



wwPDB EM Validation Summary Report ⓘ

Jul 21, 2025 – 11:04 AM EDT

PDB ID : 9MKK / pdb_00009mkk
EMDB ID : EMD-48329
Title : Structure of arbekacin bound Escherichia coli 70S ribosome
Authors : Majumdar, S.; Parajuli, N.P.; Ge, X.; Emmerich, A.; Sanyal, S.
Deposited on : 2024-12-17
Resolution : 3.20 Å(reported)
Based on initial model : 7K00

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:

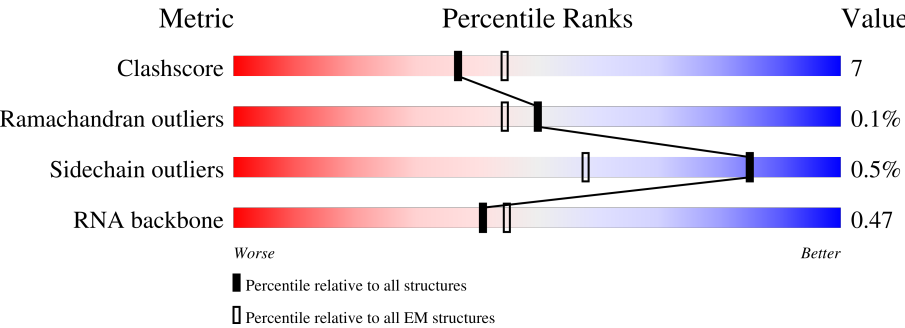
EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

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 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	
4	3	38	
5	4	70	
6	B	241	
7	C	233	



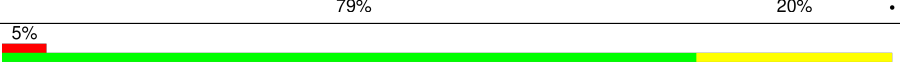
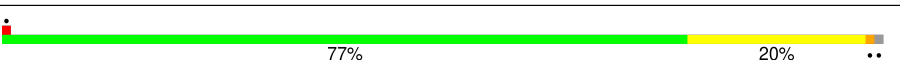


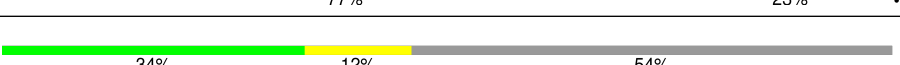

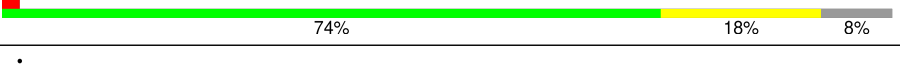

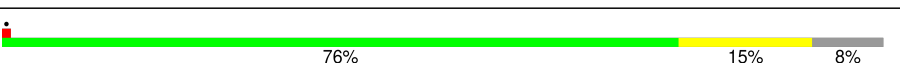


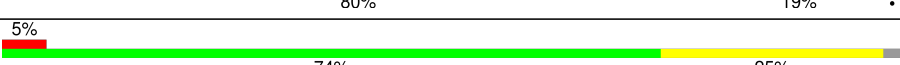

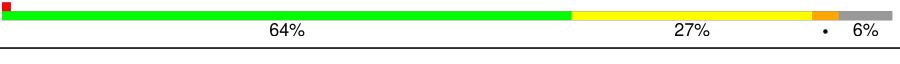




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Mol	Chain	Length	Quality of chain
8	D	206	
9	E	167	
10	F	135	
11	G	179	
12	H	130	
13	I	130	
14	J	103	
15	K	129	
16	L	124	
17	M	118	
18	N	101	
19	O	89	
20	P	82	
21	Q	84	
22	R	75	
23	S	92	
24	T	87	
25	U	71	
26	X	28	
27	Z	76	
28	b	120	
29	c	273	
30	d	209	
31	e	201	
32	f	179	

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Mol	Chain	Length	Quality of chain
33	g	177	
34	i	142	
35	j	123	
36	k	144	
37	l	136	
38	m	127	
39	n	117	
40	o	115	
41	p	118	
42	q	103	
43	s	100	
44	t	104	
45	u	94	
46	v	85	
47	w	78	
48	x	63	
49	y	59	
50	z	57	
51	A	1542	
52	a	2904	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 137440 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

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

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called 30S ribosomal protein S2.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 10 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 11 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	153	Total	C	N	O	S	0	0
			1197	747	228	218	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	127	Total	C	N	O	S	0	0
			1019	632	206	179	2		

- Molecule 14 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	116	Total	C	N	O	S	0	0
			869	536	172	158	3		

- Molecule 16 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	122	Total	C	N	O	S	0	0
			944	583	195	162	4		

- Molecule 17 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 21 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 22 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 24 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 25 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 26 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 27 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 28 is a RNA chain called 5S rRNA.

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

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	208	Total	C	N	O	S	0	0
			1556	974	286	292	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	142	Total	C	N	O	S	0	0
			1123	711	209	199	4		

- Molecule 35 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	134	Total	C	N	O	S	0	0
			1055	675	200	175	5		

- Molecule 38 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	p	54	Total	C	N	O	0	0
			431	270	96	65		

- Molecule 42 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	62	Total	C	N	O	S	0	0
			485	300	91	93	1		

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

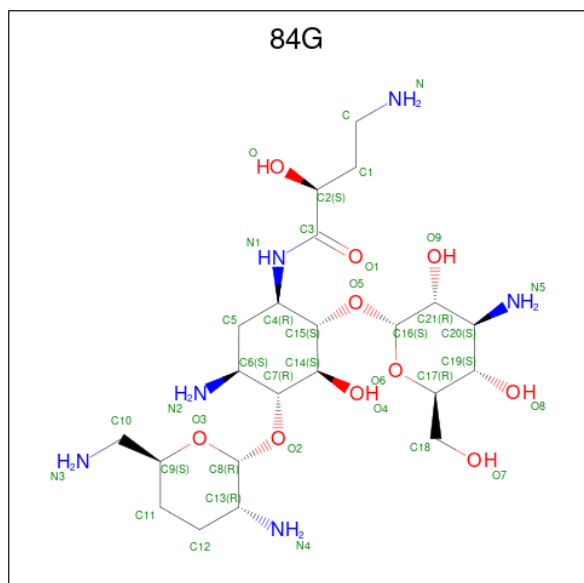
- Molecule 51 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A	1512	Total	C	N	O	P	0	0
			32450	14473	5962	10503	1512		

- Molecule 52 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	2732	Total	C	N	O	P	0	0
			58675	26173	10829	18941	2732		

- Molecule 53 is Arbekacin (CCD ID: 84G) (formula: $C_{22}H_{44}N_6O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
53	A	1	Total	C	N	O	0
			38	22	6	10	

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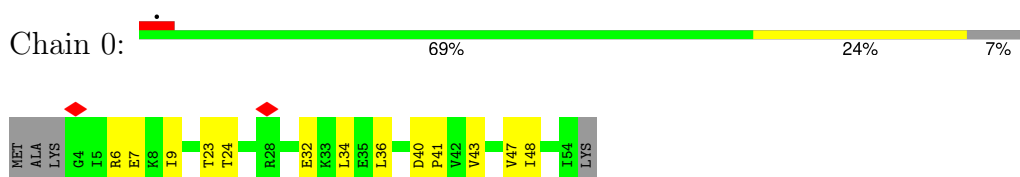
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
53	a	1	38	22	6	10	0

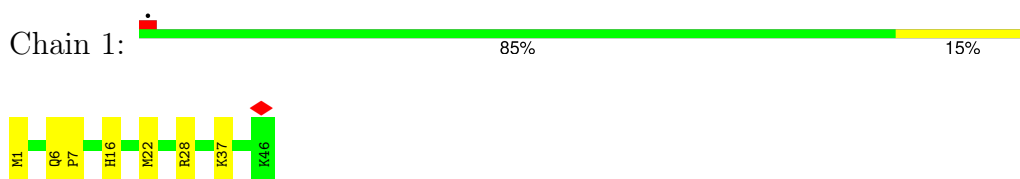
3 Residue-property plots [i](#)

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

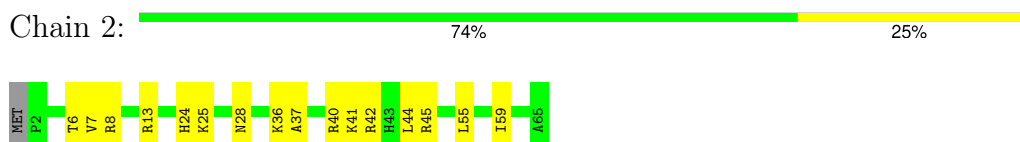
- Molecule 1: 50S ribosomal protein L33



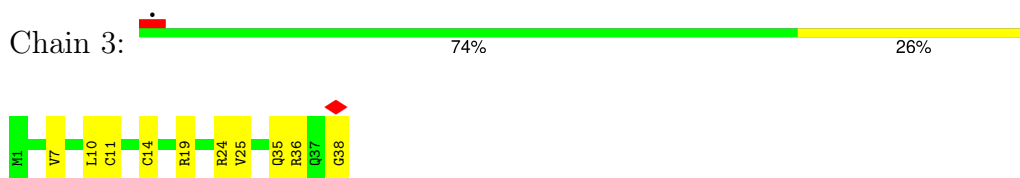
- Molecule 2: 50S ribosomal protein L34



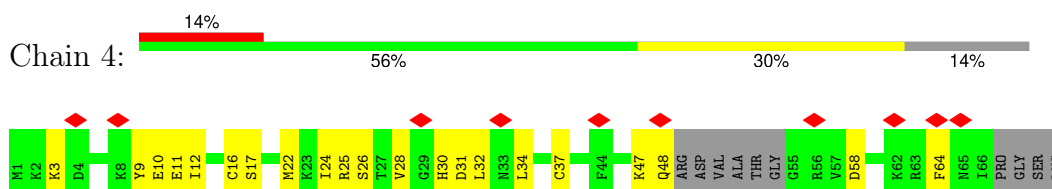
- Molecule 3: 50S ribosomal protein L35



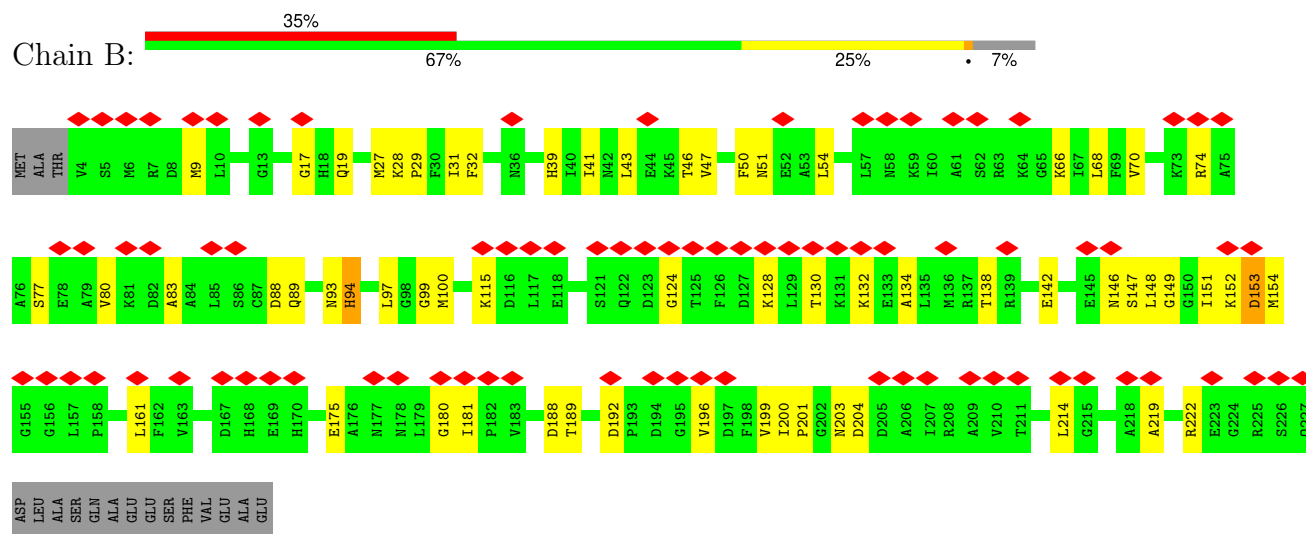
- Molecule 4: 50S ribosomal protein L36



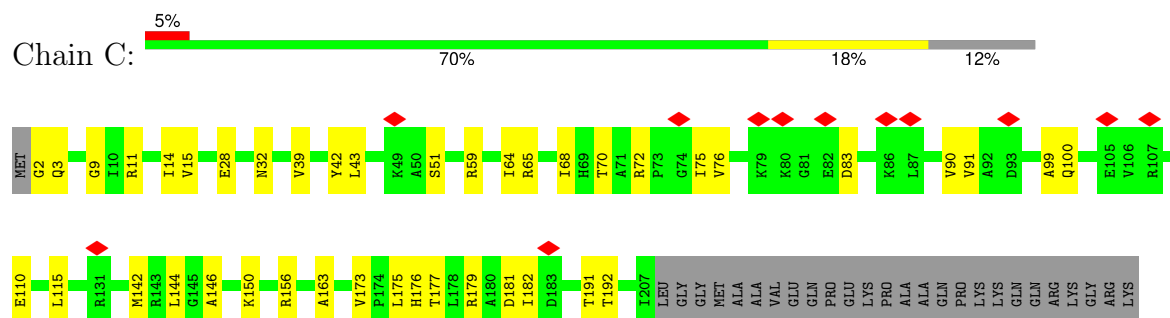
- Molecule 5: 50S ribosomal protein L31



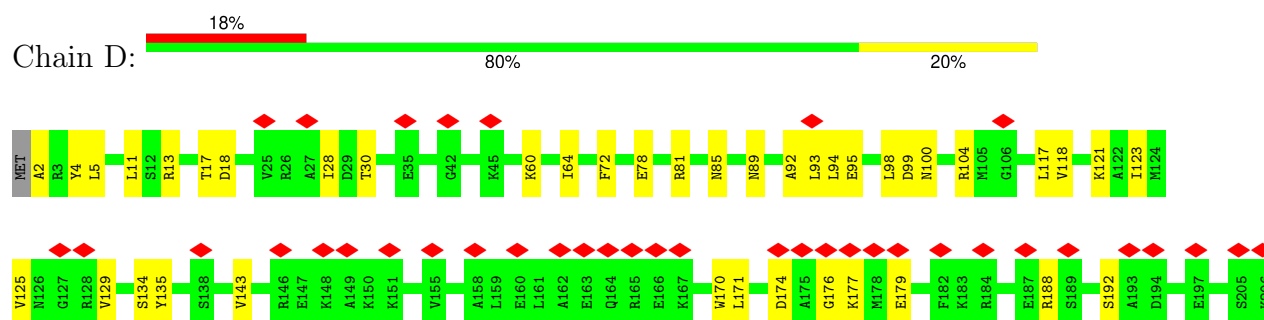
- Molecule 6: 30S ribosomal protein S2



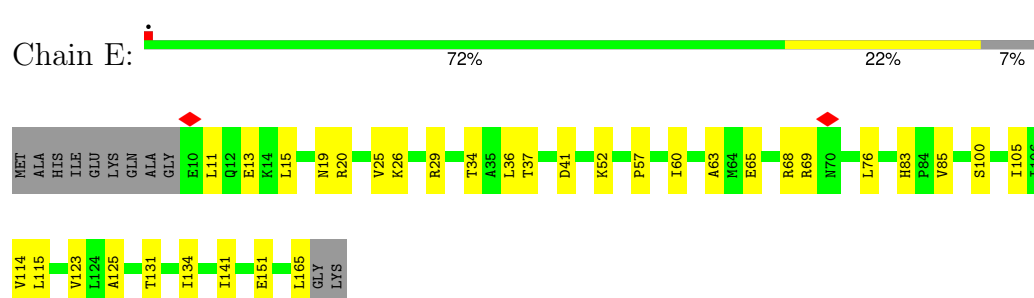
- Molecule 7: Small ribosomal subunit protein uS3



