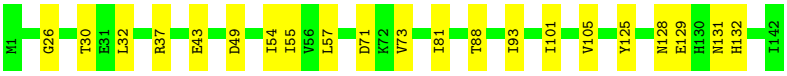
• Molecule 18: 50S ribosomal protein L31



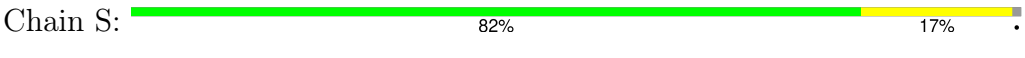


• Molecule 19: 50S ribosomal protein L13



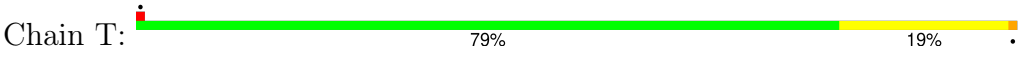


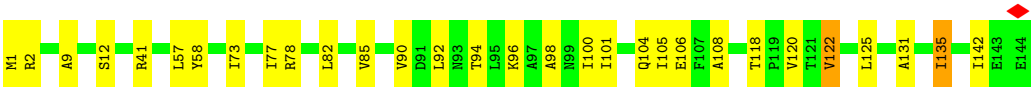
• Molecule 20: 50S ribosomal protein L14





• Molecule 21: 50S ribosomal protein L15

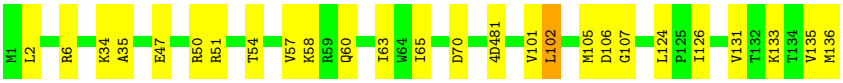




• Molecule 22: 50S ribosomal protein L16

Chain U:

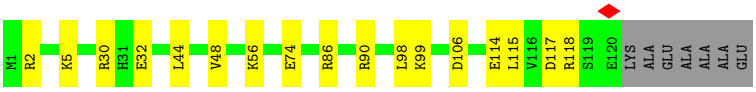




• Molecule 23: 50S ribosomal protein L17

Chain V:

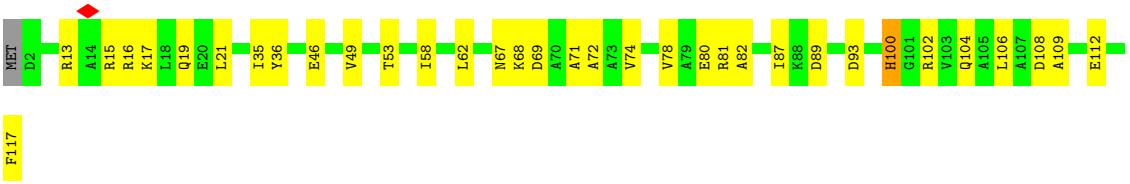




• Molecule 24: 50S ribosomal protein L18

Chain W:





• Molecule 25: 50S ribosomal protein L19

Chain X:





• Molecule 26: 50S ribosomal protein L20

Chain Y:





• Molecule 27: Ribosomal protein L21

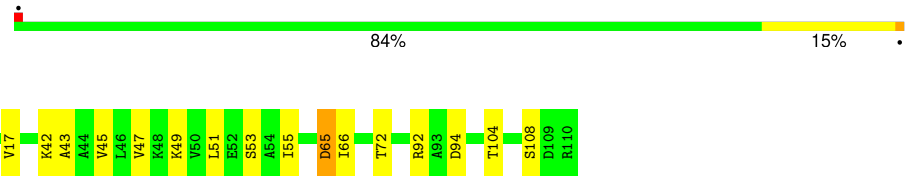
Chain Z:





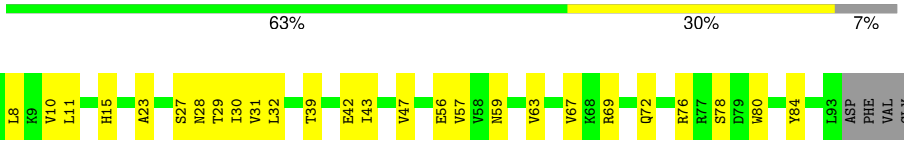
• Molecule 28: 50S ribosomal protein L22

Chain a:



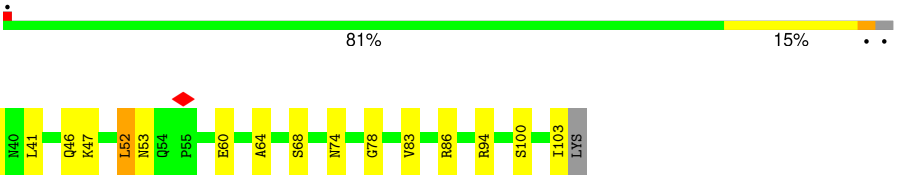
• Molecule 29: 50S ribosomal protein L23

Chain b:



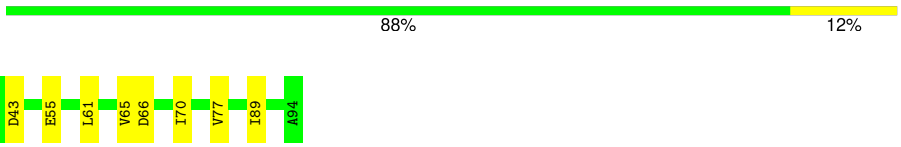
• Molecule 30: 50S ribosomal protein L24

Chain c:



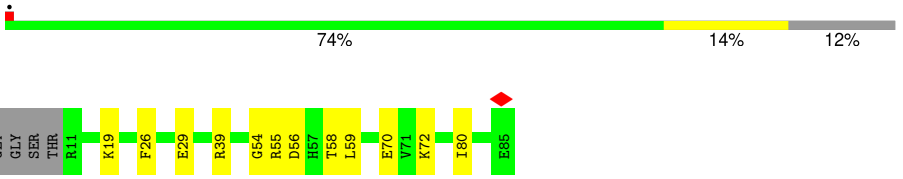
• Molecule 31: 50S ribosomal protein L25

Chain d:



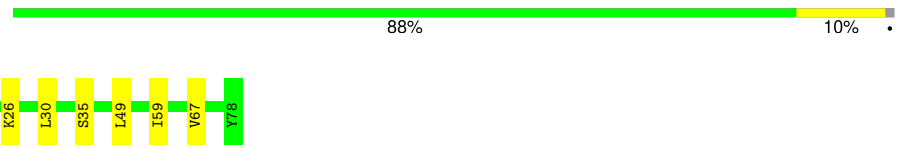
• Molecule 32: 50S ribosomal protein L27

Chain e:



• Molecule 33: 50S ribosomal protein L28

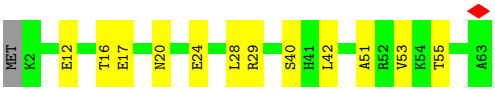
Chain f:



• Molecule 34: 50S ribosomal protein L29

Chain g:

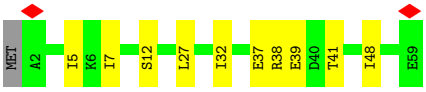




• Molecule 35: 50S ribosomal protein L30

Chain h:

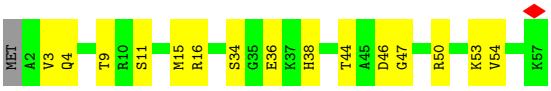




• Molecule 36: 50S ribosomal protein L32

Chain i:

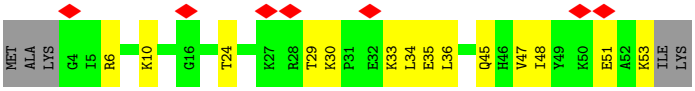




• Molecule 37: 50S ribosomal protein L33

Chain j:

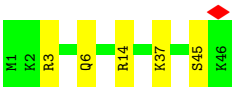




• Molecule 38: 50S ribosomal protein L34

Chain k:





• Molecule 39: 50S ribosomal protein L35

Chain l:

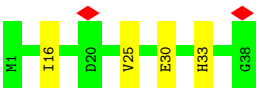




• Molecule 40: 50S ribosomal protein L36

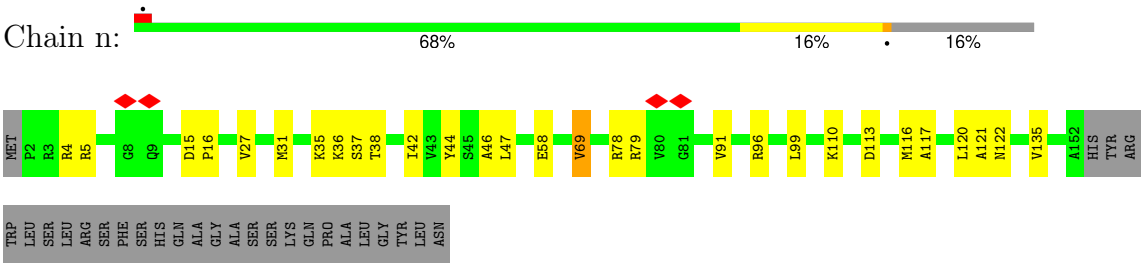
Chain m:





