



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 02:35 pm BST

PDB ID : 7PJU / pdb_00007pju
EMDB ID : EMD-13460
Title : Structure of the 70S ribosome with tRNAs in hybrid state 2 (H2)
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.;
Fischer, N.
Deposited on : 2021-08-24
Resolution : 9.50 Å (reported)
Based on initial models : 5LZD, 4AQY, 6YSS

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

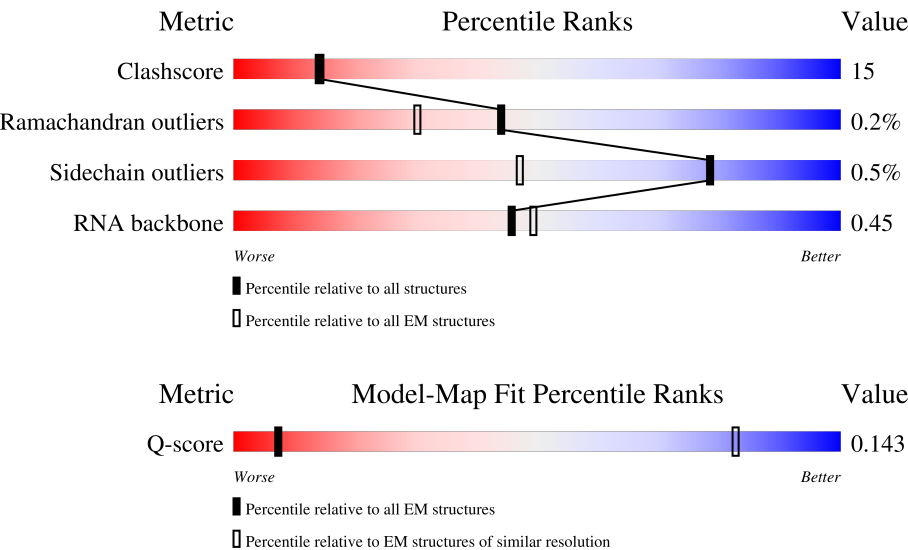
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 9.50 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	234 (9.00 - 10.00)

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	57	37% 65% 33% .
2	1	55	16% 58% 33% 9%
3	2	46	20% 74% 26%

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Mol	Chain	Length	Quality of chain
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	
9	B	120	
10	C	273	
11	D	209	
12	E	201	
13	F	179	
14	G	177	
15	H	149	
16	I	142	
17	J	142	
18	K	123	
19	L	144	
20	M	136	
21	N	127	
22	O	117	
23	P	115	
24	Q	118	
25	R	103	
26	S	110	
27	T	100	
28	U	104	

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Mol	Chain	Length	Quality of chain
29	V	94	
30	W	85	
31	X	78	
32	Y	63	
33	Z	59	
34	a	1542	
35	b	240	
36	c	233	
37	d	206	
38	e	167	
39	f	135	
40	g	179	
41	h	130	
42	i	130	
43	j	103	
44	k	129	
45	l	124	
46	m	118	
47	n	102	
48	o	89	
49	p	82	
50	q	84	
51	r	75	
52	s	92	
53	t	87	

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Mol	Chain	Length	Quality of chain
54	u	71	
55	v	77	
56	w	76	
57	y	2	
58	z	33	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	FME	y	101	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 147243 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 L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	131	Total	C	N	O	0	0
			647	385	131	131		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2903	Total	C	N	O	P	0	0
			62339	27816	11471	20149	2903		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 16 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	141	Total	C	N	O		0	0
			693	411	141	141			

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

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

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

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

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

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

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called Ribosomal protein L22.