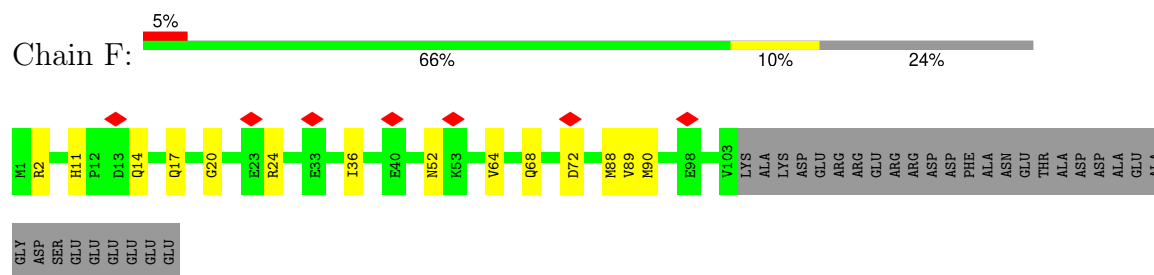
- Molecule 8: Small ribosomal subunit protein uS4



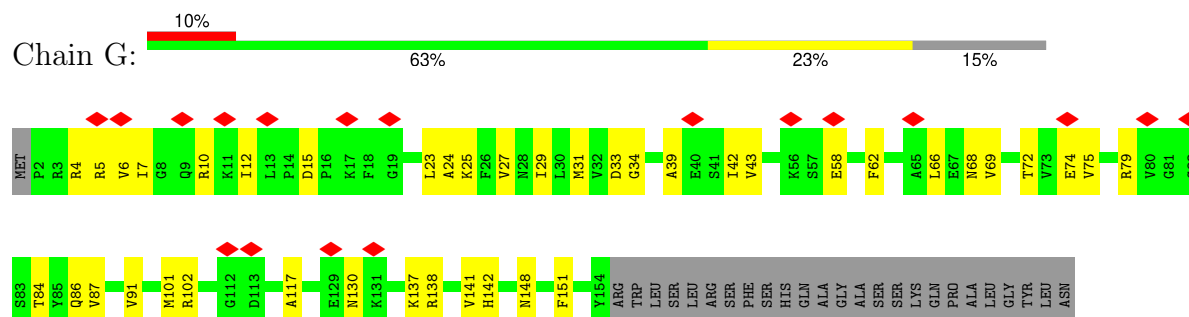
- Molecule 9: Small ribosomal subunit protein uS5



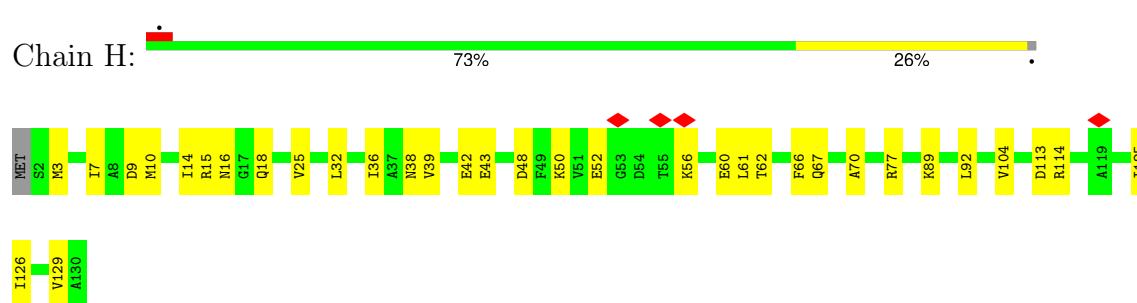
- Molecule 10: Small ribosomal subunit protein bS6



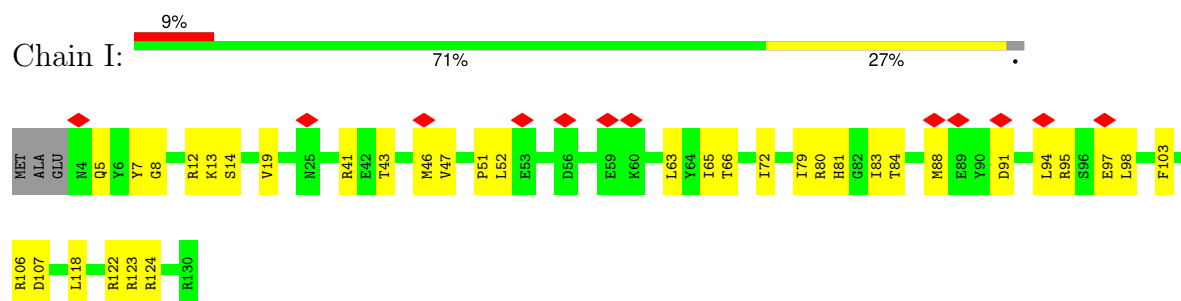
- Molecule 11: Small ribosomal subunit protein uS7



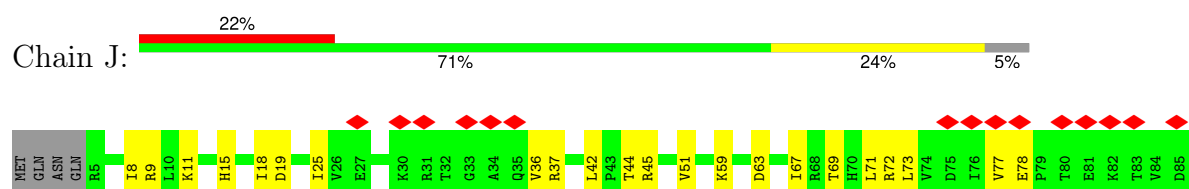
- Molecule 12: Small ribosomal subunit protein uS8

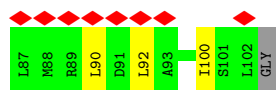


- Molecule 13: Small ribosomal subunit protein uS9



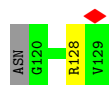
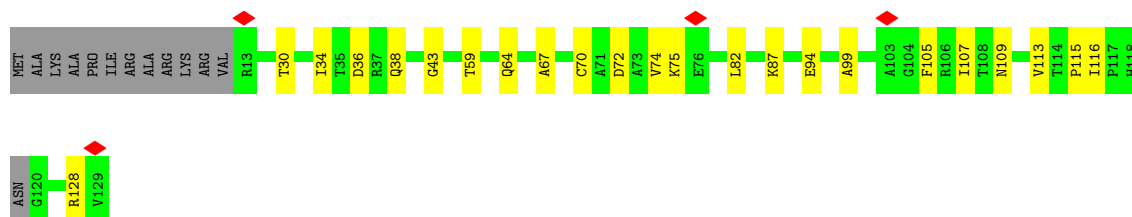
- Molecule 14: Small ribosomal subunit protein uS10





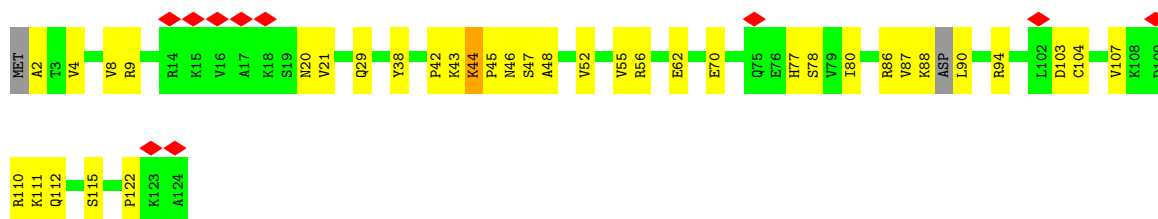
- Molecule 15: 30S ribosomal protein S11

Chain K: 72% 18% 10%



- Molecule 16: 30S ribosomal protein S12

Chain L: 8% 69% 28% ..



- Molecule 17: Small ribosomal subunit protein uS13

Chain M: 10% 80% 17% ..



- Molecule 18: Small ribosomal subunit protein uS14

Chain N: 73% 25% ..

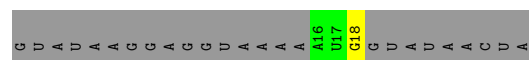
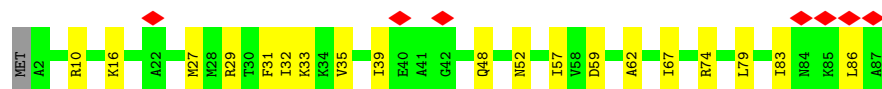
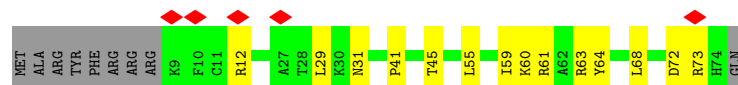


- Molecule 19: Small ribosomal subunit protein uS15

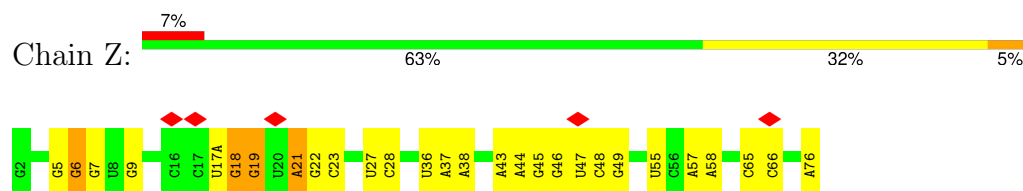
Chain O: 70% 29% .



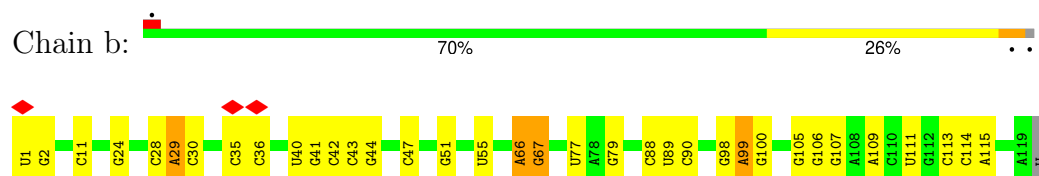
- Molecule 20: Small ribosomal subunit protein bS16



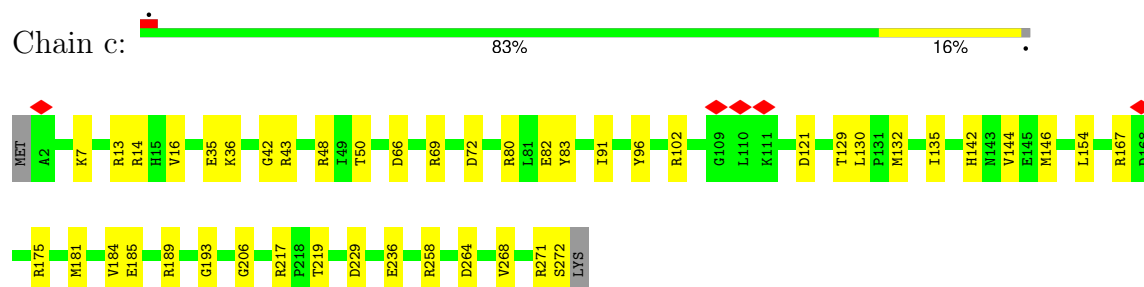
- Molecule 27: tRNA-fMet



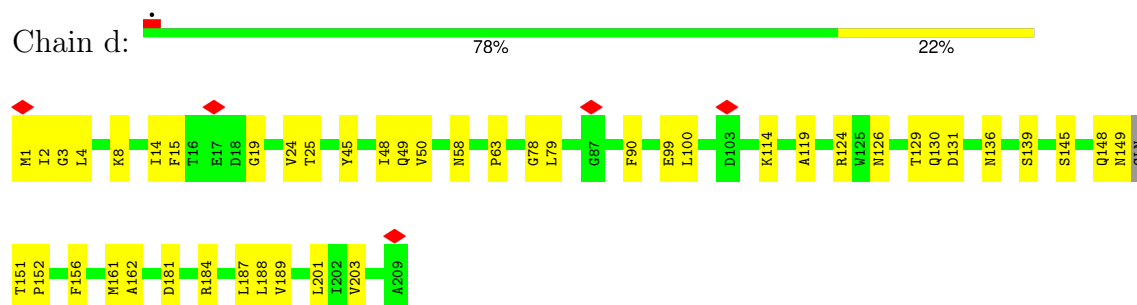
- Molecule 28: 5S rRNA



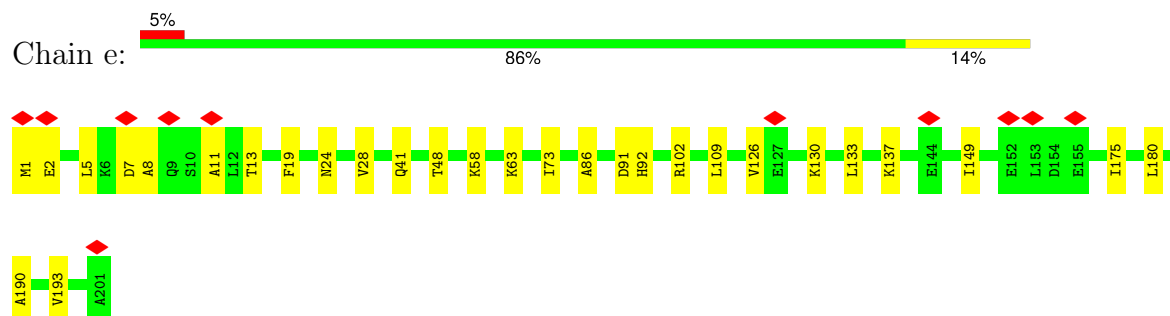
- Molecule 29: 50S ribosomal protein L2



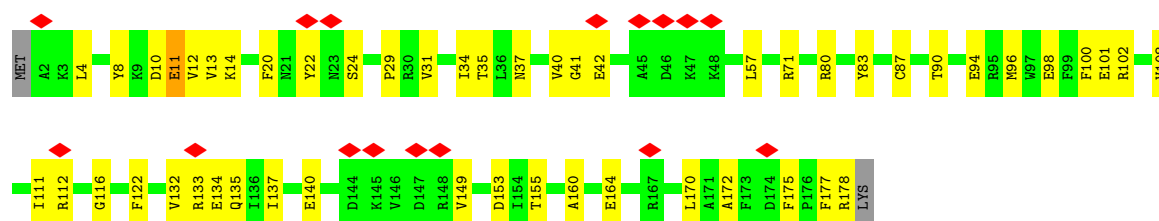
- Molecule 30: 50S ribosomal protein L3



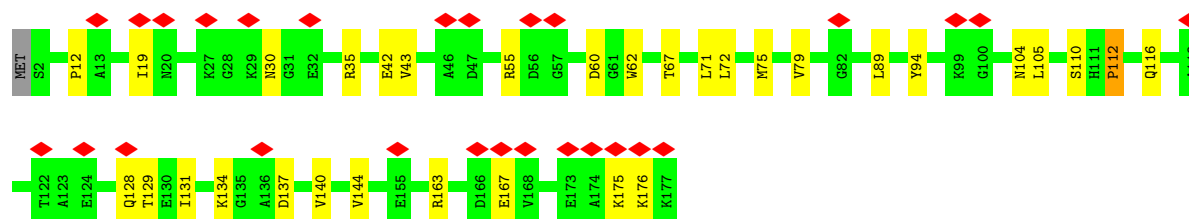
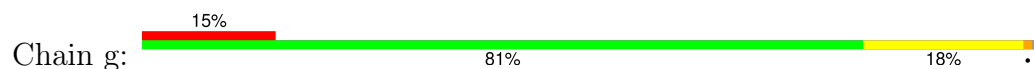
- Molecule 31: Large ribosomal subunit protein uL4