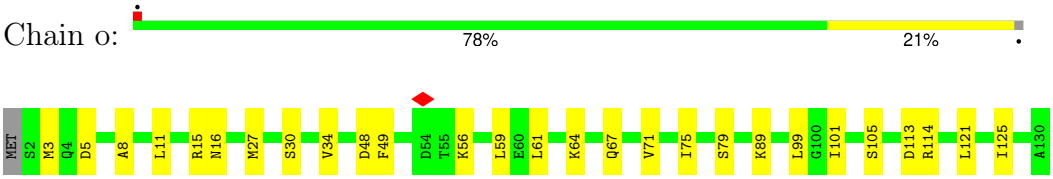
• Molecule 41: 30S ribosomal protein S7

Chain n:



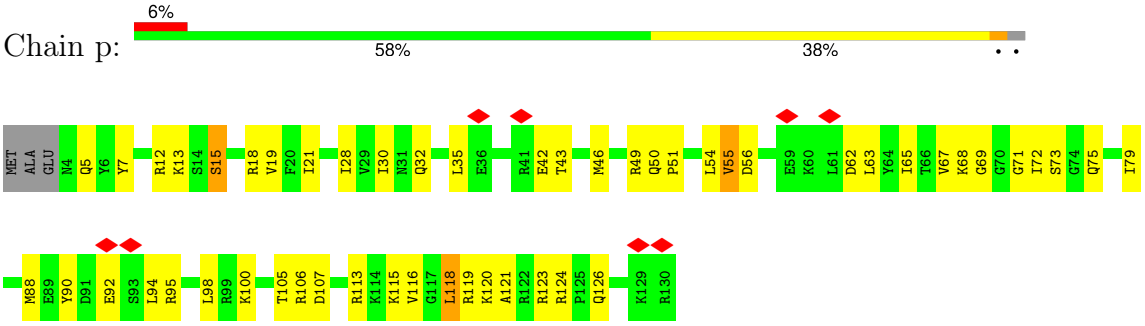
• Molecule 42: 30S ribosomal protein S8

Chain o:



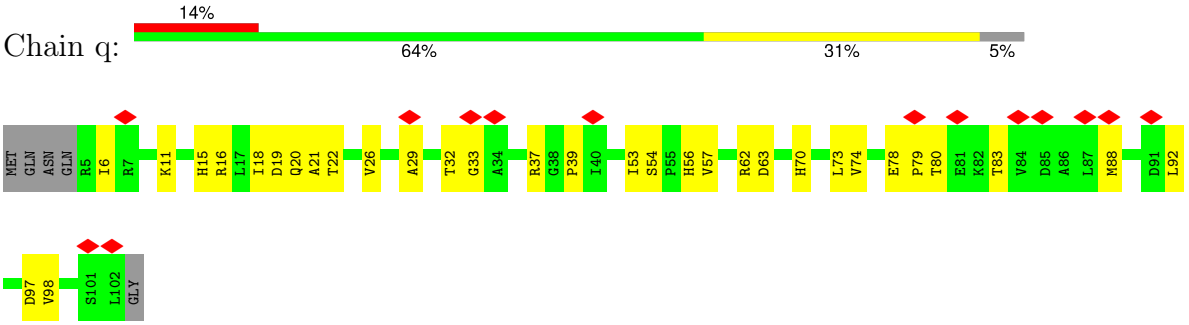
• Molecule 43: 30S ribosomal protein S9

Chain p:



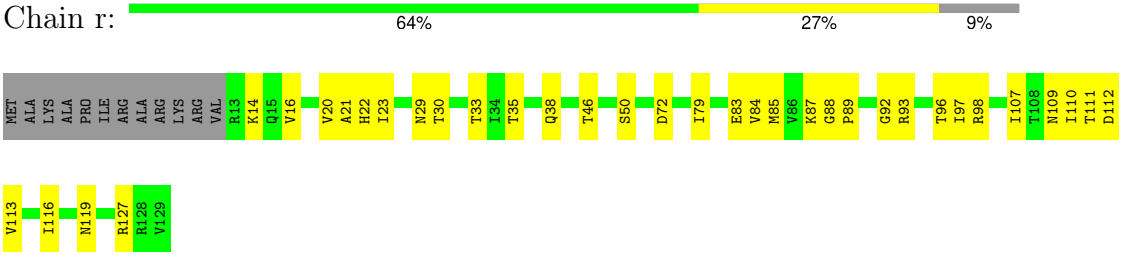
• Molecule 44: 30S ribosomal protein S10

Chain q:



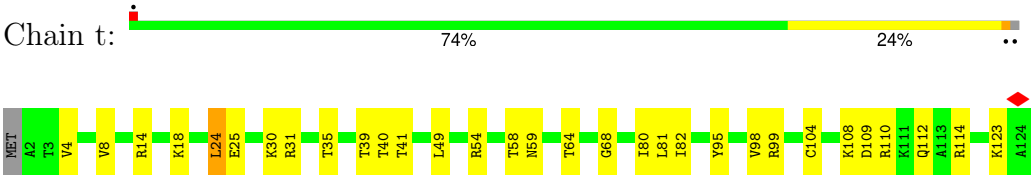
• Molecule 45: 30S ribosomal protein S11

Chain r:



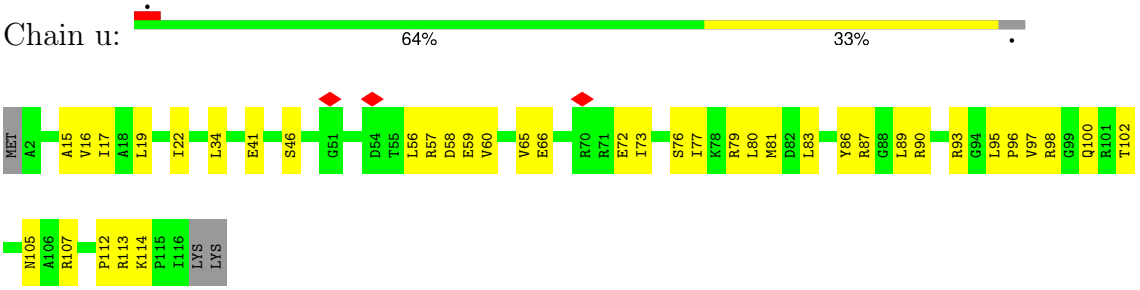
• Molecule 46: 30S ribosomal protein S12

Chain t:



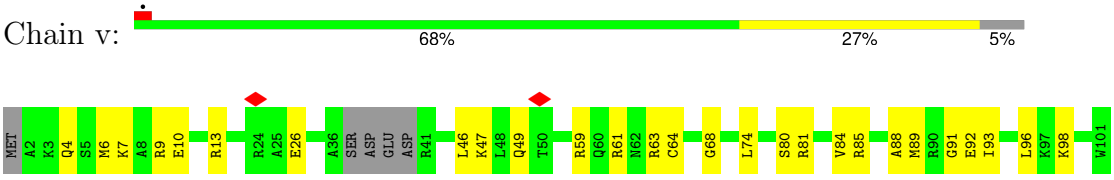
• Molecule 47: 30S ribosomal protein S13

Chain u:



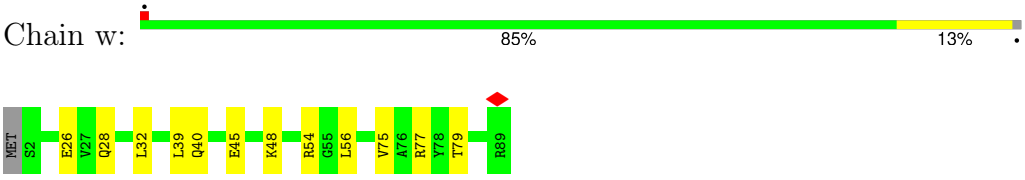
• Molecule 48: 30S ribosomal protein S14

Chain v:



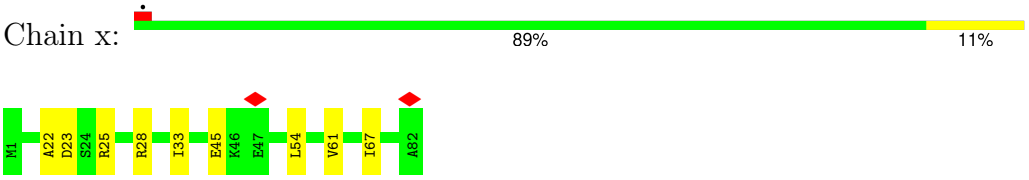
• Molecule 49: 30S ribosomal protein S15

Chain w:



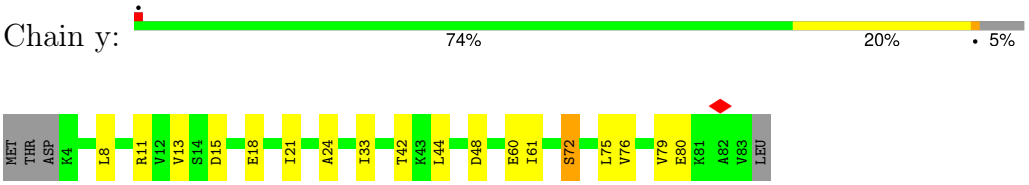
• Molecule 50: 30S ribosomal protein S16