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

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

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

- Molecule 28 is a protein called Ribosomal protein L24.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total	C	N	O	S		
			575	356	116	102	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

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

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P		
			33050	14748	6057	10705	1540	0	0

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called Ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

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

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a RNA chain called P-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	2	Total	C	N	O	S	0	0
			20	15	2	2	1		

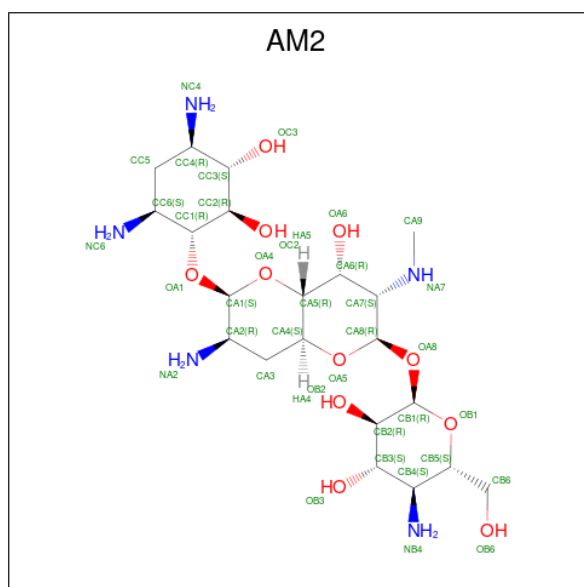
- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	11	Total	C	N	O	P	0	0
			230	103	35	81	11		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	4	1	Total	Zn	0
			1	1	
59	6	1	Total	Zn	0
			1	1	

- Molecule 60 is APRAMYCIN (CCD ID: AM2) (formula: C₂₁H₄₁N₅O₁₁).

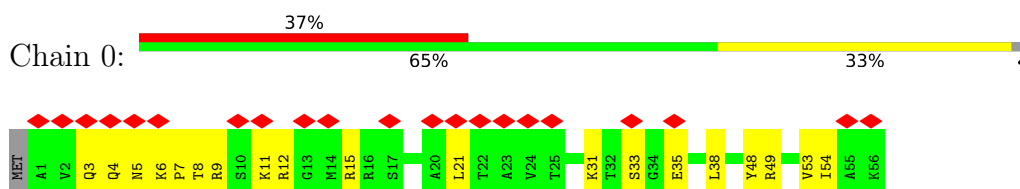


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
60	a	1	37	21	5	11	0

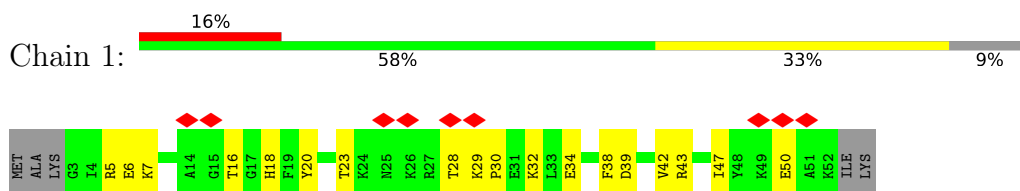
3 Residue-property plots [i](#)

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.