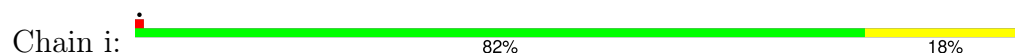
- Molecule 32: Large ribosomal subunit protein uL5



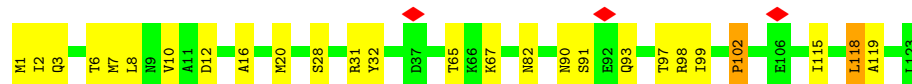
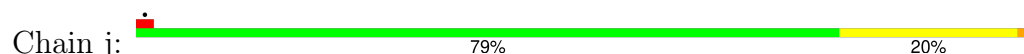
- Molecule 33: Large ribosomal subunit protein uL6



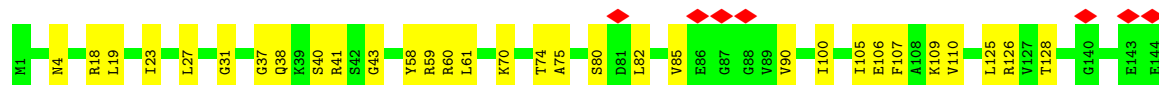
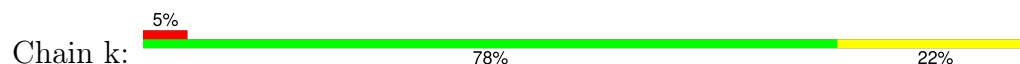
- Molecule 34: Large ribosomal subunit protein uL13



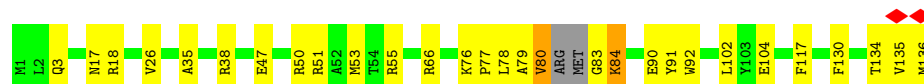
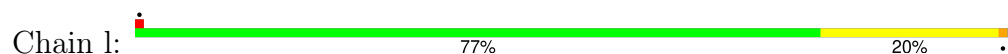
- Molecule 35: Large ribosomal subunit protein uL14




- Molecule 36: Large ribosomal subunit protein uL15



- Molecule 37: 50S ribosomal protein L16




- Molecule 38: Large ribosomal subunit protein bL17

Chain m: 




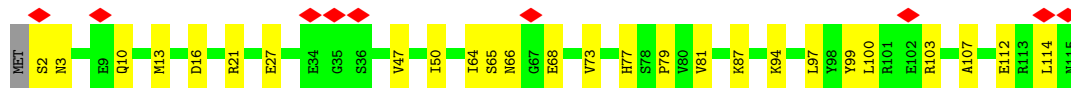
- Molecule 39: Large ribosomal subunit protein uL18

Chain n: 




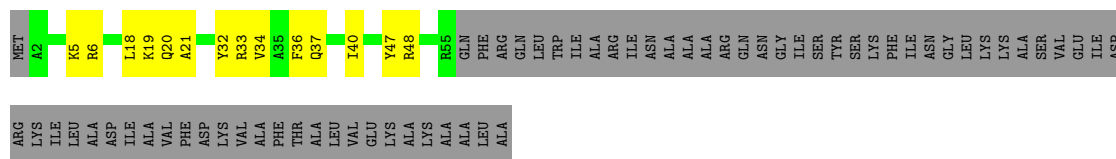
- Molecule 40: Large ribosomal subunit protein bL19

Chain o: 




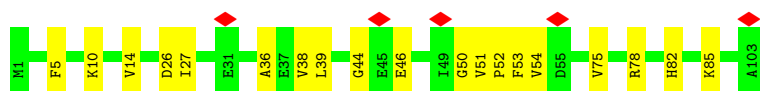
- Molecule 41: 50S ribosomal protein L20

Chain p: 



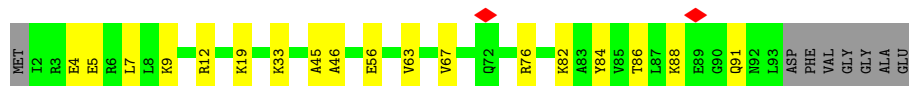
- Molecule 42: Large ribosomal subunit protein bL21

Chain q: 




- Molecule 43: 50S ribosomal protein L23

Chain s: 

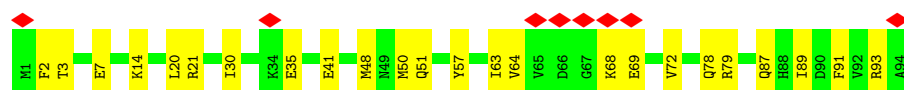
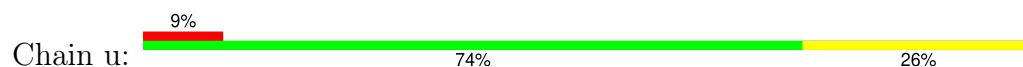


- Molecule 44: 50S ribosomal protein L24

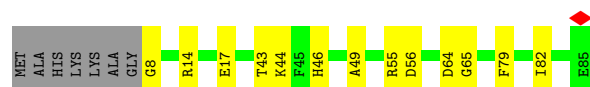
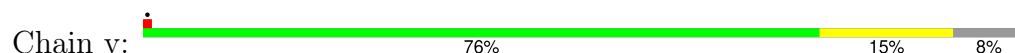
Chain t: 



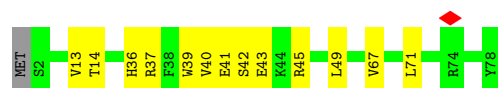
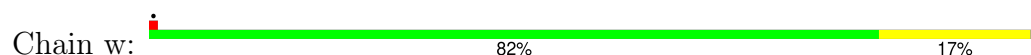
- Molecule 45: Large ribosomal subunit protein bL25



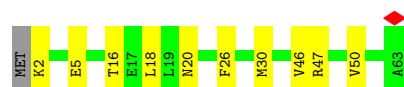
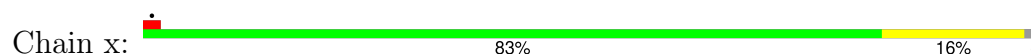
- Molecule 46: Large ribosomal subunit protein bL27



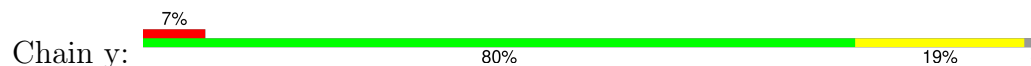
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: Large ribosomal subunit protein uL29



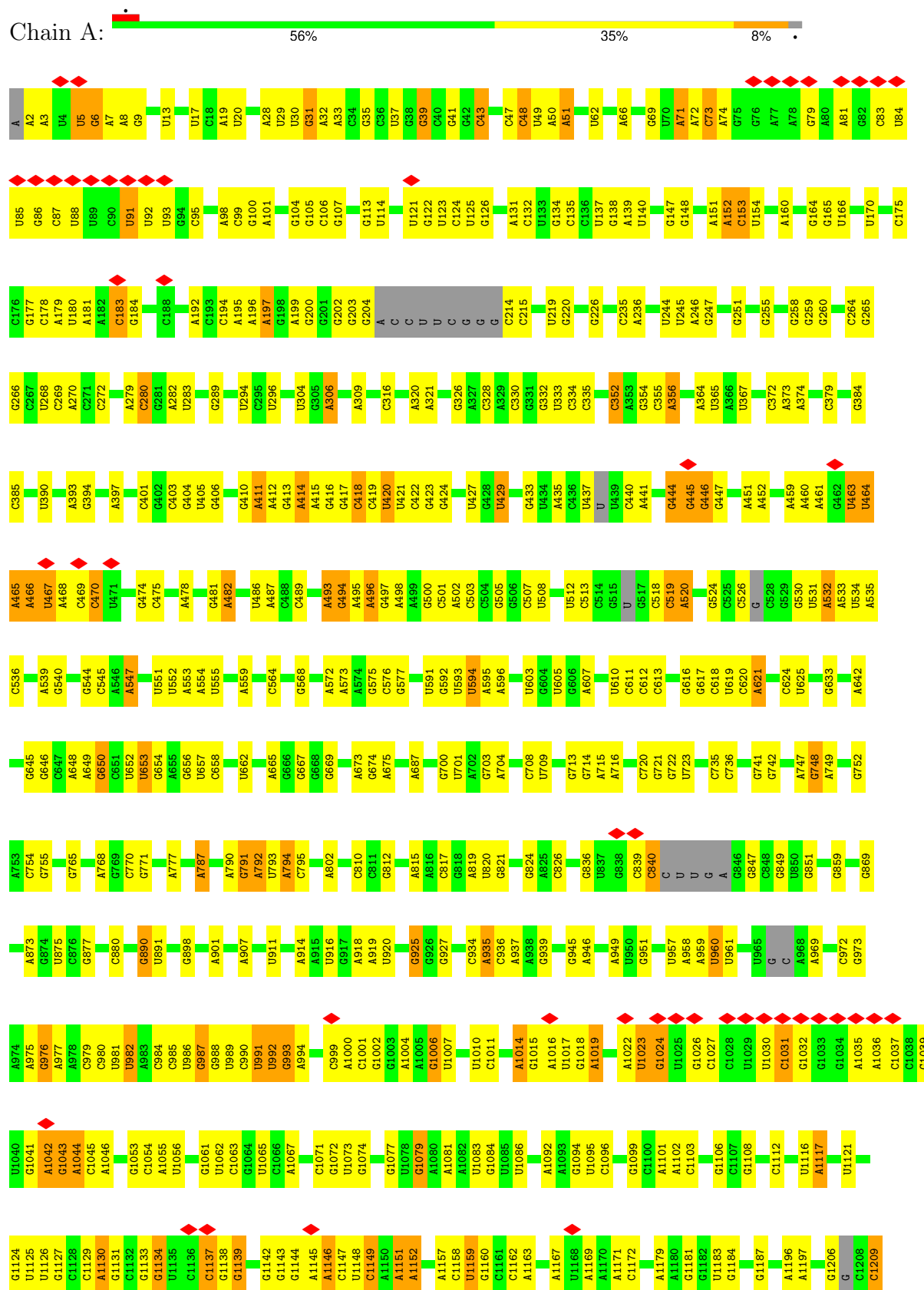
- Molecule 49: 50S ribosomal protein L30