Chain x:



• Molecule 51: 30S ribosomal protein S17

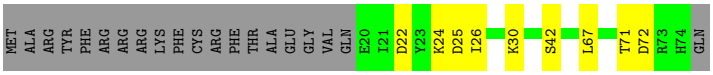
Chain y:



• Molecule 52: 30S ribosomal protein S18

Chain z:




MET
ALA
ARG
TYR
PHE
ARG
ARG
ARG
LYS
PHE
CYS
ARG
PHE
THR
ALA
GLU
GLY
VAL
GLN
E20
I21
D22
Y23
K24
D25
I26
K30
S42
L67
T71
D72
R73
H74
GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146245	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	23.964	Depositor
Minimum map value	-9.815	Depositor
Average map value	-0.022	Depositor
Map value standard deviation	0.807	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	422.4, 422.4, 422.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 2MG, PSU, 4D4, 1MG, 5MC, 5MU, 6MZ, 3TD, MG, OMU, 2MA, ZN, G7M, RD8, H2U, OMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.16	0/652	0.38	0/877
2	2	0.15	0/671	0.35	0/888
3	3	0.10	0/598	0.24	0/792
4	C	0.07	0/36991	0.15	0/57705
5	D	0.12	0/1735	0.31	0/2338
6	E	0.12	0/1651	0.29	0/2225
7	F	0.11	0/1665	0.30	0/2227
8	G	0.11	0/1118	0.28	0/1504
9	H	0.11	0/835	0.33	0/1128
10	I	0.09	0/69168	0.17	0/107901
11	J	0.07	0/2828	0.14	0/4410
12	K	0.11	0/2121	0.27	0/2852
13	L	0.10	0/1586	0.26	0/2134
14	M	0.11	0/1571	0.29	0/2113
15	N	0.12	0/1434	0.30	0/1926
16	O	0.11	0/1343	0.26	0/1816
17	P	0.10	0/1122	0.27	0/1515
18	Q	0.12	0/488	0.31	0/649
19	R	0.09	0/1152	0.24	0/1551
20	S	0.13	0/947	0.34	0/1268
21	T	0.10	0/1062	0.27	0/1413
22	U	0.11	0/1081	0.30	0/1443
23	V	0.08	0/973	0.22	0/1301
24	W	0.14	0/902	0.36	0/1209
25	X	0.12	0/929	0.28	0/1242
26	Y	0.11	0/960	0.21	0/1278
27	Z	0.13	0/829	0.37	0/1107
28	a	0.08	0/864	0.22	0/1156
29	b	0.11	0/744	0.32	0/994
30	c	0.12	0/787	0.28	0/1051
31	d	0.11	0/766	0.29	0/1025

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.11	0/582	0.24	0/769
33	f	0.12	0/635	0.27	0/848
34	g	0.13	0/502	0.31	0/667
35	h	0.12	0/453	0.27	0/605
36	i	0.12	0/450	0.25	0/599
37	j	0.17	0/416	0.31	0/554
38	k	0.09	0/380	0.23	0/498
39	l	0.12	0/513	0.30	0/676
40	m	0.10	0/303	0.23	0/397
41	n	0.11	0/1195	0.29	0/1602
42	o	0.11	0/989	0.26	0/1326
43	p	0.15	0/1034	0.41	0/1375
44	q	0.14	0/796	0.34	0/1077
45	r	0.13	0/893	0.31	0/1205
46	t	0.12	0/969	0.29	0/1300
47	u	0.14	0/900	0.38	0/1204
48	v	0.13	0/785	0.33	0/1043
49	w	0.11	0/718	0.23	0/959
50	x	0.09	0/659	0.25	0/884
51	y	0.15	0/657	0.35	0/881
52	z	0.15	0/462	0.38	0/621
All	All	0.10	0/153864	0.21	0/230128

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
27	Z	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	Z	51	VAL	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	1	637	666	665	23	0
2	2	665	715	714	18	0
3	3	590	629	629	17	0
4	C	33037	16628	16626	187	0
5	D	1704	1733	1732	56	0
6	E	1624	1697	1696	35	0
7	F	1643	1708	1707	42	0
8	G	1105	1149	1148	31	0
9	H	817	808	808	22	0
10	I	62271	31341	31338	276	0
11	J	2529	1280	1281	14	0
12	K	2082	2155	2145	45	0
13	L	1565	1618	1616	28	0
14	M	1552	1619	1619	40	0
15	N	1410	1445	1444	67	0
16	O	1323	1372	1371	11	0
17	P	1111	1148	1148	19	0
18	Q	480	483	478	16	0
19	R	1129	1162	1162	16	0
20	S	938	1012	1012	19	0
21	T	1053	1129	1129	25	0
22	U	1075	1155	1154	19	0
23	V	960	1000	1000	11	0
24	W	892	924	923	35	0
25	X	917	963	962	17	0
26	Y	947	1021	1019	8	0
27	Z	816	839	839	13	0
28	a	857	922	922	11	0
29	b	738	807	807	20	0
30	c	779	832	831	12	0
31	d	753	780	780	7	0
32	e	575	593	592	9	0
33	f	625	653	652	3	0
34	g	501	533	531	10	0
35	h	449	489	488	6	0
36	i	444	459	458	10	0
37	j	409	441	440	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	k	377	418	418	3	0
39	l	504	573	572	9	0
40	m	302	343	340	2	0
41	n	1181	1238	1238	29	0
42	o	979	1032	1031	22	0
43	p	1022	1071	1070	51	0
44	q	786	829	828	30	0
45	r	877	888	887	42	0
46	t	955	1017	1016	19	0
47	u	891	953	952	38	0
48	v	774	826	823	33	0
49	w	710	729	728	10	0
50	x	649	666	666	7	0
51	y	648	692	691	14	0
52	z	455	479	478	7	0
53	C	84	0	0	0	0
53	I	111	0	0	0	0
53	K	1	0	0	0	0
53	L	1	0	0	0	0
53	T	1	0	0	0	0
53	v	1	0	0	0	0
54	I	32	22	0	0	0
55	Q	1	0	0	0	0
55	m	1	0	0	0	0
56	C	3	6	0	0	0
56	I	31	62	0	1	0
56	c	1	2	0	0	0
All	All	142380	95754	95604	1313	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1313 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:51:VAL:HG23	27:Z:52:PRO:HD2	1.28	1.09
4:C:421:U:O2	6:E:127:ARG:NH2	2.00	0.94
32:e:56:ASP:OD1	32:e:58:THR:OG1	1.88	0.92
7:F:13:ARG:NH2	7:F:37:ALA:O	2.03	0.92
4:C:1098:C:OP1	5:D:143:LYS:NZ	2.07	0.87

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
2	2	83/87 (95%)	82 (99%)	1 (1%)	0	100	100
3	3	68/71 (96%)	68 (100%)	0	0	100	100
5	D	216/241 (90%)	208 (96%)	8 (4%)	0	100	100
6	E	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
7	F	203/206 (98%)	195 (96%)	7 (3%)	1 (0%)	24	40
8	G	148/167 (89%)	142 (96%)	6 (4%)	0	100	100
9	H	98/135 (73%)	97 (99%)	1 (1%)	0	100	100
12	K	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
13	L	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
14	M	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
15	N	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
16	O	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
17	P	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
18	Q	56/70 (80%)	56 (100%)	0	0	100	100
19	R	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
20	S	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
21	T	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
22	U	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
23	V	118/127 (93%)	117 (99%)	1 (1%)	0	100	100
24	W	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
25	X	112/115 (97%)	112 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Y	115/118 (98%)	115 (100%)	0	0	100	100
27	Z	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
28	a	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
29	b	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
30	c	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
31	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
32	e	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
33	f	75/78 (96%)	75 (100%)	0	0	100	100
34	g	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
35	h	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
36	i	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
37	j	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
38	k	44/46 (96%)	44 (100%)	0	0	100	100
39	l	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
40	m	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
41	n	149/179 (83%)	146 (98%)	3 (2%)	0	100	100
42	o	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
43	p	125/130 (96%)	116 (93%)	8 (6%)	1 (1%)	16	28
44	q	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	22
45	r	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
46	t	121/124 (98%)	114 (94%)	7 (6%)	0	100	100
47	u	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
48	v	92/101 (91%)	88 (96%)	4 (4%)	0	100	100
49	w	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
50	x	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
51	y	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
52	z	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
All	All	5553/5913 (94%)	5405 (97%)	145 (3%)	3 (0%)	49	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	F	28	ILE