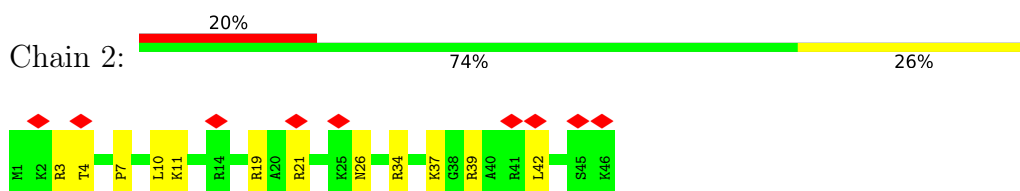
- Molecule 1: 50S ribosomal protein L32



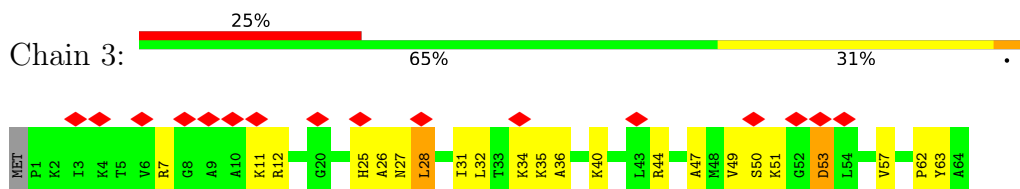
- Molecule 2: 50S ribosomal protein L33



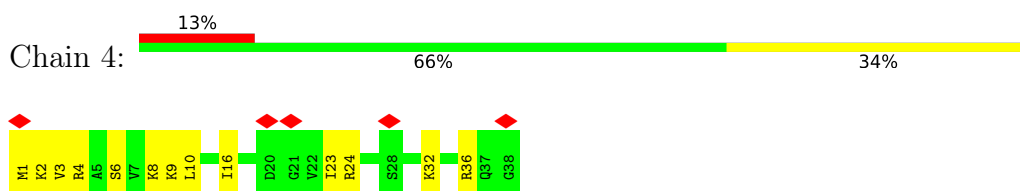
- Molecule 3: 50S ribosomal protein L34



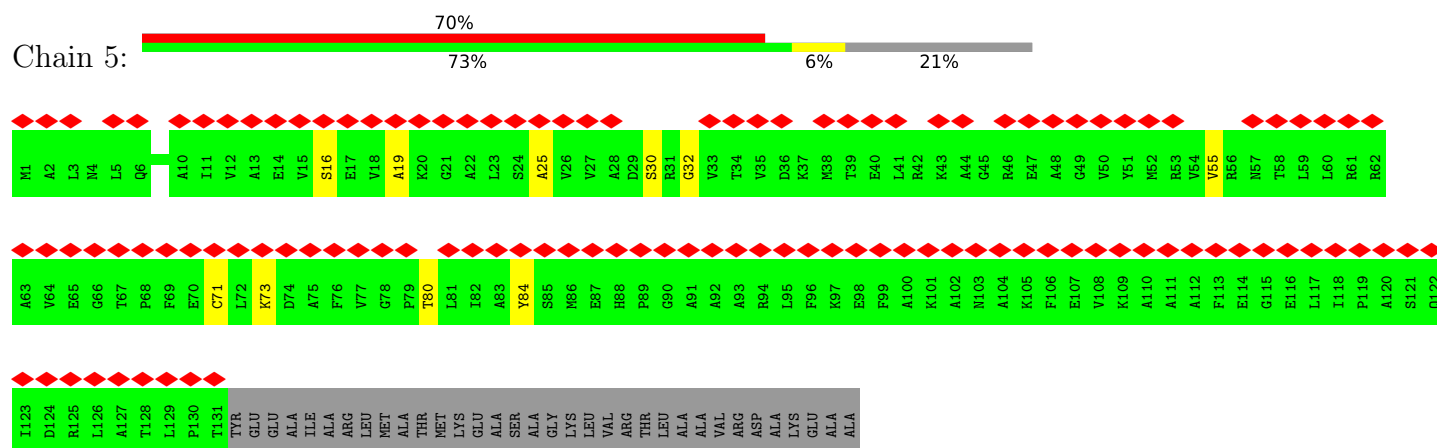
- Molecule 4: 50S ribosomal protein L35



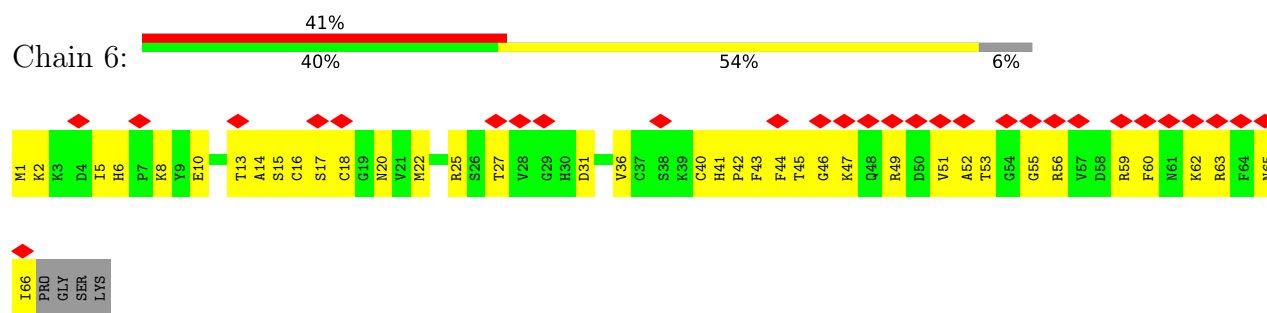
- Molecule 5: 50S ribosomal protein L36



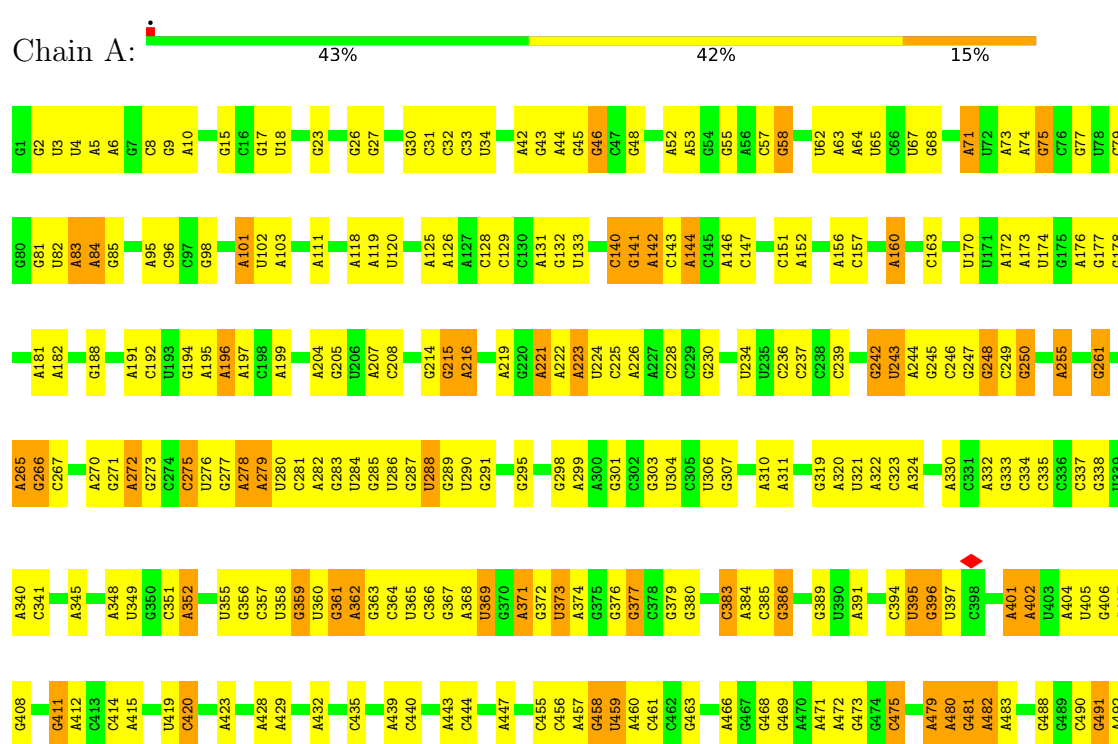
- Molecule 6: 50S ribosomal protein L10



- Molecule 7: 50S ribosomal protein L31

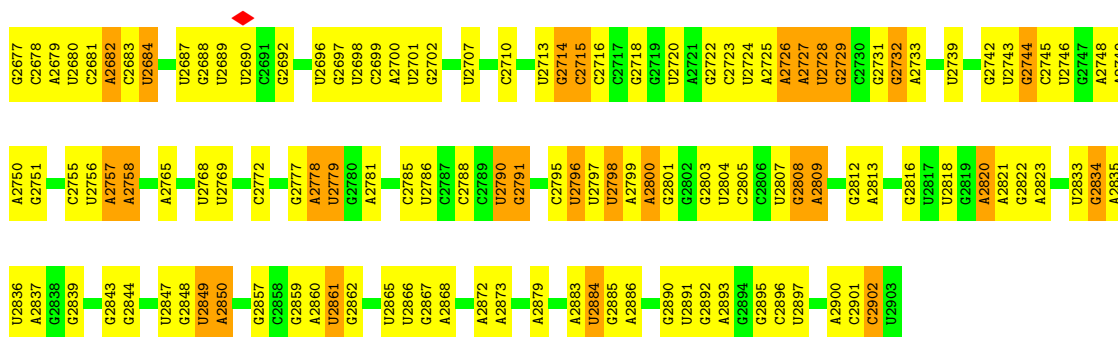


- Molecule 8: 23S ribosomal RNA



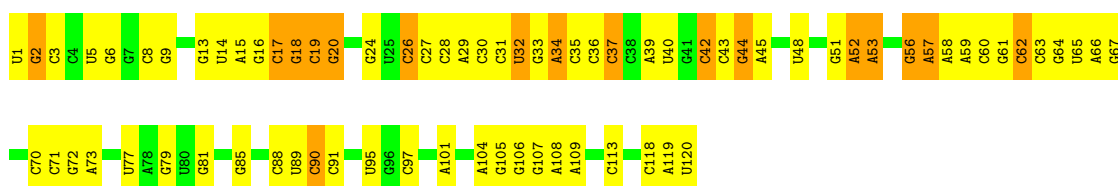