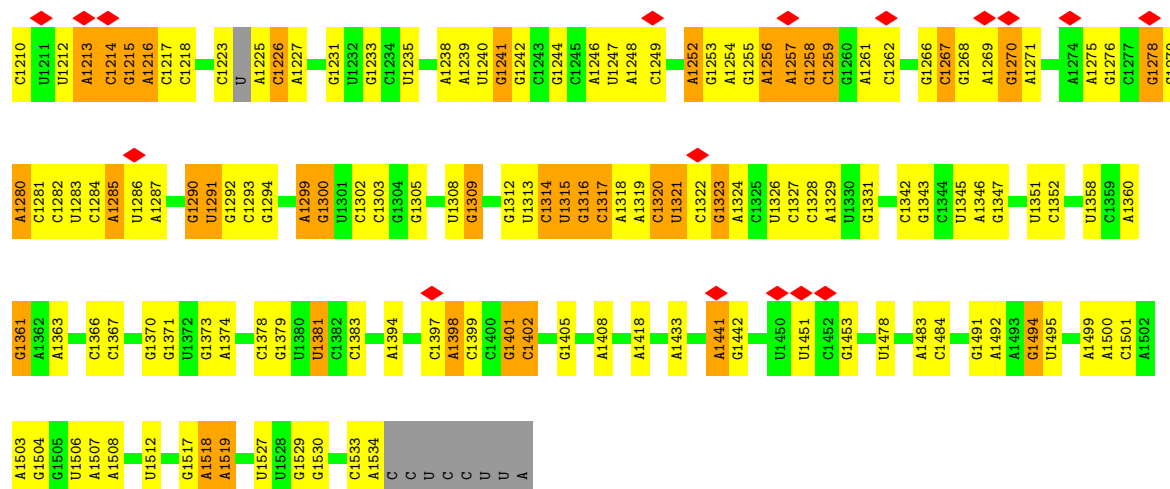


- Molecule 50: 50S ribosomal protein L32

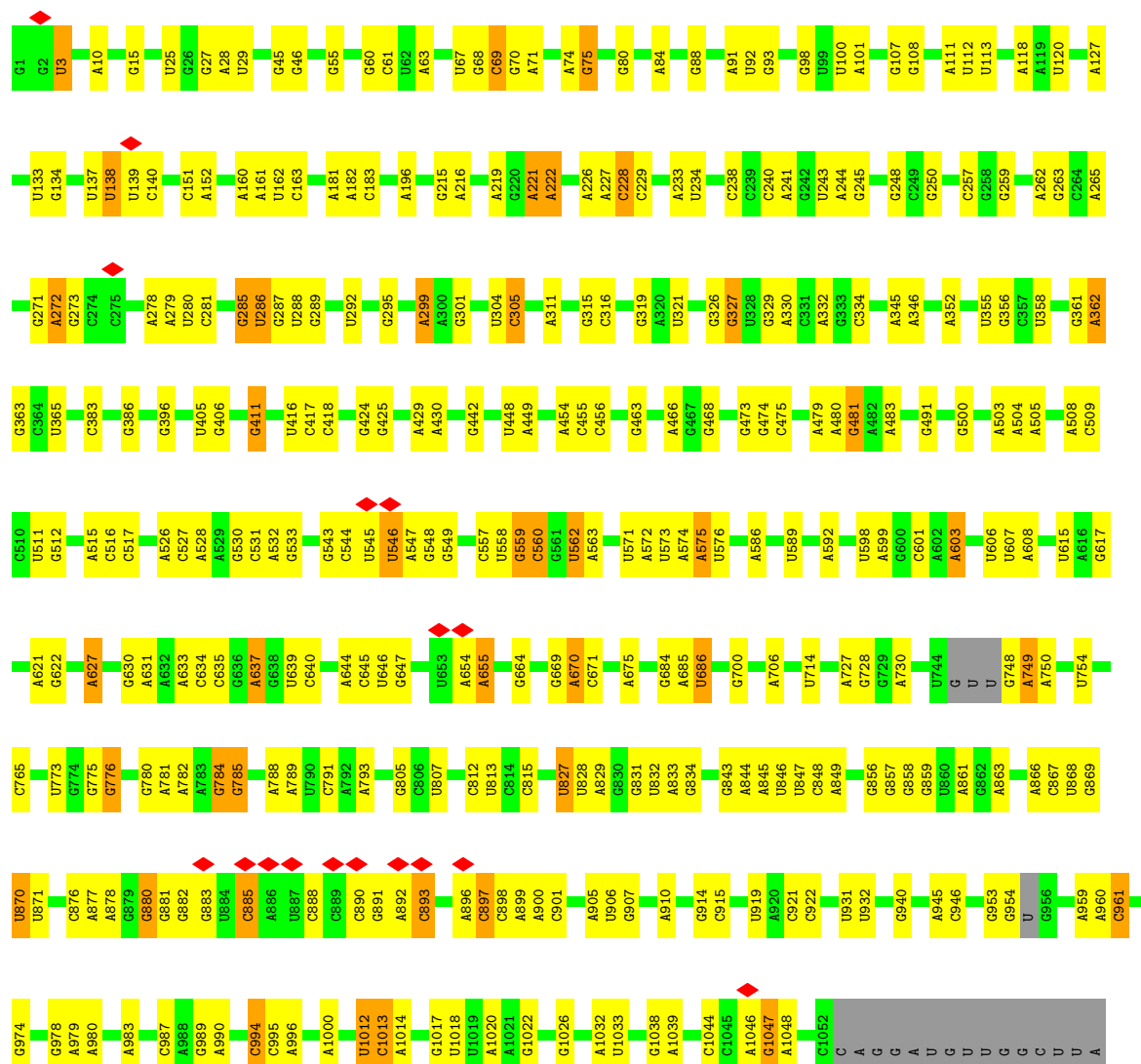


- Molecule 51: 16S rRNA

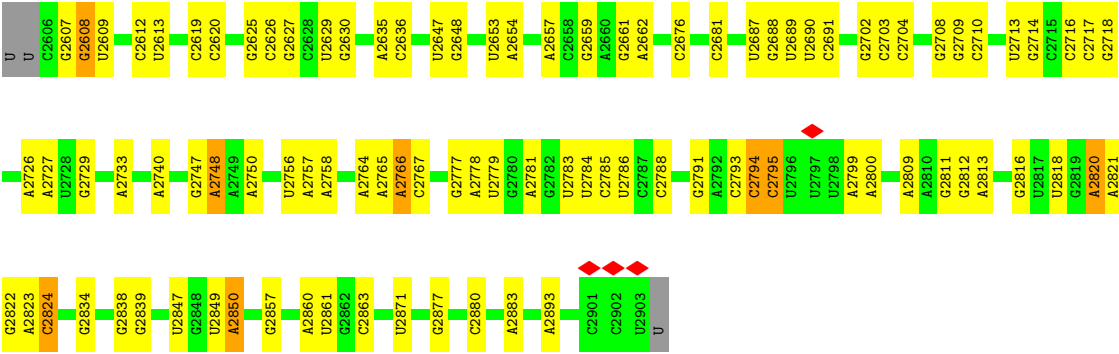




• Molecule 52: 23S rRNA



G2502	G2396	C2285	A	G	C2047	C1958	U1841	A1713	A1551	G1418	G1299	U1141	G
G2503	U2402	G2286	A	G	G2048	G1959	G1942	U1714	A1552	A1419	G1299	A1141	A
G2504	A2406	A2287	U	G	G2049	G1960	C1843	G1715	U1562	A1420	G1300	A1143	A
G2505	U2291	U2292	U	G	C2050	C1961	C1844	G1720	A1566	A1421	A1302	A1144	C
G2506	G2293	G2294	U	G	A2051	U1963	A1848	G1721	G1567	C1428	G1309	C1146	C
G2507	G2294	G2295	U	C	A2052	U1964	A1849	U1729	G1568	G1432	G1309	A1151	A
U2514	G2295	U2302	G	U	C2055	G1965	A1854	C1730	G1569	A1433	U1312	A1152	C
G2515	G2296	U2192	U	U	G2056	C1966	A1855	G1731	A1570	A1434	U1313	C1153	C
G2516	G2297	G2193	U	G	G2057	C1967	G1857	C1732	A1571	A1435	G1332	G1171	U
G2517	G2298	G2194	U	G	A2058	A1970	A1858	G1733	C1577	G1452	G1333	G1172	C
G2518	U2197	U2198	A	A	A2059	U1971	U1859	G1734	U1578	A1453	G1334	U	U
G2519	A2198	A2199	G	G	A2060	U1972	U1864	G1737	U1584	C1462	U1340	U	U
G2520	G2200	G2201	U	U	A2061	G1973	U1865	G1738	C1585	A1469	U1340	U	A
G2521	U2202	U2203	U	U	A2062	G1974	U1866	A1739	C1586	A1470	C1348	G1177	A
G2522	G2204	G2205	G	G	C2066	U1981	G1867	A1754	A1590	A1471	C1349	U	A
G2523	G2206	U2068	U	U	G2067	U1982	G1868	A1755	A1591	A1472	C1350	U	G
G2524	A2311	A2312	A	C	G	A1987	G1869	A1756	U1599	A1473	C1351	U	A
G2525	U2321	U2322	C	G	A2070	G1988	A1871	U1758	C1600	A1474	U1352	U	A
G2526	A2211	A2212	C	C	A2071	G1989	A1872	U1759	A1603	A1475	A1353	U	A
G2527	G2213	G2214	U	A	C2072	U1990	A1873	C1764	A1604	A1476	A1354	U	G
G2528	G2215	G2216	G	G	U2075	U1991	A1874	U1769	A1605	A1477	U1355	U	C
G2529	G2217	G2218	U	U	G	G1992	A1875	U1770	C1606	A1478	A1356	U	G
G2530	G2219	U2219	C	U	U2076	U1993	G1884	U1771	C1607	A1479	G1358	U	G
G2531	A2225	A2226	U	U	C2077	U1994	A1885	A1773	A1608	A1480	A1359	U	A
G2532	G2227	G2228	C	C	U2078	C1995	G1886	C1774	A1609	A1481	G1360	U	U
G2533	G2229	G2230	U	U	A2082	C1996	G1887	U1779	A1610	U1497	C1362	G1206	U
G2534	G2231	G2232	C	C	G	U1997	A1890	U1780	C1617	A1498	C1363	U	A
G2535	U2321	U2322	A	A	A2083	C2006	G1891	U1781	A	C1499	G1364	G1212	G
G2536	G2233	G2234	U	U	U2084	U2007	G1906	A1782	G1622	G1500	A1365	A1213	C
G2537	G2235	G2236	G	G	U2085	C2008	A1913	A1783	G1623	A1509	C1370	U	U
G2538	G2237	G2238	U	U	G	A2013	C1914	A1784	U1821	G1510	G1371	U	A
G2539	U2243	U2244	C	C	U	A2014	G1915	U1798	G1624	A1515	U1372	U	C
G2540	G2245	G2246	C	C	G	G2018	U1916	G1799	A1641	G1524	A1378	A1246	G
G2541	G2247	G2248	U	U	A	A2019	A1917	C1800	G1642	G1525	U1379	A1247	C
G2542	G2249	G2250	C	C	U	G2019	A1918	A1801	C1643	G1526	A1383	U	U
G2543	G	G	C	C	C	C2023	A1919	A1802	U1647	G1527	A1392	G1250	A
G2544	G2252	G2253	C	C	U	G2024	C1920	A1803	U1648	G1528	A1393	A1253	C
G2545	G2254	G2255	U	U	U	C2025	U1926	A1804	G1649	G1529	A1394	G1256	U
G2546	G2256	G2257	U	U	G	U2026	G1929	A1805	U1649	G1530	U1395	G1261	C
G2547	G2258	G2259	A	A	A	G2029	G1930	A1806	G1653	C1531	U1396	U1262	U
G2548	G2260	G2261	G	G	U	A2031	A1936	A1807	G1674	G1532	U1397	A1263	A
G2549	G2262	G2263	U	U	U	G2032	A1937	A1808	U1675	A1533	G1407	G1266	U
G2550	G2264	G2265	A	A	G	A2033	U	A1809	G1676	U1534	G1408	U	U
G2551	A2268	A2269	U	U	U	U2034	A1938	A1810	G1677	C1536	U1409	A1129	C
G2552	G2270	G2271	C	C	A	G2035	U	A1811	U1678	G1537	G1410	U1130	U
G2553	U2272	U2273	C	C	G	C2036	U1940	A1812	A1689	G1538	G1411	U1131	C
G2554	A2274	A2275	A	A	U	A2037	C1941	A1813	U1690	G1539	G1412	U1132	U
G2555	G2276	G2277	C	C	U	G2038	C1942	A1814	A1691	C1541	G1413	A1133	C
G2556	G2278	G2279	C	C	U	U2039	U1943	A1815	U1692	A1542	A1414	A1134	U
G2557	G2280	G2281	U	U	G	C2040	U1944	A1816	C1694	A1543	G1415	C1135	C
G2558	U2393	U2394	U	U	U	C2041	U1945	A1817	U1695	A1544	G1416	G1292	U
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G2560	G2397	G2398	U	U	U	C2043	U1947	A1819	U1697	A1546	G1418	U	U
G2561	G2399	G2400	U	U	G	C2044	U1948	A1820	U1698	A1547	G1419	U	U
G2562	G2401	G2402	U	U	U	U2045	U1949	A1821	U1699	A1548	G1420	U	U
G2563	U2403	U2404	C	C	U	U2046	U1950	A1822	U1700	A1549	G1421	U	U
G2564	G2405	G2406	U	U	U	U2047	U1951	A1823	U1701	A1550	G1422	U	U
G2565	G2407	G2408	C	C	U	U2048	U1952	A1824	U1702	A1551	G1423	U	U
G2566	G2409	G2410	C	C	U	U2049	U1953	A1825	U1703	A1552	G1424	U	U
G2567	U2411	U2412	U	U	U	U2050	U1954	A1826	U1704	A1553	G1425	U	U
G2568	G2413	G2414	U	U	U	U2051	U1955	A1827	U1705	A1554	G1426	U	U
G2569	G2415	G2416	C	C	U	U2052	U1956	A1828	U1706	A1555	G1427	U	U
G2570	U2417	U2418	C	C	U	U2053	U1957	A1829	U1707	A1556	G1428	U	U
G2571	G2419	G2420	C	C	U	U2054	U1958	A1830	U1708	A1557	G1429	U	U
G2572	G2421	G2422	U	U	U	U2055	U1959	A1831	U1709	A1558	G1430	U	U
G2573	G2423	G2424	C	C	U	U2056	U1960	A1832	U1710	A1559	G1431	U	U
G2574	U2425	U2426	C	C	U	U2057	U1961	A1833	U1711	A1560	G1432	U	U
G2575	G2427	G2428	U	U	U	U2058	U1962	A1834	U1712	A1561	G1433	U	U
G2576	G2429	G2430	C	C	U	U2059	U1963	A1835	U1713	A1562	G1434	U	U
G2577	U2431	U2432	C	C	U	U2060	U1964	A1836	U1714	A1563	G1435	U	U
G2578	G2433	G2434	U	U	U	U2061	U1965	A1837	U1715	A1564	G1436	U	U
G2579	G2435	G2436	C	C	U	U2062	U1966	A1838	U1716	A1565	G1437	U	U
G2580	U2437	U2438	C	C	U	U2063	U1967	A1839	U1717	A1566	G1438	U	U
G2581	G2439	G2440	U	U	U	U2064	U1968	A1840	U1718	A1567	G1439	U	U
G2582	G2441	G2442	C	C	U	U2065	U1969	A1841	U1719	A1568	G1440	U	U
G2583	U2443	U2444	C	C	U	U2066	U1970	A1842	U1720	A1569	G1441	U	U
G2584	G2445	G2446	U	U	U	U2067	U1971	A1843	U1721	A1570	G1442	U	U
G2585	G2447	G2448	C	C	U	U2068	U1972	A1844	U1722	A1571	G1443	U	U
G2586	U2449	U2450	C	C	U	U2069	U1973	A1845	U1723	A1572	G1444	U	U
G2587	G2451	G2452	U	U	U	U2070	U1974	A1846	U1724	A1573	G1445	U	U
G2588	G2453	G2454	C	C	U	U2071	U1975	A1847	U1725	A1574	G1446	U	U
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G2590	G2457	G2458	U	U	U	U2073	U1977	A1849	U1727	A1576	G1448	U	U
G2591	U2459	U2460	C	C	U	U2074	U1978	A1850	U1728	A1577	G1449	U	U
G2592	G2461	G2462	C	C	U	U2075	U1979	A1851	U1729	A1578	G1450	U	U
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G2594	G2465	G2466	C	C	U	U2077	U1981	A1853	U1731	A1580	G1452	U	U
G2595	U2467	U2468	C	C	U	U2078	U1982	A1854	U1732	A1581	G1453	U	U
G2596	G2469	G2470	U	U	U	U2079	U1983	A1855	U1733	A1582	G1454	U	U
G2597	U2471	U2472	C	C	U	U2080	U1984	A1856	U1734	A1583	G1455	U	U
G2598	G2473	G2474	C	C	U	U2081	U1985	A1857	U1735	A1584	G1456	U	U
G2599	U2475	U2476	U	U	U	U2082	U1986	A1858	U1736	A1585	G1457	U	U
G2600	G2477	G2478	C	C	U	U2083	U1987	A1859	U1737	A1586	G1458	U	U
G2601	A2479	A2480	C	C	U	U2084	U1988	A1860	U1738	A1587	G1459	U	U
G2602	U2481	U2482	U	U	U	U2085	U1989	A1861	U1739	A1588	G1460	U	U
G2603	G2483	G2484	C	C	U	U2086	U1990	A1862	U1740	A1589	G1461	U	U
G2604	U2485	U2486	C	C	U	U2087	U1991	A1863	U1741	A1590	G1462	U	U
G2605	G2487	G2488	U	U	U	U2088	U1992	A1864	U1742	A1591	G1463	U	U
G2606	A2489	A2490	C	C	U	U2089	U1993	A1865	U1743	A1592	G1464	U	U
G2607	U2491	U2492	C	C	U	U2090	U1994	A1866	U1744	A1593	G1465	U	U
G2608	G2493	G2494	U	U	U	U2091	U1995	A1867	U1745	A1594	G1466	U	U
G2609	U2495	U2496	C	C	U	U2092	U1996	A1868	U1746	A1595	G1467	U	U
G2610	G2497	G2498	C	C	U	U2093	U1997	A1869	U1747	A1596	G1468	U	U
G2611	A2499	A2500	U	U	U	U2094	U1998	A1870	U1748	A1597	G1469	U	U
G2612	U2501												



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46282	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.37	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	425.0, 425.0, 425.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 84G