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Mol	Chain	Res	Type
43	p	55	VAL
44	q	57	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	70/79 (89%)	69 (99%)	1 (1%)	59	79
2	2	65/66 (98%)	63 (97%)	2 (3%)	35	60
3	3	60/61 (98%)	59 (98%)	1 (2%)	53	75
5	D	180/199 (90%)	177 (98%)	3 (2%)	53	75
6	E	170/190 (90%)	168 (99%)	2 (1%)	63	81
7	F	172/173 (99%)	169 (98%)	3 (2%)	53	75
8	G	113/126 (90%)	111 (98%)	2 (2%)	51	74
9	H	87/116 (75%)	86 (99%)	1 (1%)	65	83
12	K	216/218 (99%)	213 (99%)	3 (1%)	59	79
13	L	164/164 (100%)	162 (99%)	2 (1%)	63	81
14	M	165/165 (100%)	163 (99%)	2 (1%)	63	81
15	N	148/150 (99%)	143 (97%)	5 (3%)	32	57
16	O	137/138 (99%)	133 (97%)	4 (3%)	37	62
17	P	114/114 (100%)	112 (98%)	2 (2%)	51	74
18	Q	55/62 (89%)	53 (96%)	2 (4%)	31	55
19	R	116/116 (100%)	116 (100%)	0	100	100
20	S	103/104 (99%)	103 (100%)	0	100	100
21	T	103/103 (100%)	99 (96%)	4 (4%)	28	52
22	U	108/108 (100%)	105 (97%)	3 (3%)	38	63
23	V	100/103 (97%)	99 (99%)	1 (1%)	68	84
24	W	86/87 (99%)	85 (99%)	1 (1%)	63	81
25	X	99/100 (99%)	96 (97%)	3 (3%)	36	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	Y	89/90 (99%)	88 (99%)	1 (1%)	65 83
27	Z	84/84 (100%)	83 (99%)	1 (1%)	63 81
28	a	93/93 (100%)	91 (98%)	2 (2%)	45 70
29	b	80/84 (95%)	77 (96%)	3 (4%)	29 53
30	c	83/85 (98%)	81 (98%)	2 (2%)	43 67
31	d	78/78 (100%)	77 (99%)	1 (1%)	61 80
32	e	57/63 (90%)	57 (100%)	0	100 100
33	f	67/68 (98%)	63 (94%)	4 (6%)	17 33
34	g	54/55 (98%)	53 (98%)	1 (2%)	50 73
35	h	48/49 (98%)	47 (98%)	1 (2%)	47 71
36	i	47/48 (98%)	47 (100%)	0	100 100
37	j	45/49 (92%)	45 (100%)	0	100 100
38	k	38/38 (100%)	37 (97%)	1 (3%)	40 65
39	l	51/52 (98%)	50 (98%)	1 (2%)	48 72
40	m	34/34 (100%)	34 (100%)	0	100 100
41	n	124/147 (84%)	123 (99%)	1 (1%)	73 87
42	o	104/105 (99%)	103 (99%)	1 (1%)	68 84
43	p	105/107 (98%)	100 (95%)	5 (5%)	23 43
44	q	86/90 (96%)	86 (100%)	0	100 100
45	r	90/99 (91%)	90 (100%)	0	100 100
46	t	103/104 (99%)	99 (96%)	4 (4%)	28 52
47	u	93/96 (97%)	91 (98%)	2 (2%)	45 70
48	v	79/84 (94%)	79 (100%)	0	100 100
49	w	75/77 (97%)	75 (100%)	0	100 100
50	x	65/65 (100%)	65 (100%)	0	100 100
51	y	74/78 (95%)	71 (96%)	3 (4%)	27 50
52	z	48/65 (74%)	47 (98%)	1 (2%)	47 71
All	All	4625/4829 (96%)	4543 (98%)	82 (2%)	51 74

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	f	3	ARG

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Mol	Chain	Res	Type
43	p	118	LEU
33	f	35	SER
41	n	69	VAL
46	t	64	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
16	O	48	ASN
46	t	72	HIS
23	V	73	ASN
49	w	42	HIS
40	m	13	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	I	2894/2904 (99%)	342 (11%)	25 (0%)
11	J	117/120 (97%)	11 (9%)	0
4	C	1539/1540 (99%)	169 (10%)	7 (0%)
All	All	4550/4564 (99%)	522 (11%)	32 (0%)

5 of 522 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	C	4	U
4	C	5	U
4	C	9	G
4	C	39	G
4	C	47	C

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	I	2447	G
10	I	2543	G
10	I	504	A
10	I	404	A
10	I	2680	U

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	5MU	I	747	10	19,22,23	1.02	2 (10%)	27,32,35	2.13	6 (22%)
22	4D4	U	81	22	9,11,12	2.14	2 (22%)	7,13,15	1.96	3 (42%)
10	6MZ	I	1618	10	22,25,26	1.08	1 (4%)	29,36,39	2.20	9 (31%)
10	PSU	I	1911	10	18,21,22	0.88	0	21,30,33	1.98	4 (19%)
10	H2U	I	2449	10	18,21,22	0.42	0	19,30,33	0.71	0
10	OMG	I	2251	10	23,26,27	0.73	0	32,38,41	1.95	10 (31%)
10	2MG	I	1835	10	23,26,27	0.77	0	33,38,41	2.17	10 (30%)
10	6MZ	I	2030	10	22,25,26	1.09	1 (4%)	29,36,39	2.24	9 (31%)
10	5MU	I	1939	10	19,22,23	1.02	2 (10%)	27,32,35	2.12	6 (22%)
10	OMU	I	2552	10	19,22,23	0.95	2 (10%)	25,31,34	1.94	6 (24%)
10	5MC	I	1962	10	19,22,23	1.22	2 (10%)	26,32,35	1.11	3 (11%)
10	PSU	I	2580	53,10	18,21,22	0.95	0	21,30,33	1.97	5 (23%)
10	OMC	I	2498	53,10	19,22,23	0.89	1 (5%)	25,31,34	0.97	1 (4%)
10	PSU	I	2605	10	18,21,22	0.92	1 (5%)	21,30,33	1.97	4 (19%)
10	PSU	I	955	10	18,21,22	0.91	0	21,30,33	1.99	4 (19%)
10	2MA	I	2503	53,10	22,25,26	1.33	3 (13%)	32,37,40	1.96	7 (21%)
10	PSU	I	2604	10	18,21,22	0.91	0	21,30,33	1.99	4 (19%)
10	PSU	I	746	53,10	18,21,22	0.99	1 (5%)	21,30,33	1.88	4 (19%)
10	3TD	I	1915	10	19,22,23	1.09	2 (10%)	23,32,35	1.88	2 (8%)
10	PSU	I	2504	53,10	18,21,22	0.88	0	21,30,33	1.97	4 (19%)
10	PSU	I	2457	10	18,21,22	0.93	1 (5%)	21,30,33	2.01	4 (19%)
10	2MG	I	2445	10	23,26,27	0.76	0	33,38,41	2.20	12 (36%)
10	PSU	I	1917	10	18,21,22	0.88	0	21,30,33	1.96	4 (19%)
10	G7M	I	2069	10	23,26,27	0.54	0	34,39,42	0.91	2 (5%)
10	1MG	I	745	10	23,26,27	0.91	2 (8%)	33,39,42	1.78	6 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	5MU	I	747	10	-	0/7/25/26	0/2/2/2
22	4D4	U	81	22	-	1/11/12/14	-
10	6MZ	I	1618	10	-	2/9/27/28	0/3/3/3
10	PSU	I	1911	10	-	0/7/25/26	0/2/2/2
10	H2U	I	2449	10	-	0/7/38/39	0/2/2/2
10	OMG	I	2251	10	-	0/9/27/28	0/3/3/3
10	2MG	I	1835	10	-	0/9/27/28	0/3/3/3
10	6MZ	I	2030	10	-	2/9/27/28	0/3/3/3
10	5MU	I	1939	10	-	0/7/25/26	0/2/2/2
10	OMU	I	2552	10	-	0/9/27/28	0/2/2/2
10	5MC	I	1962	10	-	0/7/25/26	0/2/2/2
10	PSU	I	2580	53,10	-	0/7/25/26	0/2/2/2
10	OMC	I	2498	53,10	-	0/9/27/28	0/2/2/2
10	PSU	I	2605	10	-	2/7/25/26	0/2/2/2
10	PSU	I	955	10	-	0/7/25/26	0/2/2/2
10	2MA	I	2503	53,10	-	2/7/25/26	0/3/3/3
10	PSU	I	2604	10	-	0/7/25/26	0/2/2/2
10	PSU	I	746	53,10	-	1/7/25/26	0/2/2/2
10	3TD	I	1915	10	-	2/7/25/26	0/2/2/2
10	PSU	I	2504	53,10	-	2/7/25/26	0/2/2/2
10	PSU	I	2457	10	-	0/7/25/26	0/2/2/2
10	2MG	I	2445	10	-	2/9/27/28	0/3/3/3
10	PSU	I	1917	10	-	0/7/25/26	0/2/2/2
10	G7M	I	2069	10	-	0/7/25/26	0/3/3/3
10	1MG	I	745	10	-	0/7/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	81	4D4	CZ-NE	5.38	1.43	1.33
10	I	2503	2MA	C6-N1	3.94	1.40	1.35
10	I	1962	5MC	C5-C4	-3.87	1.41	1.44
10	I	1618	6MZ	C6-N6	3.81	1.38	1.34
10	I	2030	6MZ	C6-N6	3.76	1.38	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	2445	2MG	C2-N3-C4	7.30	121.13	112.00
10	I	1835	2MG	C2-N3-C4	7.26	121.08	112.00
10	I	1915	3TD	N1-C2-N3	6.59	120.92	116.13
10	I	2503	2MA	C5-C4-N3	-5.93	120.93	127.18
10	I	2457	PSU	N1-C2-N3	5.63	121.11	115.17

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	2030	6MZ	1	0
10	I	2503	2MA	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 202 ligands modelled in this entry, 201 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	RD8	I	3112	53	35,35,35	1.33	4 (11%)	45,48,48	1.77	8 (17%)

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
54	RD8	I	3112	53	-	0/19/31/31	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	I	3112	RD8	C30-N21	3.70	1.40	1.36
54	I	3112	RD8	C24-C23	3.27	1.55	1.51
54	I	3112	RD8	O29-C23	-3.12	1.41	1.46
54	I	3112	RD8	C13-N17	-2.61	1.31	1.36

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	I	3112	RD8	C13-N17-N16	-5.60	102.97	109.01
54	I	3112	RD8	C23-O29-C30	4.50	113.70	110.10
54	I	3112	RD8	C22-N21-C30	-4.07	108.16	111.17
54	I	3112	RD8	O29-C23-C22	-2.91	101.68	104.50
54	I	3112	RD8	O29-C30-N21	-2.91	107.47	109.92

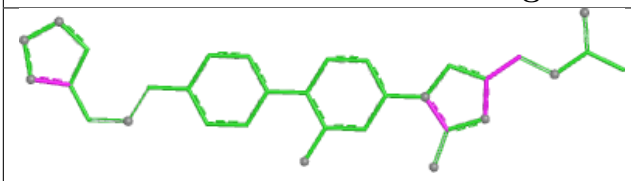
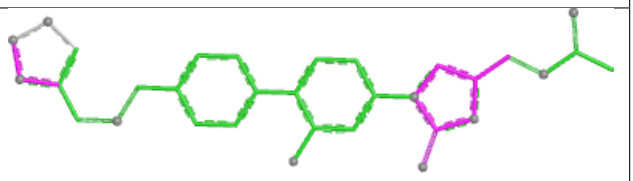
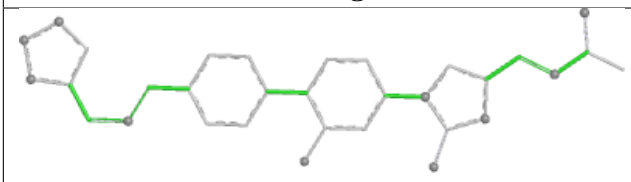
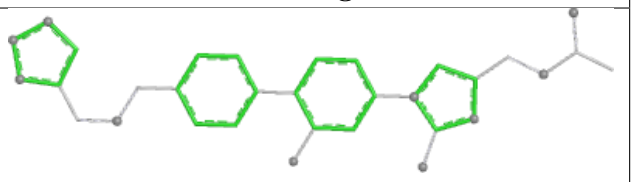
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand RD8 I 3112	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

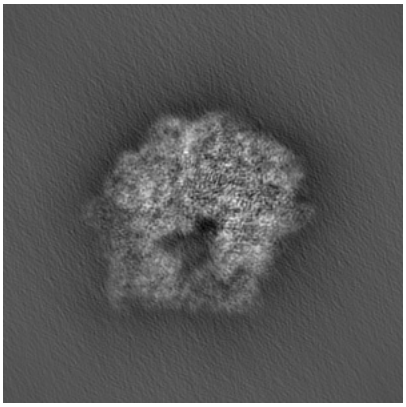
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24803. These allow visual inspection of the internal detail of the map and identification of artifacts.

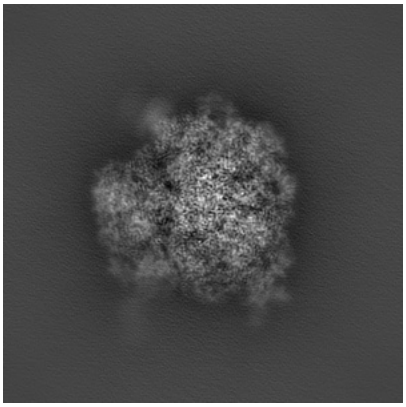
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

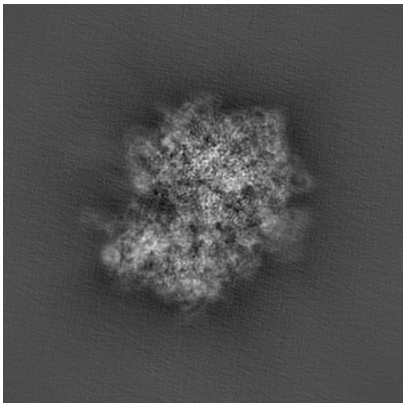
6.1.1 Primary map



X



Y

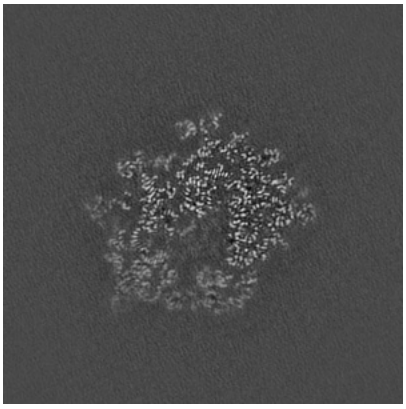


Z

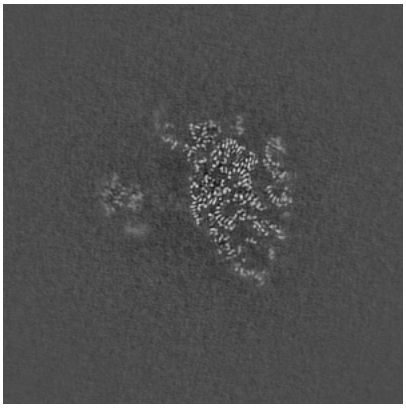
The images above show the map projected in three orthogonal directions.

6.2 Central slices

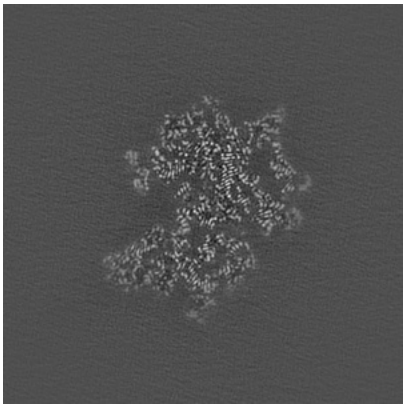
6.2.1 Primary map



X Index: 256



Y Index: 256

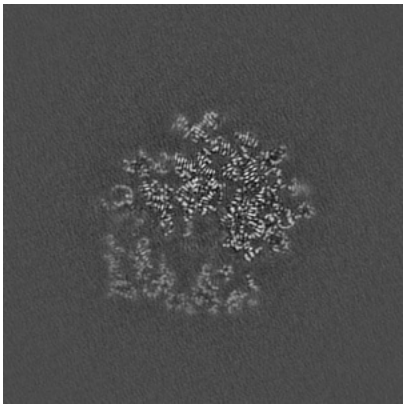


Z Index: 256

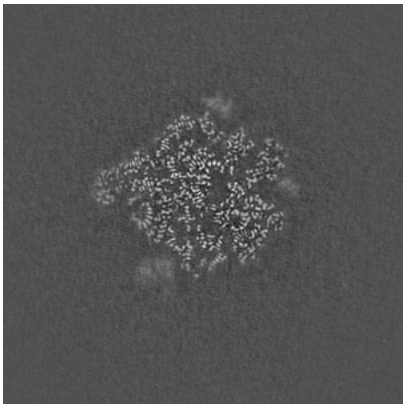
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

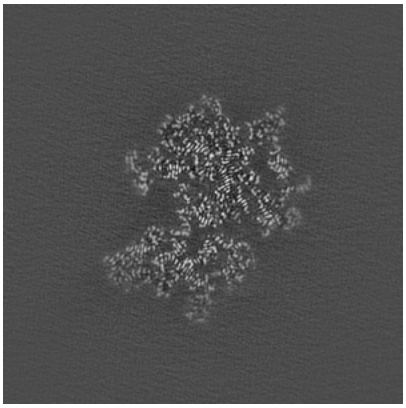
6.3.1 Primary map



X Index: 264



Y Index: 292

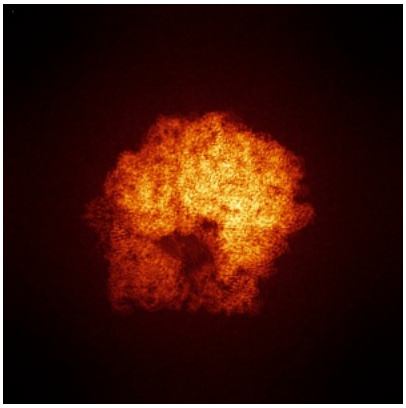


Z Index: 254

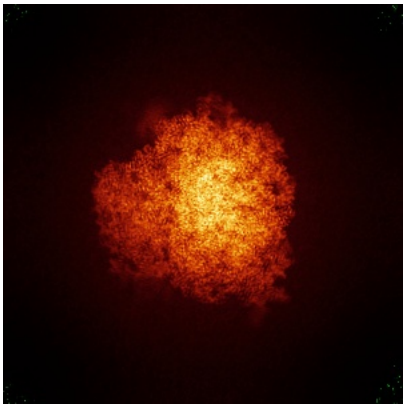
The images above show the largest variance slices of the map in three orthogonal directions.