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.46	1/424 (0.2%)	0.81	2/565 (0.4%)
2	1	0.25	0/380	0.41	0/498
3	2	0.22	0/513	0.43	0/676
4	3	0.23	0/303	0.48	0/397
5	4	0.24	0/488	0.51	0/649
6	B	0.21	0/1784	0.46	0/2403
7	C	0.20	0/1651	0.40	0/2225
8	D	0.19	0/1665	0.40	0/2227
9	E	0.24	0/1165	0.46	0/1568
10	F	0.22	0/858	0.44	0/1160
11	G	0.22	0/1213	0.42	0/1628
12	H	0.22	0/989	0.43	0/1326
13	I	0.26	0/1031	0.55	0/1372
14	J	0.23	0/796	0.41	0/1077
15	K	0.22	0/884	0.46	0/1191
16	L	0.26	0/957	0.48	0/1282
17	M	0.20	0/900	0.41	0/1204
18	N	0.20	0/817	0.43	0/1088
19	O	0.24	0/722	0.43	0/964
20	P	0.21	0/653	0.45	0/877
21	Q	1.21	4/650 (0.6%)	1.31	5/871 (0.6%)
22	R	0.18	0/553	0.45	0/742
23	S	0.20	0/685	0.41	0/922
24	T	0.23	0/676	0.44	0/895
25	U	0.20	0/597	0.42	0/792
26	X	0.17	0/72	0.26	0/110
27	Z	0.17	0/1813	0.33	0/2825
28	b	0.18	0/2850	0.30	0/4444
29	c	0.24	0/2121	0.43	0/2852
30	d	0.27	0/1576	0.48	0/2119
31	e	0.23	0/1571	0.40	0/2113
32	f	0.21	0/1434	0.45	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.47	3/1343 (0.2%)	0.82	6/1816 (0.3%)
34	i	0.30	0/1146	0.47	0/1544
35	j	0.26	0/955	0.57	1/1279 (0.1%)
36	k	0.25	0/1062	0.45	0/1413
37	l	0.32	0/1073	0.53	1/1433 (0.1%)
38	m	0.76	1/958 (0.1%)	1.22	7/1281 (0.5%)
39	n	0.21	0/902	0.42	0/1209
40	o	0.22	0/929	0.42	0/1242
41	p	0.27	0/436	0.55	1/578 (0.2%)
42	q	0.24	0/829	0.44	0/1107
43	s	0.22	0/736	0.40	0/984
44	t	0.21	0/787	0.42	0/1051
45	u	0.23	0/766	0.43	0/1025
46	v	0.22	0/593	0.43	0/785
47	w	0.34	0/635	0.43	0/848
48	x	0.21	0/486	0.44	0/648
49	y	0.22	0/453	0.39	0/605
50	z	0.22	0/450	0.44	0/599
51	A	0.19	1/36330 (0.0%)	0.32	0/56657
52	a	0.20	0/65703	0.31	0/102459
All	All	0.23	10/149363 (0.0%)	0.38	23/223551 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Q	32	PRO	CB-CG	22.09	2.60	1.49
38	m	50	PRO	CG-CD	-20.28	0.81	1.50
21	Q	32	PRO	CG-CD	-18.25	0.88	1.50
33	g	112	PRO	CG-CD	-8.93	1.20	1.50
1	0	41	PRO	CG-CD	-7.24	1.26	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Q	32	PRO	CB-CG-CD	-29.43	11.92	106.10
38	m	50	PRO	CB-CG-CD	23.07	179.91	106.10
38	m	50	PRO	N-CD-CG	-19.44	74.03	103.20
33	g	112	PRO	CA-N-CD	-15.69	90.04	112.00
38	m	50	PRO	CA-CB-CG	-15.44	75.17	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	9	0
2	1	377	0	418	6	0
3	2	504	0	572	14	0
4	3	302	0	340	8	0
5	4	480	0	482	26	0
6	B	1753	0	1780	50	0
7	C	1624	0	1696	28	0
8	D	1643	0	1707	26	0
9	E	1152	0	1196	26	0
10	F	839	0	833	11	0
11	G	1197	0	1243	29	0
12	H	979	0	1031	25	0
13	I	1019	0	1063	30	0
14	J	786	0	828	37	0
15	K	869	0	880	18	0
16	L	944	0	1002	30	0
17	M	891	0	952	18	0
18	N	805	0	844	19	0
19	O	714	0	734	26	0
20	P	643	0	661	21	0
21	Q	641	0	682	34	0
22	R	544	0	565	12	0
23	S	668	0	693	10	0
24	T	670	0	719	13	0
25	U	589	0	629	7	0
26	X	65	0	33	1	0
27	Z	1623	0	825	16	0
28	b	2549	0	1291	18	0
29	c	2082	0	2154	37	0
30	d	1556	0	1607	35	0
31	e	1552	0	1619	21	0
32	f	1410	0	1444	44	0
33	g	1323	0	1371	21	0
34	i	1123	0	1151	24	0
35	j	946	0	1023	21	0
36	k	1053	0	1129	33	0
37	l	1055	0	1134	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	945	0	989	19	0
39	n	892	0	923	19	0
40	o	917	0	962	19	0
41	p	431	0	454	10	0
42	q	816	0	839	15	0
43	s	730	0	795	12	0
44	t	779	0	831	19	0
45	u	753	0	780	20	0
46	v	586	0	596	14	0
47	w	625	0	652	14	0
48	x	485	0	503	7	0
49	y	449	0	488	12	0
50	z	444	0	458	10	0
51	A	32450	0	16337	409	0
52	a	58675	0	29536	426	0
53	A	38	0	0	2	0
53	a	38	0	0	1	0
All	All	137440	0	91925	1659	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 7.

The worst 5 of 1659 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)
21:Q:32:PRO:N	21:Q:32:PRO:CG	1.75	1.47
33:g:112:PRO:CB	33:g:112:PRO:CG	1.79	1.42
21:Q:32:PRO:CD	21:Q:32:PRO:HG3	1.65	1.06
21:Q:32:PRO:CG	21:Q:32:PRO:HD3	1.57	1.05
21:Q:32:PRO:CD	21:Q:32:PRO:HG2	1.65	1.04

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
2	1	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
3	2	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
4	3	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
5	4	56/70 (80%)	48 (86%)	8 (14%)	0	100	100
6	B	222/241 (92%)	197 (89%)	25 (11%)	0	100	100
7	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
8	D	203/206 (98%)	188 (93%)	15 (7%)	0	100	100
9	E	154/167 (92%)	140 (91%)	14 (9%)	0	100	100
10	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
11	G	151/179 (84%)	140 (93%)	11 (7%)	0	100	100
12	H	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
13	I	125/130 (96%)	110 (88%)	14 (11%)	1 (1%)	16	51
14	J	96/103 (93%)	88 (92%)	8 (8%)	0	100	100
15	K	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
16	L	118/124 (95%)	104 (88%)	13 (11%)	1 (1%)	16	51
17	M	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
18	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
19	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
20	P	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
21	Q	77/84 (92%)	65 (84%)	12 (16%)	0	100	100
22	R	64/75 (85%)	57 (89%)	7 (11%)	0	100	100
23	S	82/92 (89%)	76 (93%)	6 (7%)	0	100	100
24	T	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
25	U	68/71 (96%)	68 (100%)	0	0	100	100
29	c	269/273 (98%)	249 (93%)	20 (7%)	0	100	100
30	d	204/209 (98%)	191 (94%)	13 (6%)	0	100	100
31	e	199/201 (99%)	175 (88%)	24 (12%)	0	100	100
32	f	175/179 (98%)	158 (90%)	17 (10%)	0	100	100
33	g	174/177 (98%)	153 (88%)	20 (12%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	i	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
35	j	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
36	k	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
37	l	130/136 (96%)	124 (95%)	5 (4%)	1 (1%)	16	51
38	m	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
39	n	114/117 (97%)	99 (87%)	15 (13%)	0	100	100
40	o	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
41	p	52/118 (44%)	37 (71%)	15 (29%)	0	100	100
42	q	101/103 (98%)	90 (89%)	11 (11%)	0	100	100
43	s	90/100 (90%)	81 (90%)	9 (10%)	0	100	100
44	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
45	u	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
46	v	76/85 (89%)	70 (92%)	6 (8%)	0	100	100
47	w	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
48	x	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
49	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
50	z	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
All	All	5263/5654 (93%)	4828 (92%)	431 (8%)	4 (0%)	50	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	g	128	GLN
37	l	84	LYS
13	I	13	LYS
16	L	44	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	55 (100%)	0	100	100
6	B	186/199 (94%)	184 (99%)	2 (1%)	70	86
7	C	170/190 (90%)	169 (99%)	1 (1%)	84	92
8	D	172/173 (99%)	170 (99%)	2 (1%)	67	85
9	E	119/126 (94%)	117 (98%)	2 (2%)	56	78
10	F	90/116 (78%)	90 (100%)	0	100	100
11	G	125/147 (85%)	124 (99%)	1 (1%)	79	90
12	H	104/105 (99%)	104 (100%)	0	100	100
13	I	104/107 (97%)	104 (100%)	0	100	100
14	J	86/90 (96%)	86 (100%)	0	100	100
15	K	89/99 (90%)	88 (99%)	1 (1%)	70	86
16	L	101/104 (97%)	100 (99%)	1 (1%)	73	87
17	M	93/96 (97%)	92 (99%)	1 (1%)	70	86
18	N	83/84 (99%)	82 (99%)	1 (1%)	67	85
19	O	76/77 (99%)	76 (100%)	0	100	100
20	P	65/65 (100%)	65 (100%)	0	100	100
21	Q	73/78 (94%)	73 (100%)	0	100	100
22	R	57/65 (88%)	57 (100%)	0	100	100
23	S	72/79 (91%)	72 (100%)	0	100	100
24	T	65/66 (98%)	64 (98%)	1 (2%)	60	81
25	U	60/61 (98%)	60 (100%)	0	100	100
29	c	216/218 (99%)	216 (100%)	0	100	100
30	d	163/164 (99%)	161 (99%)	2 (1%)	67	85
31	e	165/165 (100%)	165 (100%)	0	100	100
32	f	148/150 (99%)	147 (99%)	1 (1%)	81	92
33	g	137/138 (99%)	135 (98%)	2 (2%)	60	81
34	i	115/116 (99%)	115 (100%)	0	100	100
35	j	104/104 (100%)	103 (99%)	1 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	103/103 (100%)	102 (99%)	1 (1%)	73	87
37	l	107/109 (98%)	106 (99%)	1 (1%)	75	89
38	m	98/103 (95%)	98 (100%)	0	100	100
39	n	86/87 (99%)	86 (100%)	0	100	100
40	o	99/100 (99%)	99 (100%)	0	100	100
41	p	37/90 (41%)	37 (100%)	0	100	100
42	q	84/84 (100%)	83 (99%)	1 (1%)	67	85
43	s	79/84 (94%)	78 (99%)	1 (1%)	65	83
44	t	83/85 (98%)	83 (100%)	0	100	100
45	u	78/78 (100%)	78 (100%)	0	100	100
46	v	58/63 (92%)	57 (98%)	1 (2%)	56	78
47	w	67/68 (98%)	67 (100%)	0	100	100
48	x	51/55 (93%)	51 (100%)	0	100	100
49	y	48/49 (98%)	48 (100%)	0	100	100
50	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4387/4623 (95%)	4363 (100%)	24 (0%)	85	93

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	d	129	THR
33	g	131	ILE
33	g	116	GLN
35	j	118	LEU
9	E	141	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
34	i	40	HIS
39	n	116	GLN
34	i	80	HIS
37	l	13	HIS
42	q	91	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	X	2/28 (7%)	0	0
27	Z	75/76 (98%)	10 (13%)	0
28	b	118/120 (98%)	16 (13%)	0
51	A	1503/1542 (97%)	288 (19%)	9 (0%)
52	a	2711/2904 (93%)	357 (13%)	0
All	All	4409/4670 (94%)	671 (15%)	9 (0%)

5 of 671 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	Z	6	G
27	Z	9	G
27	Z	17(A)	U
27	Z	18	G
27	Z	19	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	A	1299	A
51	A	1518	A
51	A	326	G
51	A	445	G
51	A	466	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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
53	84G	A	1601	-	39,40,40	1.87	8 (20%)	48,57,57	1.21	5 (10%)
53	84G	a	3001	-	39,40,40	1.85	7 (17%)	48,57,57	1.13	6 (12%)

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
53	84G	A	1601	-	-	4/23/76/76	0/3/3/3
53	84G	a	3001	-	-	7/23/76/76	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	1601	84G	C3-N1	7.25	1.49	1.34
53	a	3001	84G	C3-N1	6.37	1.47	1.34
53	a	3001	84G	C21-C20	-4.56	1.47	1.53
53	A	1601	84G	C21-C20	-3.78	1.48	1.53
53	a	3001	84G	C19-C20	-3.66	1.48	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	1601	84G	C16-O5-C15	-3.71	109.17	117.98
53	A	1601	84G	C8-O2-C7	-3.26	110.25	117.98
53	a	3001	84G	O6-C17-C19	2.39	114.01	109.70
53	a	3001	84G	C-C1-C2	-2.39	109.26	112.52
53	a	3001	84G	C7-C14-C15	2.36	113.89	109.11

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	a	3001	84G	C-C1-C2-O

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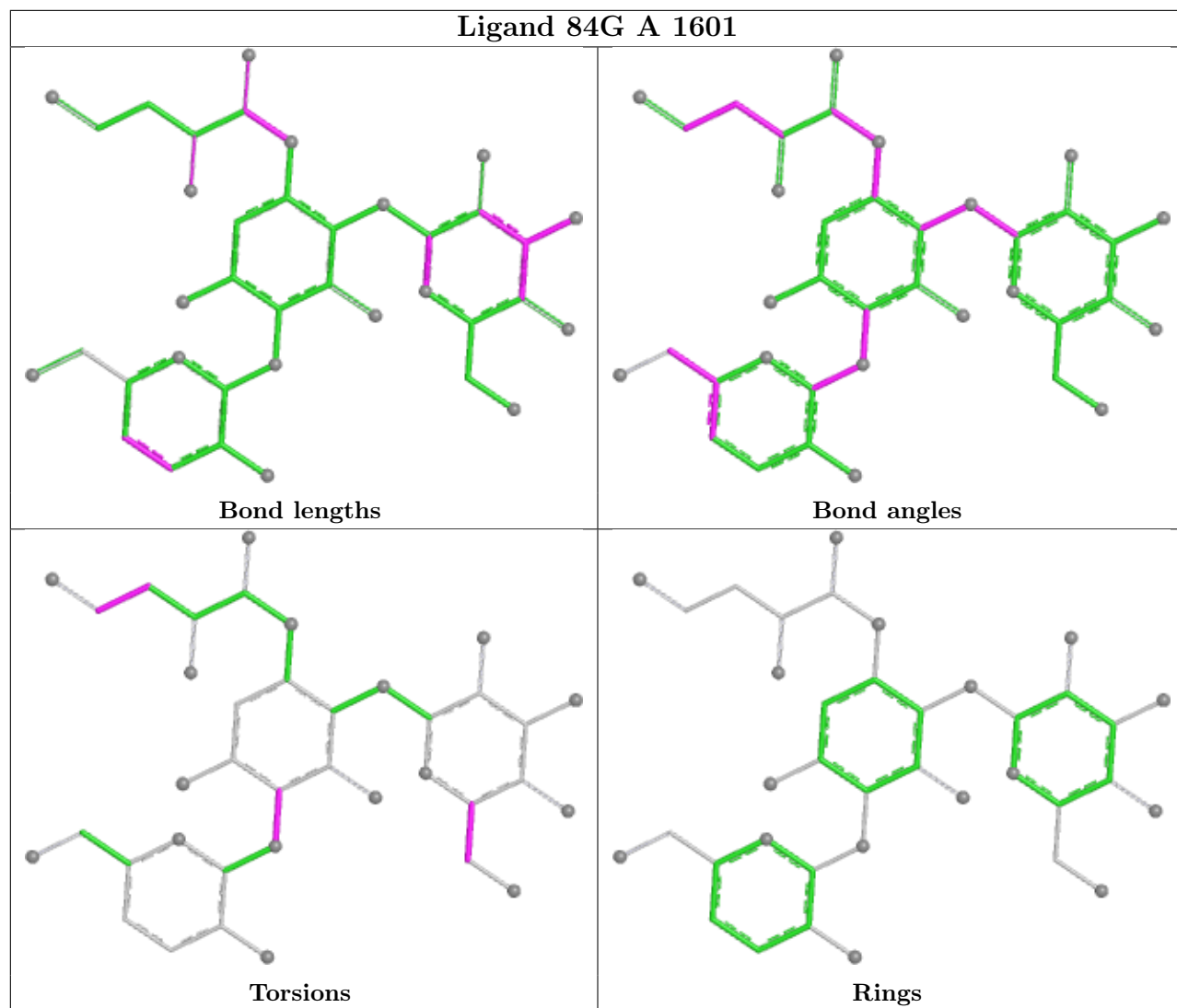
Mol	Chain	Res	Type	Atoms
53	a	3001	84G	N3-C10-C9-O3
53	a	3001	84G	N3-C10-C9-C11
53	a	3001	84G	O6-C17-C18-O7
53	A	1601	84G	C19-C17-C18-O7

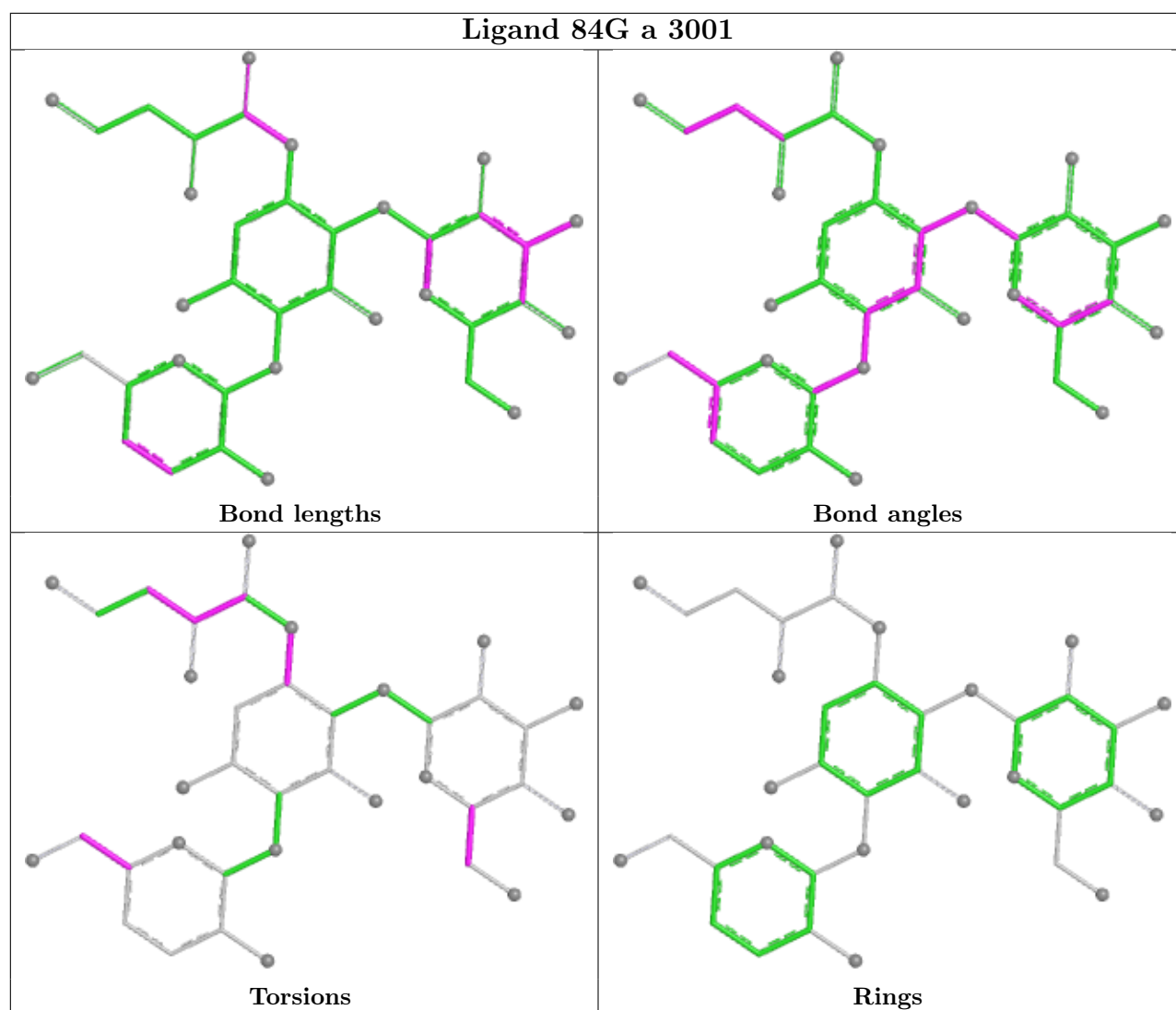
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	A	1601	84G	2	0
53	a	3001	84G	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

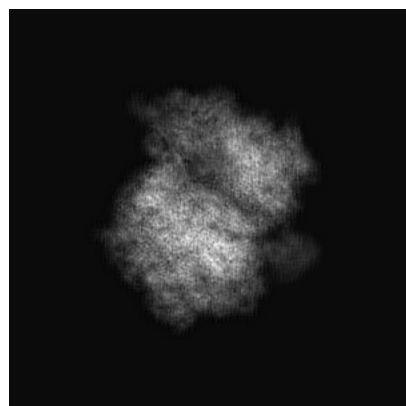
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48329. These allow visual inspection of the internal detail of the map and identification of artifacts.

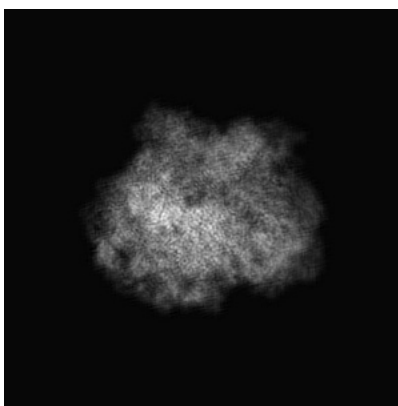
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

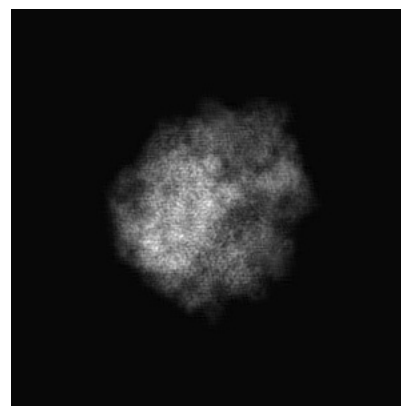
6.1.1 Primary map



X

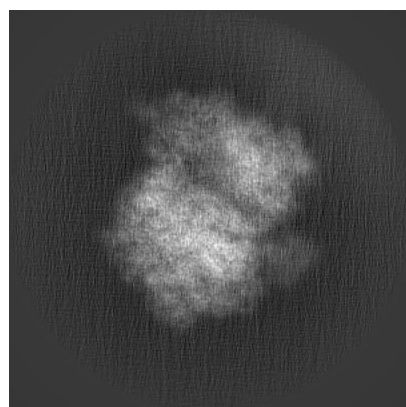


Y

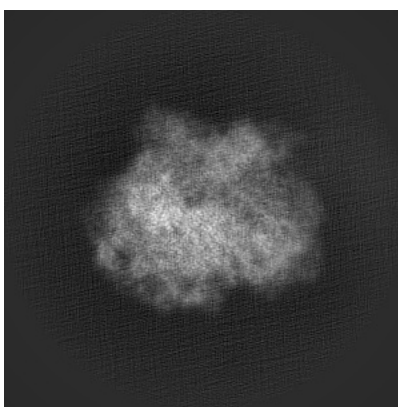


Z

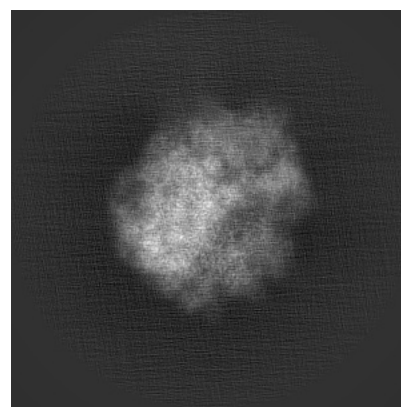
6.1.2 Raw map



X



Y

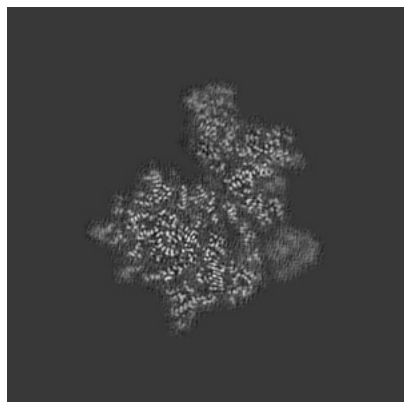


Z

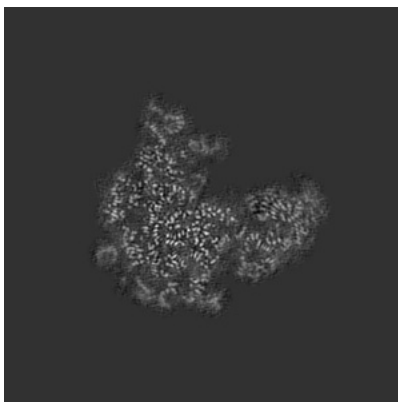
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

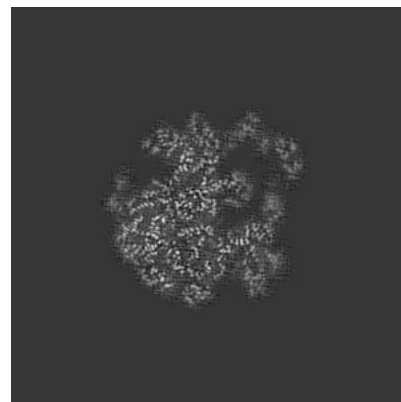
6.2.1 Primary map



X Index: 250

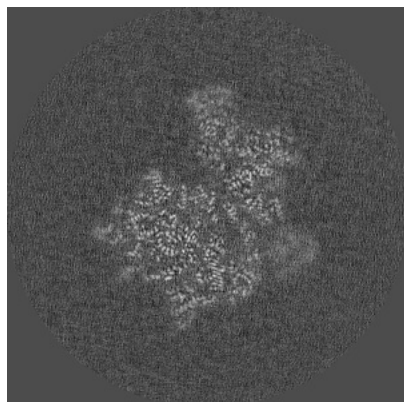


Y Index: 250

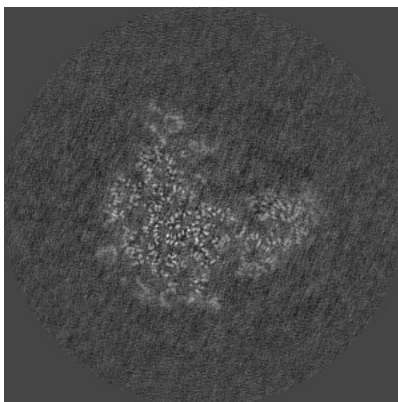


Z Index: 250

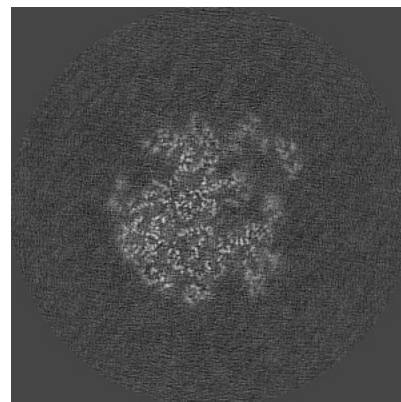
6.2.2 Raw map



X Index: 250



Y Index: 250

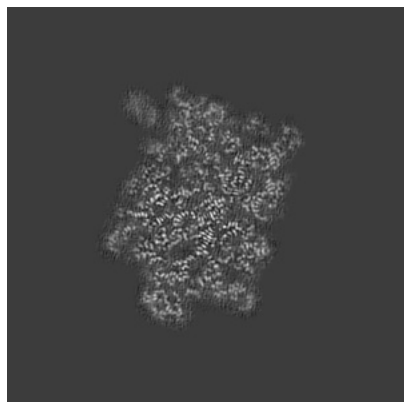


Z Index: 250

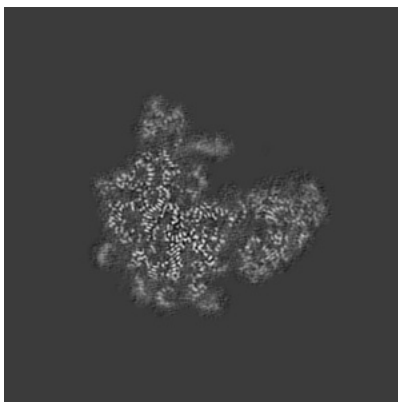
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

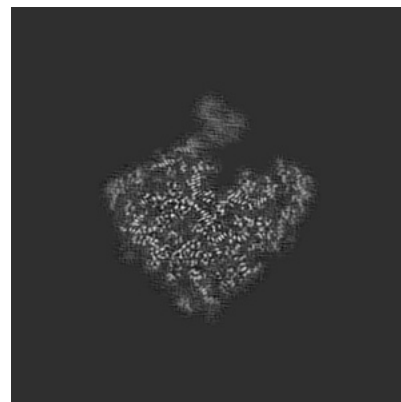
6.3.1 Primary map



X Index: 212

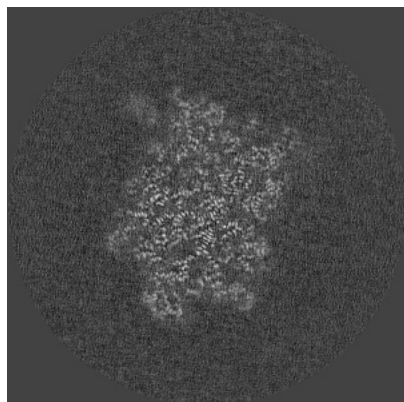


Y Index: 255

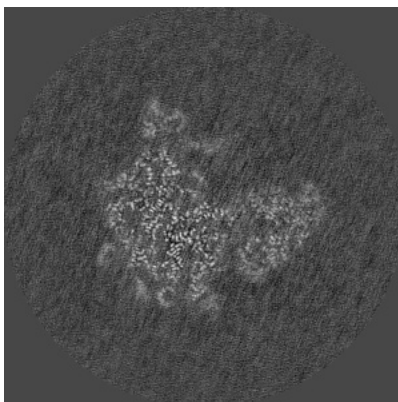


Z Index: 205

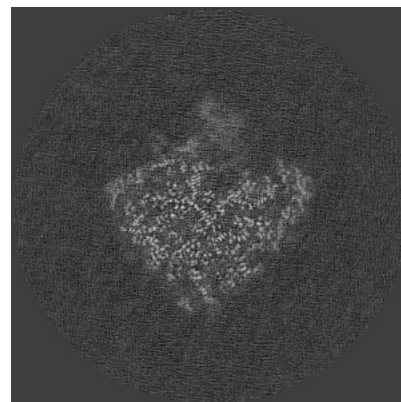
6.3.2 Raw map



X Index: 212



Y Index: 254

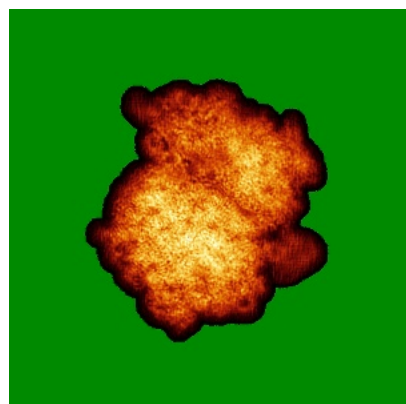


Z Index: 205

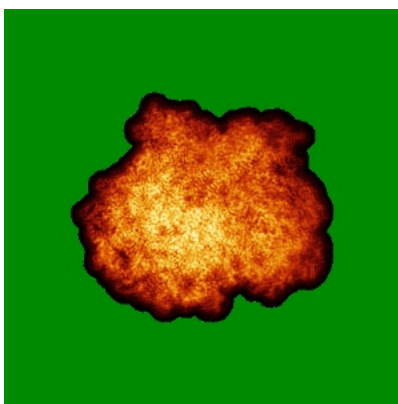
The images above show the largest variance slices of the map in three orthogonal directions.