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

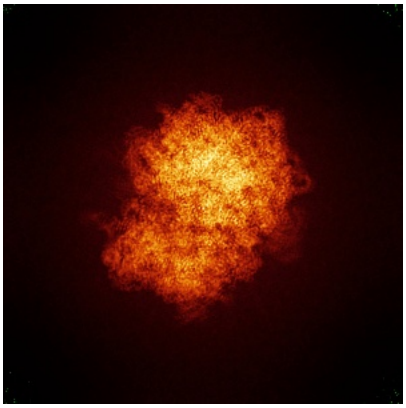
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

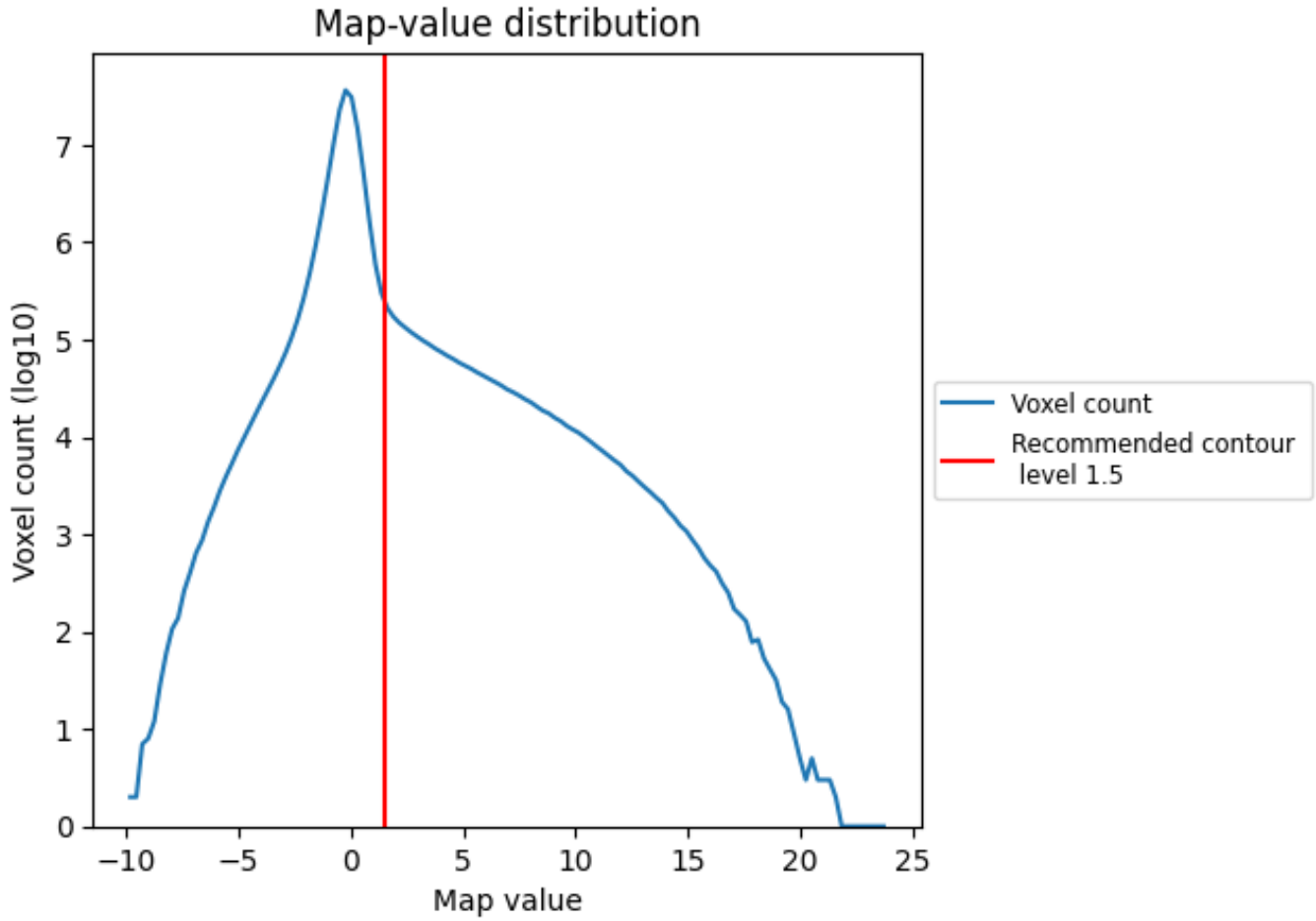
6.6 Mask visualisation (i)

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

7 Map analysis

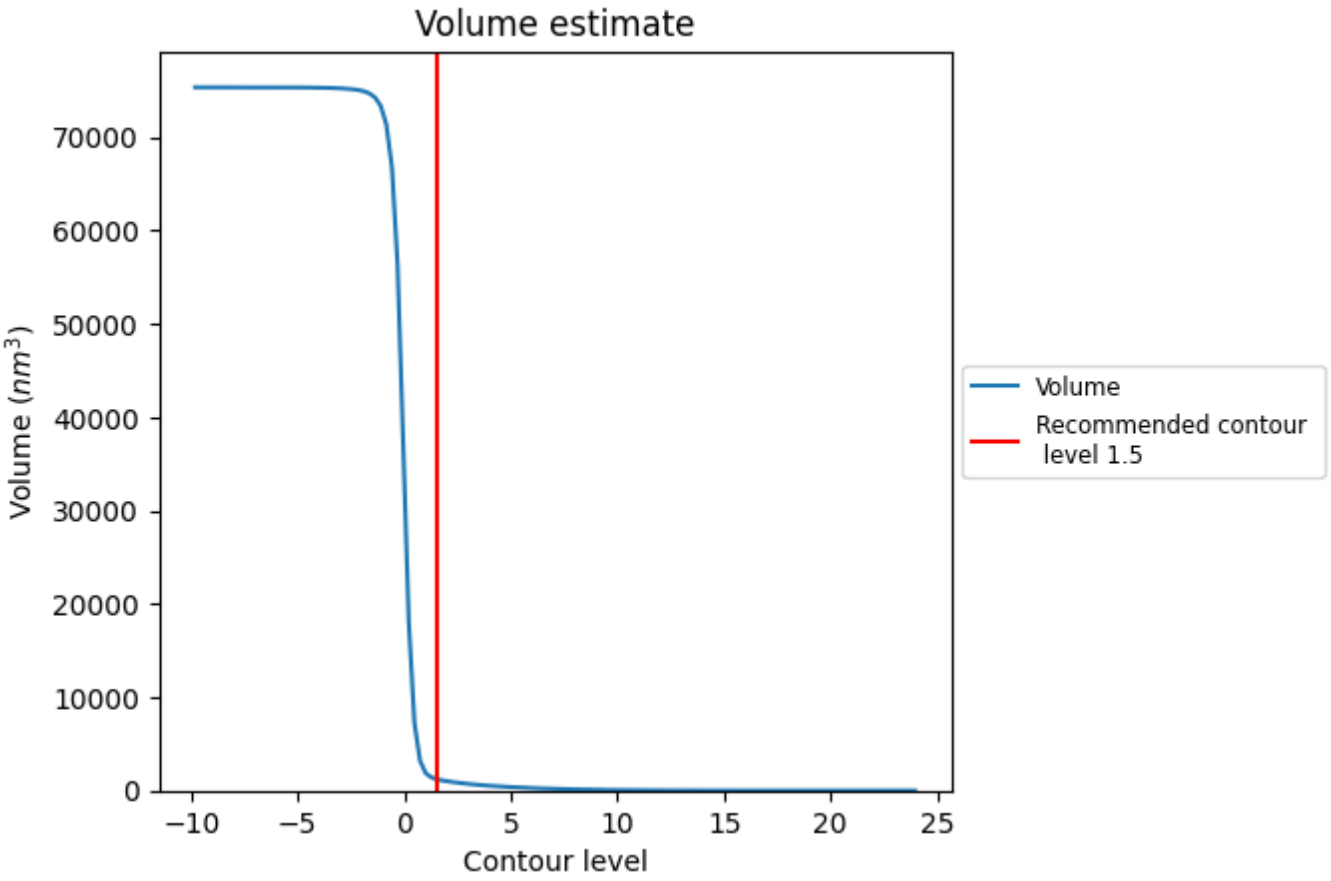
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