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

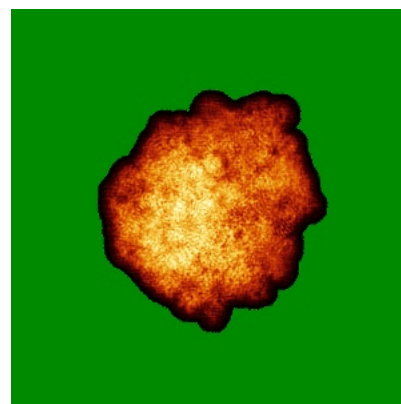
6.4.1 Primary map



X

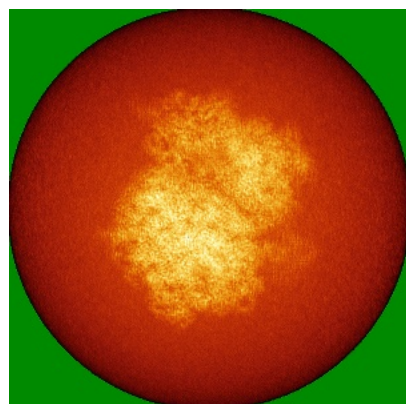


Y

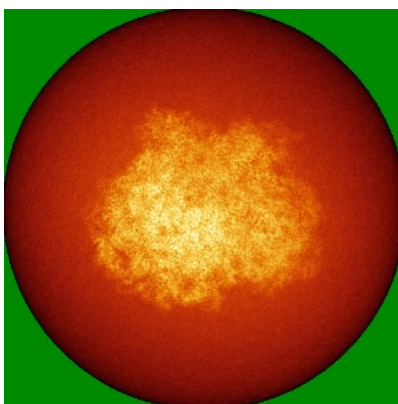


Z

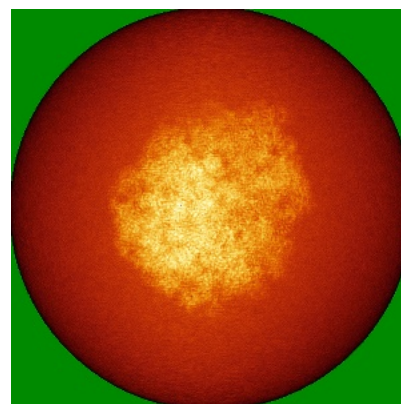
6.4.2 Raw map



X



Y

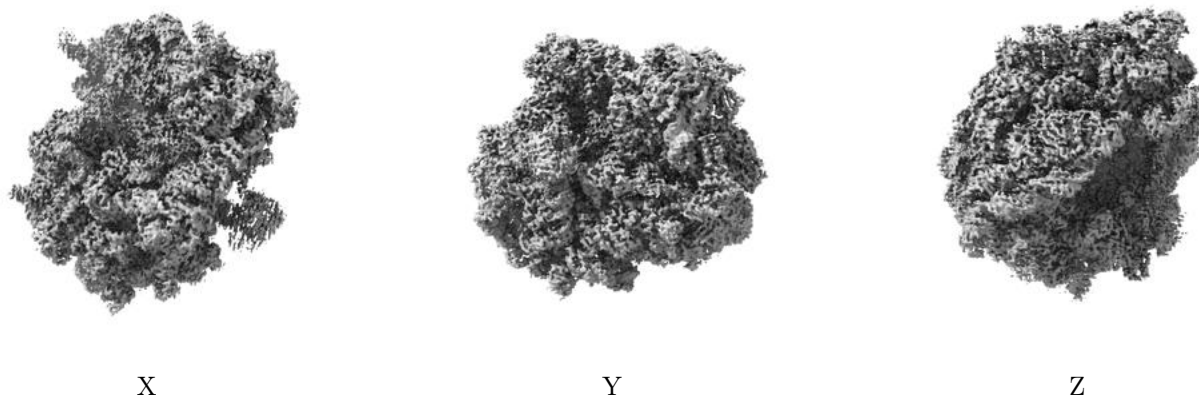


Z

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

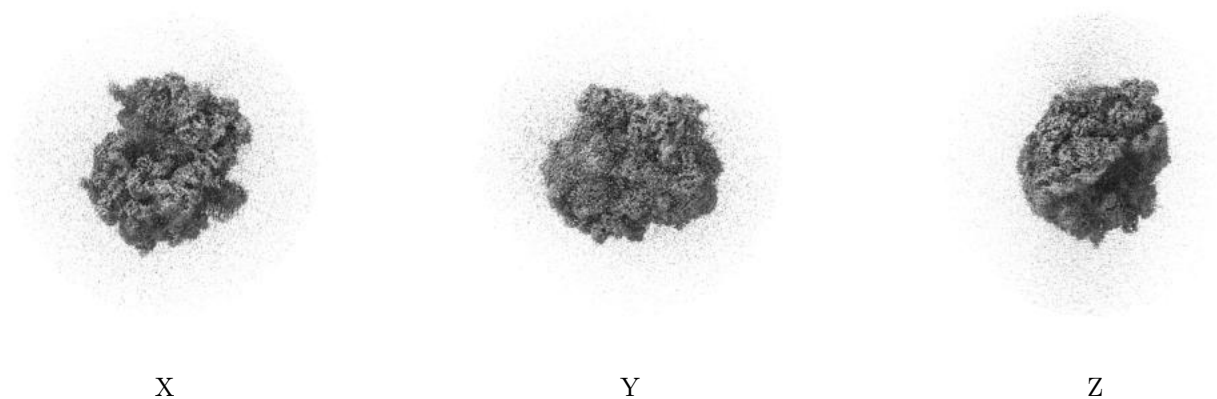
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

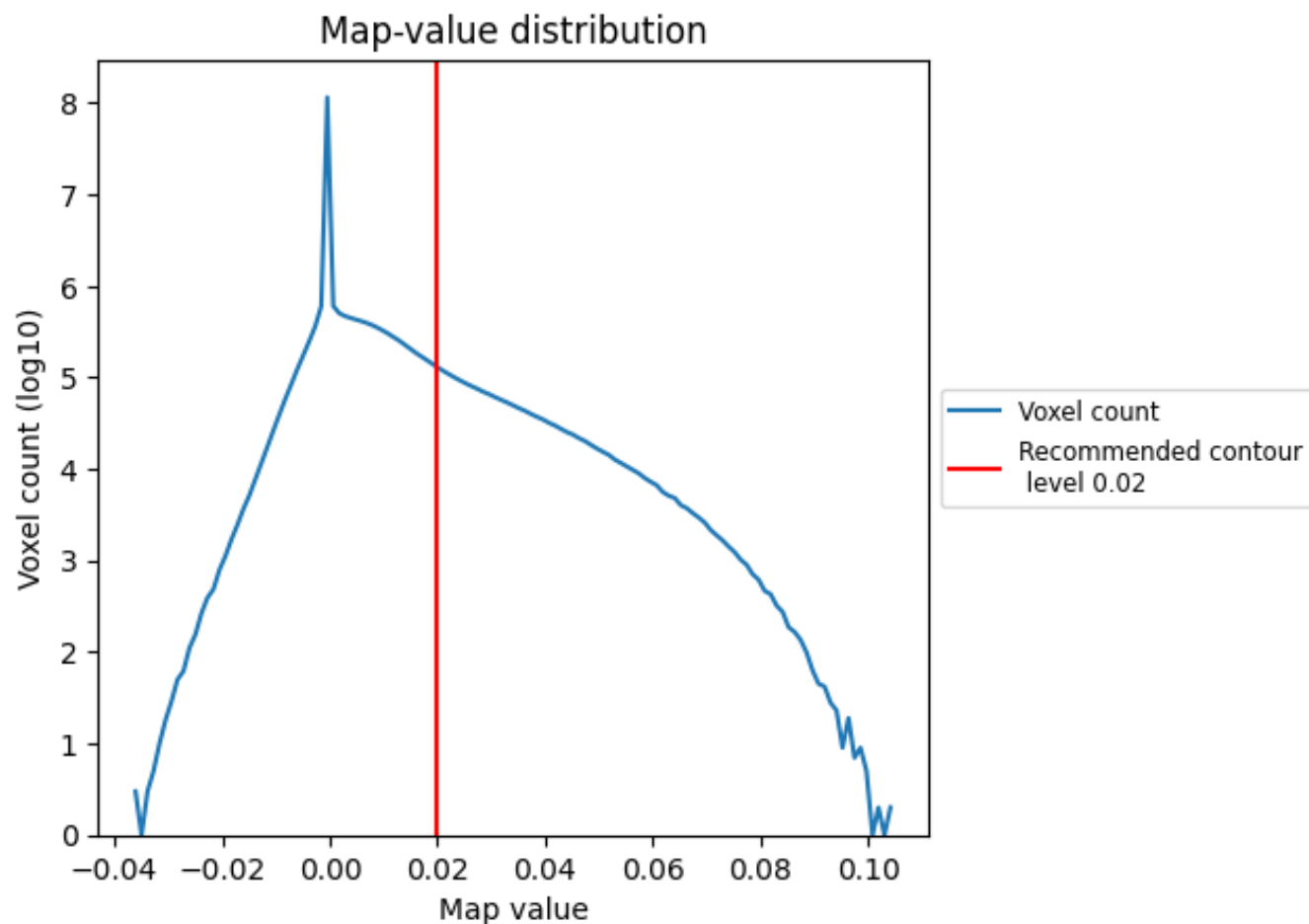
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

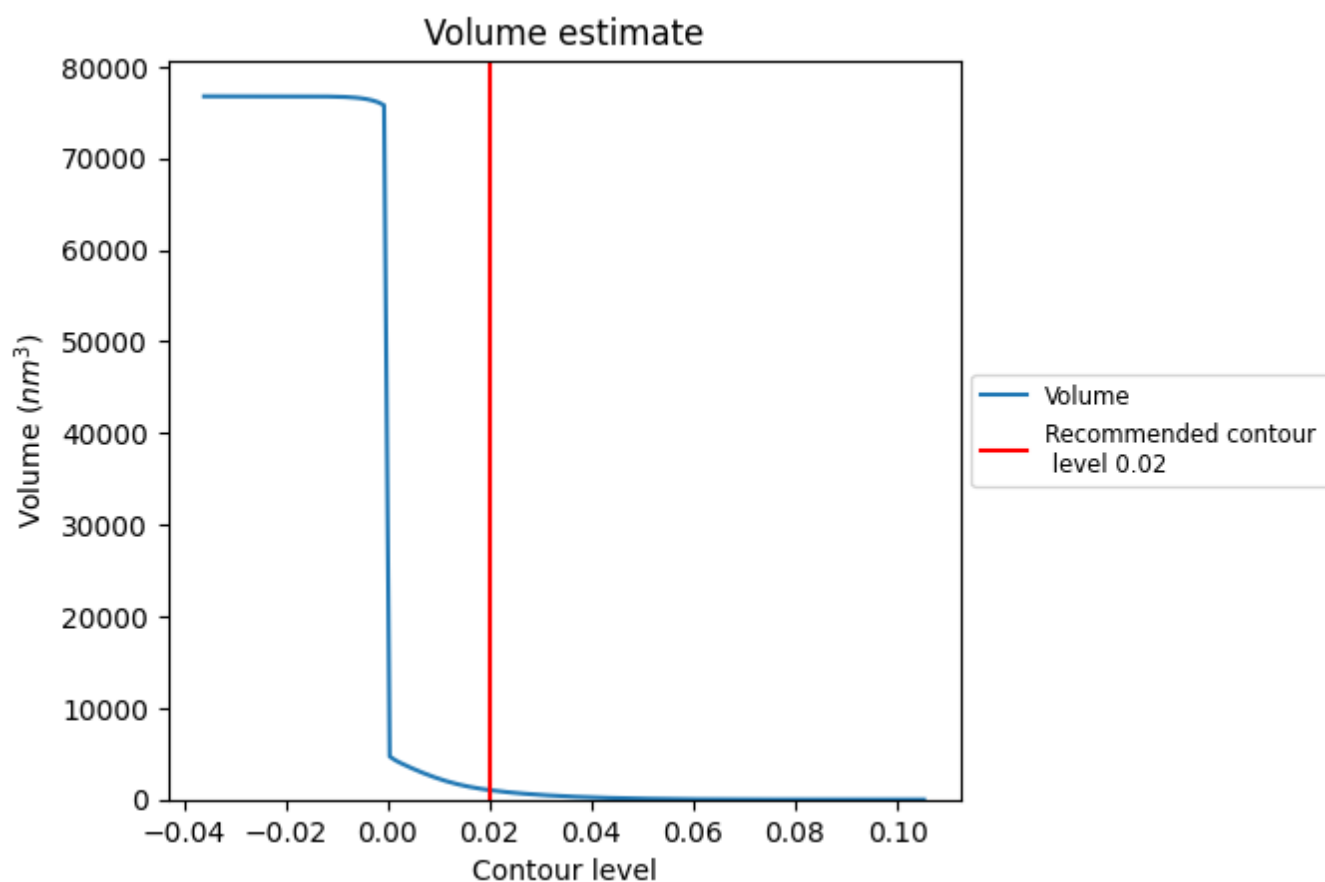
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

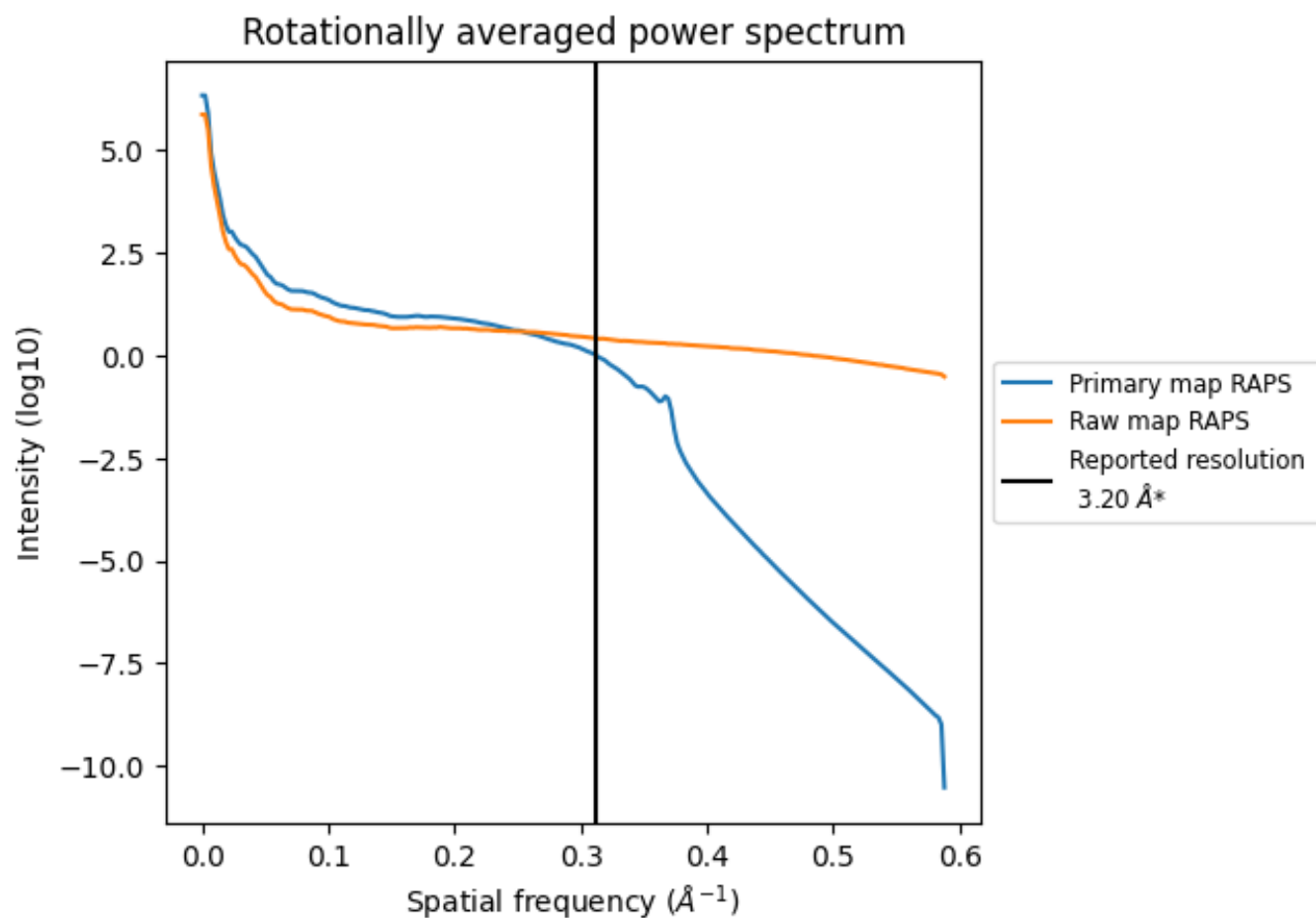
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1035 nm³; this corresponds to an approximate mass of 935 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 ⓘ