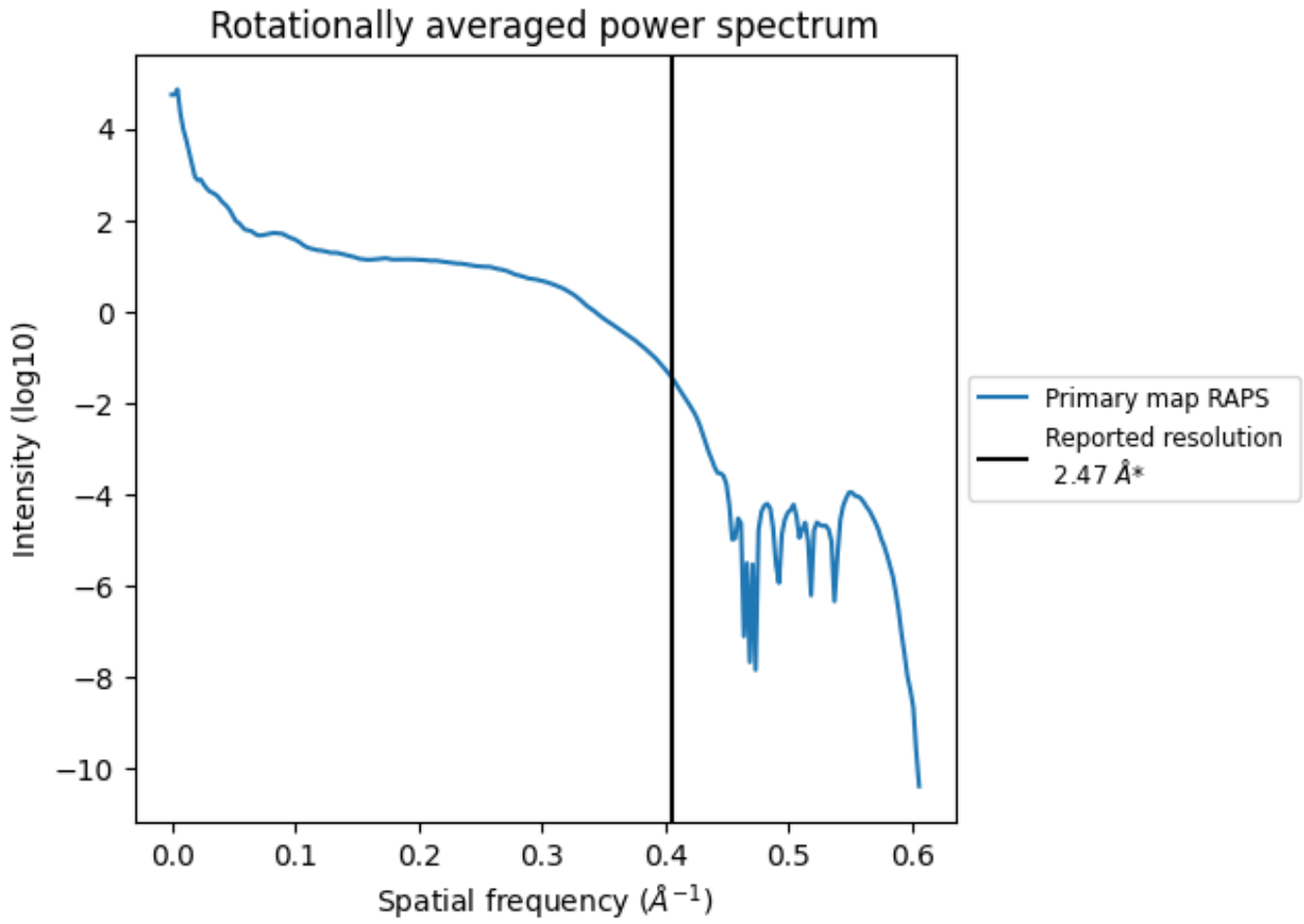
7.2 Volume estimate (i)



The volume at the recommended contour level is 1235 nm^3; this corresponds to an approximate mass of 1116 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

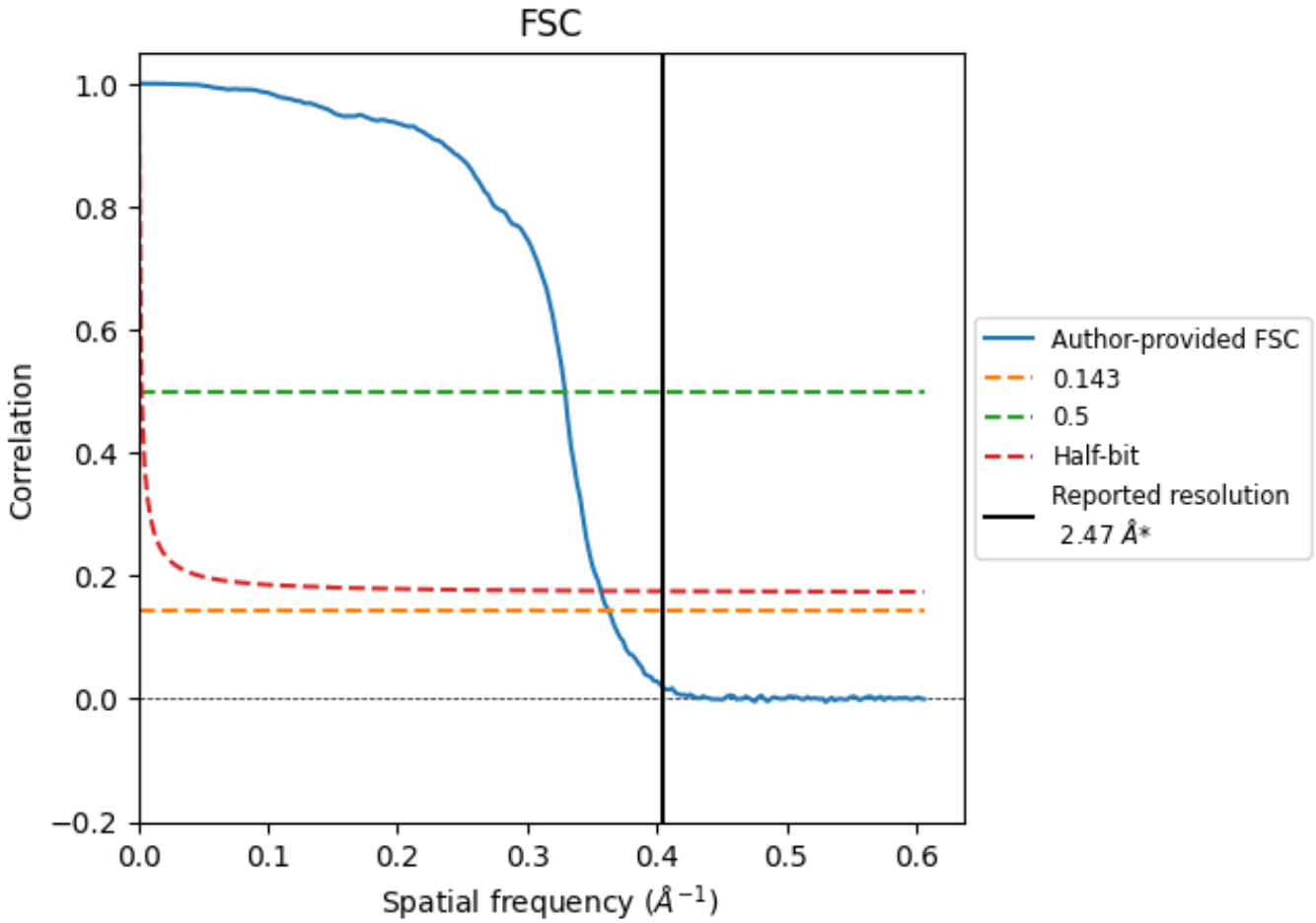


*Reported resolution corresponds to spatial frequency of 0.405 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.405 Å^{-1}

8.2 Resolution estimates (i)

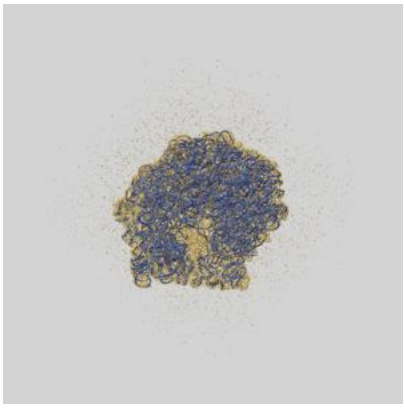
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	2.76	3.04	2.80
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.76 differs from the reported value 2.47 by more than 10 %

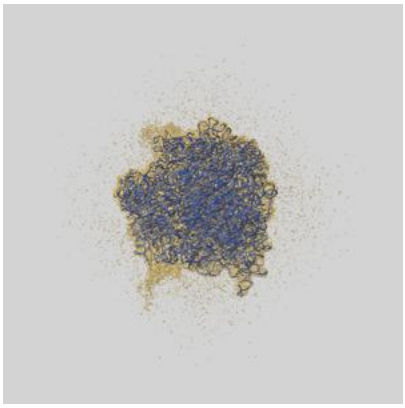
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24803 and PDB model 7S1J. Per-residue inclusion information can be found in section 3 on page 14.

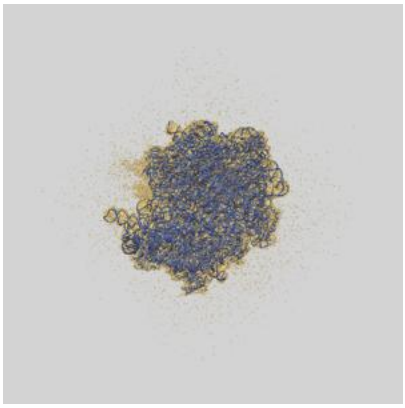
9.1 Map-model overlay



X



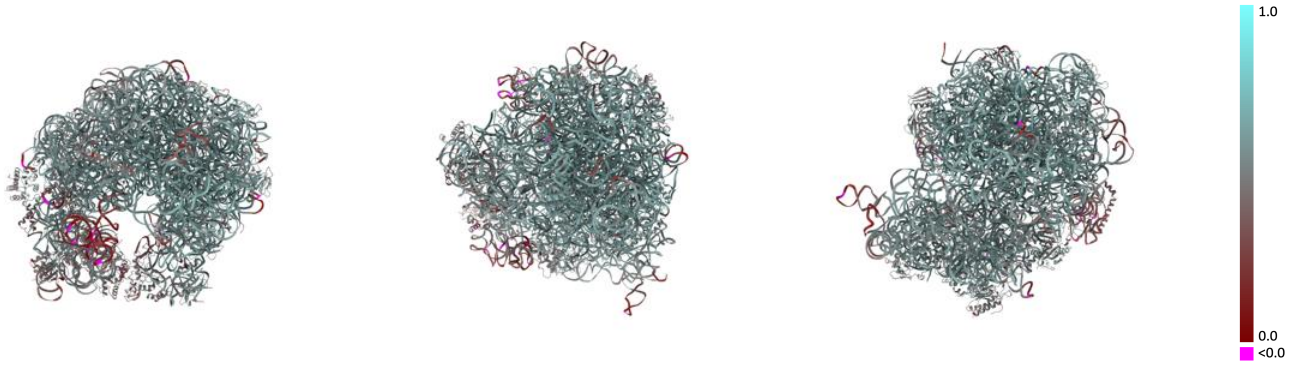
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5 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.

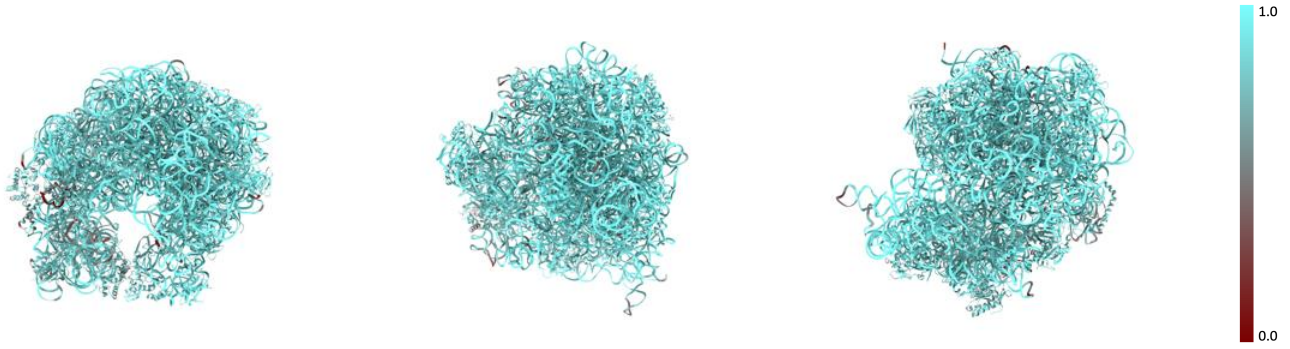
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

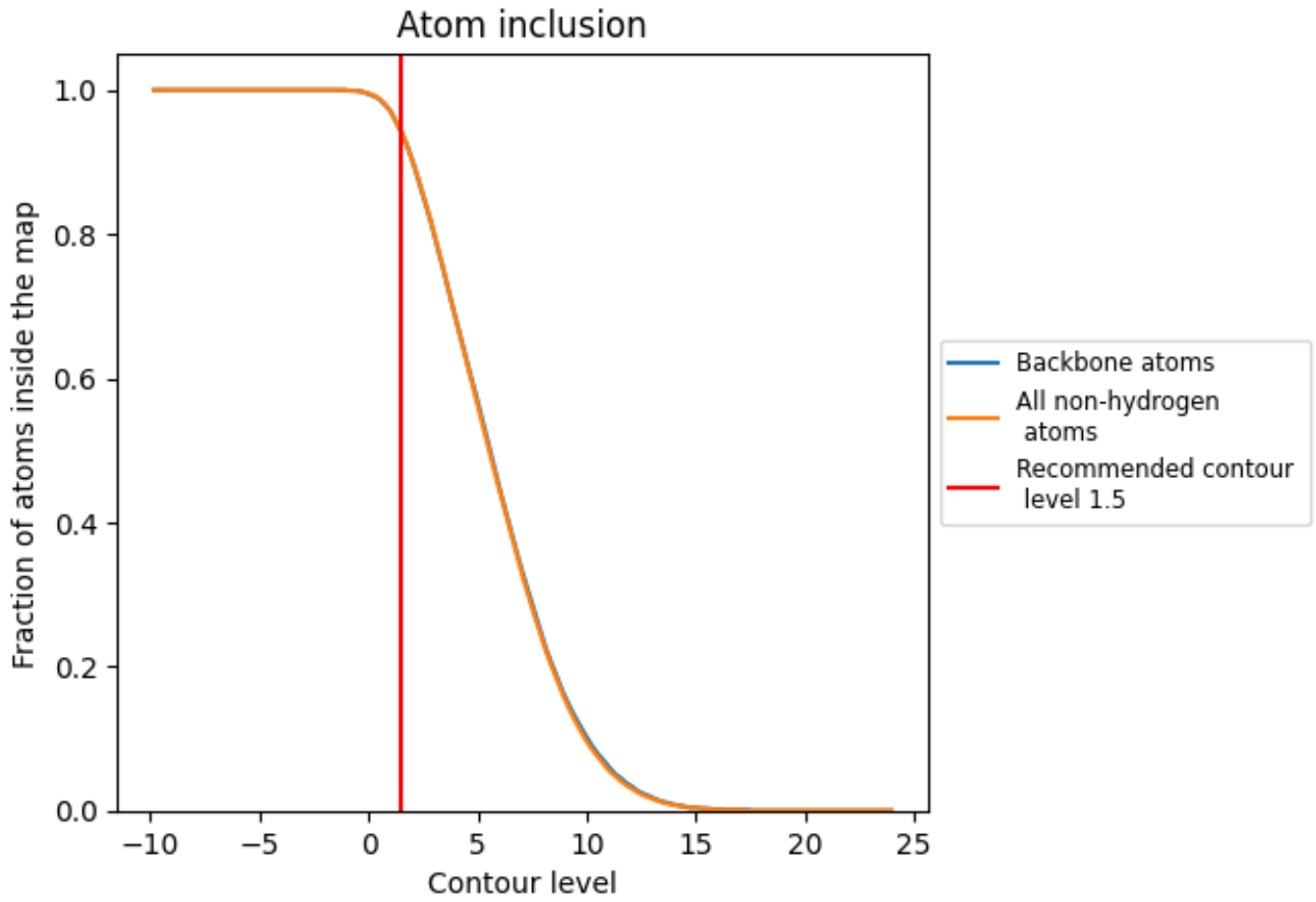
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9430	0.5520
1	0.7500	0.3490
2	0.8970	0.5170
3	0.5610	0.4060
C	0.9610	0.5470
D	0.7640	0.4660
E	0.8490	0.5190
F	0.8610	0.5120
G	0.9090	0.5590
H	0.9270	0.5170
I	0.9710	0.5670
J	0.9890	0.5600
K	0.9660	0.6030
L	0.9530	0.5980
M	0.9070	0.5510
N	0.8560	0.4480
O	0.8890	0.5010
P	0.7980	0.4400
Q	0.8410	0.4040
R	0.9490	0.6010
S	0.9500	0.5970
T	0.9400	0.5860
U	0.9360	0.5850
V	0.9760	0.6100
W	0.9260	0.5120
X	0.9370	0.5960
Y	0.9650	0.6080
Z	0.9440	0.5790
a	0.9280	0.5990
b	0.9070	0.5530
c	0.9060	0.5360
d	0.9160	0.5630
e	0.9500	0.6060
f	0.9580	0.5940
g	0.9040	0.5190



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Chain	Atom inclusion	Q-score
h	0.9340	0.5750
i	0.9420	0.5990
j	0.6410	0.4730
k	0.9660	0.6170
l	0.9610	0.6120
m	0.9450	0.6010
n	0.8410	0.4620
o	0.9210	0.5740
p	0.8020	0.4360
q	0.6910	0.4280
r	0.9190	0.5110
t	0.9320	0.5660
u	0.8310	0.4400
v	0.8480	0.4750
w	0.9640	0.5570
x	0.8990	0.5450
y	0.9070	0.5340
z	0.9520	0.5500