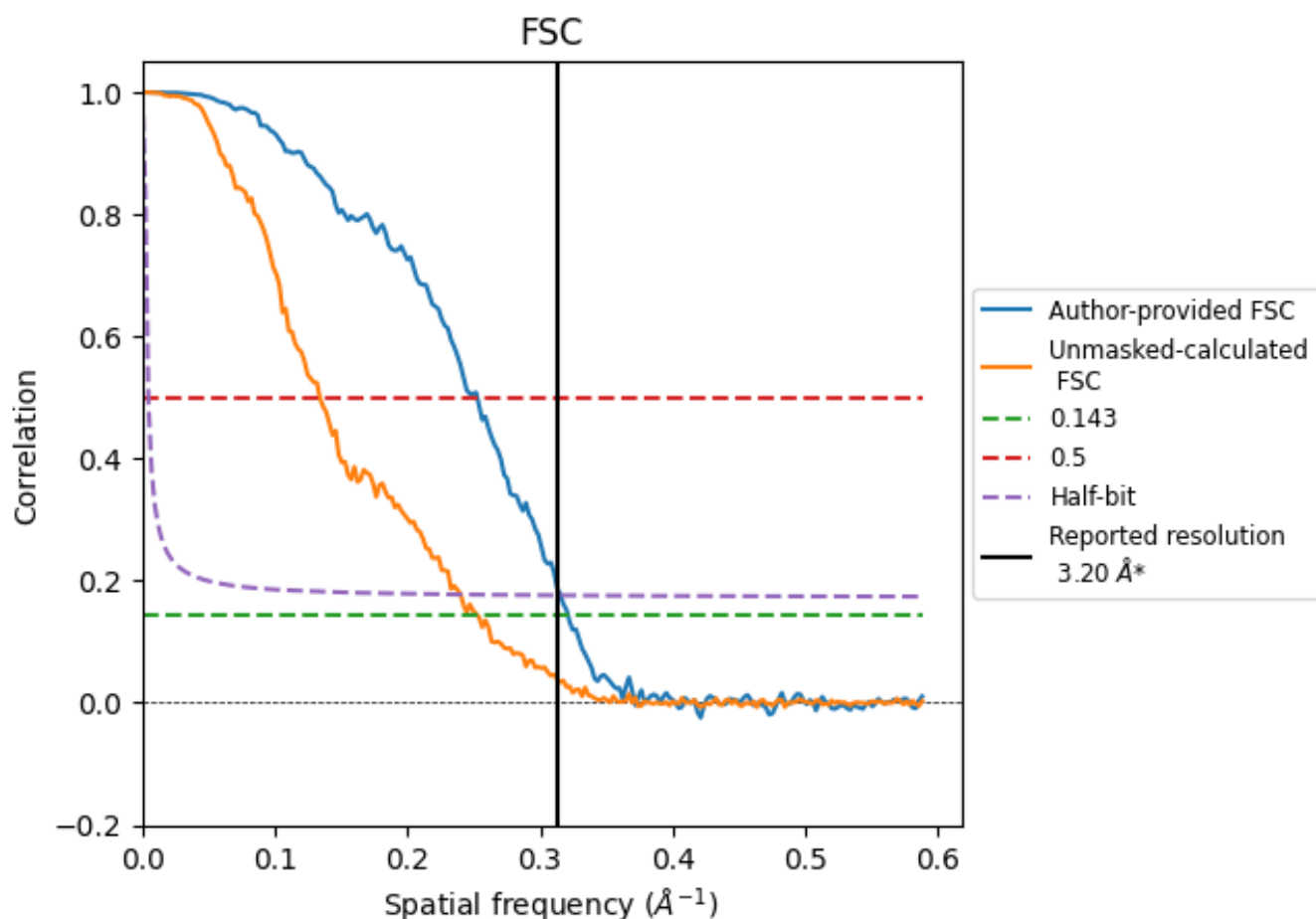


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

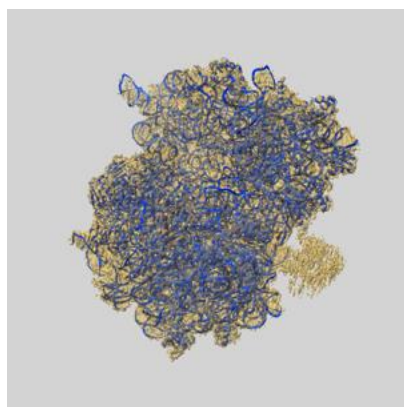
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.11	3.96	3.17
Unmasked-calculated*	3.96	7.46	4.16

*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 3.96 differs from the reported value 3.2 by more than 10 %

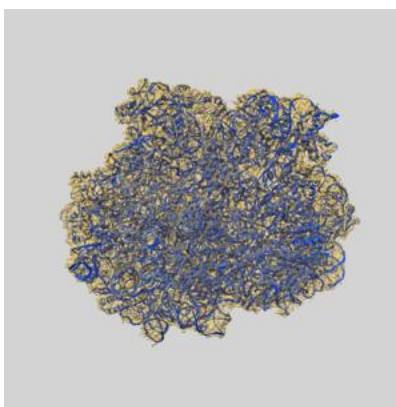
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48329 and PDB model 9MKK. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

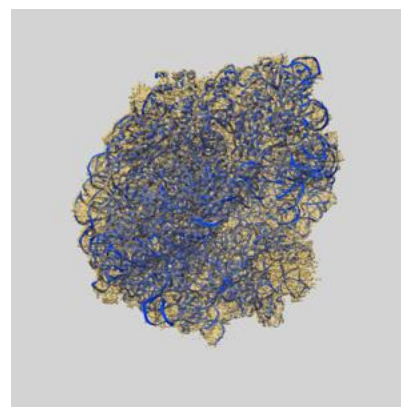
9.1 Map-model overlay [i](#)



X



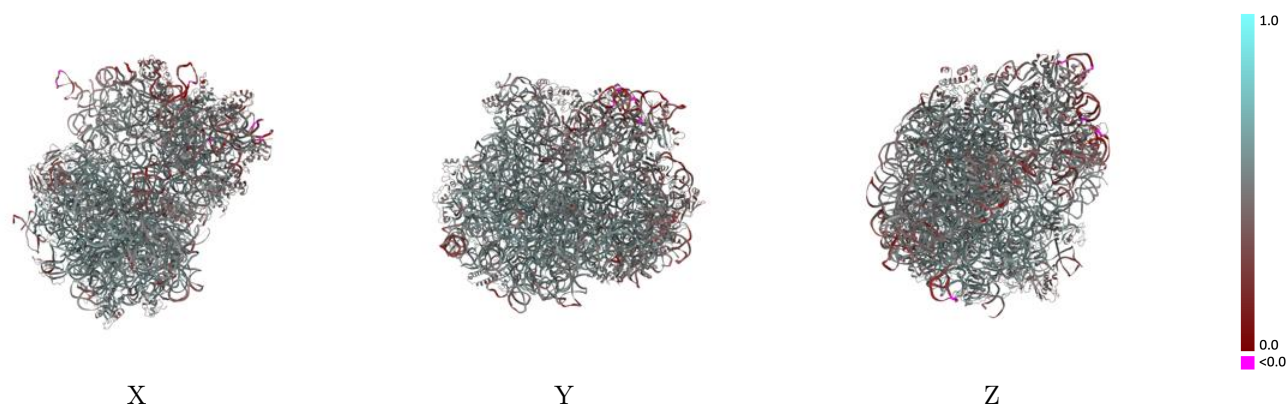
Y



Z

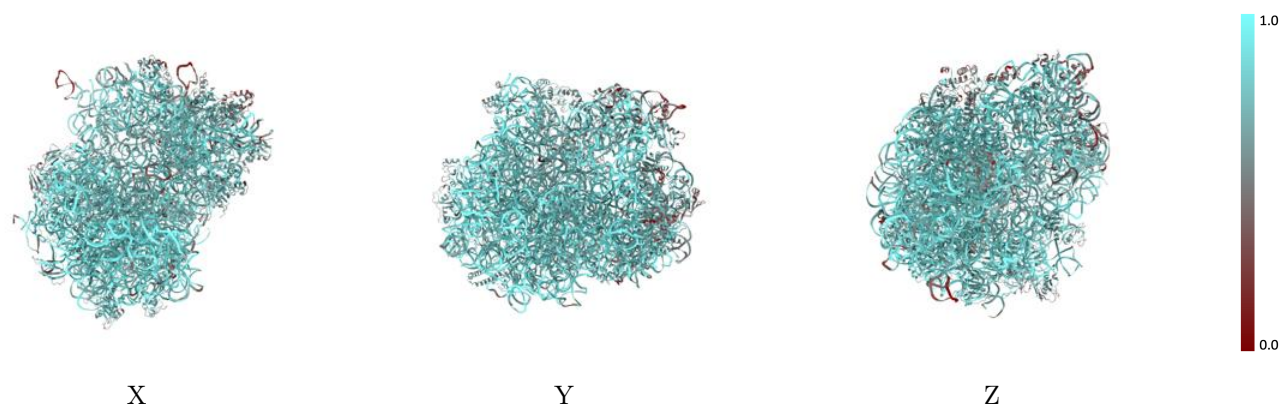
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



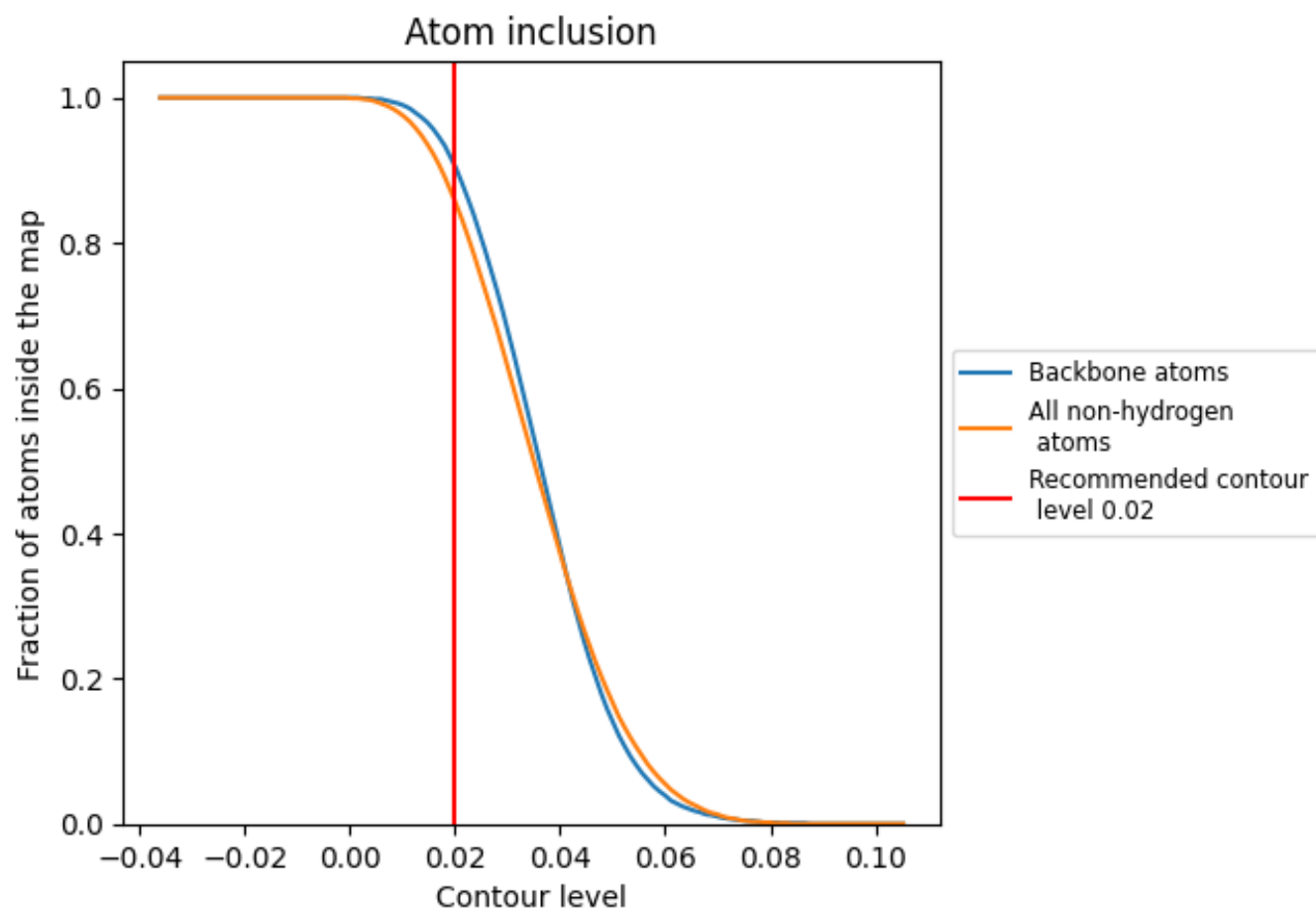
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.5030
0	 0.7310	 0.4900
1	 0.8930	 0.5630
2	 0.8600	 0.5420
3	 0.8250	 0.5070
4	 0.5880	 0.4020
A	 0.8730	 0.4720
B	 0.4890	 0.4100
C	 0.7230	 0.4720
D	 0.6260	 0.4240
E	 0.7700	 0.5000
F	 0.6780	 0.4620
G	 0.6710	 0.4400
H	 0.7530	 0.4890
I	 0.6990	 0.4560
J	 0.6030	 0.4260
K	 0.7630	 0.4990
L	 0.7140	 0.4550
M	 0.6890	 0.4610
N	 0.7560	 0.4640
O	 0.7840	 0.5020
P	 0.7330	 0.4480
Q	 0.6640	 0.4350
R	 0.7210	 0.4720
S	 0.7120	 0.4560
T	 0.7050	 0.4420
U	 0.6300	 0.4310
X	 0.9540	 0.5530
Z	 0.7980	 0.4710
a	 0.9350	 0.5370
b	 0.9120	 0.5030
c	 0.8490	 0.5510
d	 0.8160	 0.5250
e	 0.7740	 0.5080
f	 0.6690	 0.4390



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Chain	Atom inclusion	Q-score
g	 0.6310	 0.4180
i	 0.8060	 0.5160
j	 0.7560	 0.5200
k	 0.7820	 0.5090
l	 0.8190	 0.5210
m	 0.8820	 0.5420
n	 0.7390	 0.4660
o	 0.7700	 0.5240
p	 0.8700	 0.4920
q	 0.7790	 0.4970
s	 0.7630	 0.4960
t	 0.7510	 0.4770
u	 0.7240	 0.4830
v	 0.8270	 0.5270
w	 0.8050	 0.4980
x	 0.7420	 0.4740
y	 0.7800	 0.5070
z	 0.7990	 0.5080