U2605	G2606	G2607	U2608	G2609	C2610	G2611	G2612	U2613	A2614	U2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	U2629	G2630	G2631	G2632	G2633	A2634	U2635	G2636	U2637	G2638	G2639	U2640	G2641	G2642	G2643	G2644	G2645	G2646	U2647	G2648	U2649	U2650	C2651	A2652	G2653	U2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	A2670	G2671	G2672	G2673	G2674	G2675	G2676																				
G1715	U1716	A1717	U1720	G1721	A1722	G1723	G1724	U1725	G1726	G1727	G1728	U1729	G1730	G1731	G1732	G1733	G1734	G1735	U1736	G1737	G1738	A1739	G1740	C1741	A1745	A1746	U1747	U1751	C1752	G1753	A1754	G1755	A1756	A1757	U1758	G1759	C1760	G1763	C1764	U1769	G1681	G1682	U1683	G1684	C1685	U1693	G1707	A1783	A1784	U1709	G1710	A1786	A1787	C1788																																					
A1789	C1790	A1791	A1794	G1795	U1796	G1797	U1798	G1799	C1800	A1801	A1802	A1803	G1807	G1808	A1809	A1810	G1811	U1812	G1813	G1816	G1817	U1818	G1824	U1827	G1828	A1829	G1835	G1838	U1841	G1842	C1843	C1844	G1845	G1846	G1847	A1848	G1849	A1853	A1854	G1857	A1858	U1859	G1860	G1861	G1862	U1863	U1864	U1865	A1866																																										
G1869	C1870	A1871	A1872	G1873	C1874	C1879	U1880	U1883	G1884	A1885	U1886	C1887	G1888	A1889	A1890	C1894	C1895	U1898	A1899	A1900	A1901	C1902	G1906	G1907	C1908	G1909	G1910	U1911	A1912	A1913	C1914	G1915	A1916	U1917	A1918	A1919	C1920	G1921	A1922	U1923	C1924	A1925	U1926	A1927	G1928	U1929	G1930	U1931	A1932	G1933	A1936	A1937																																							
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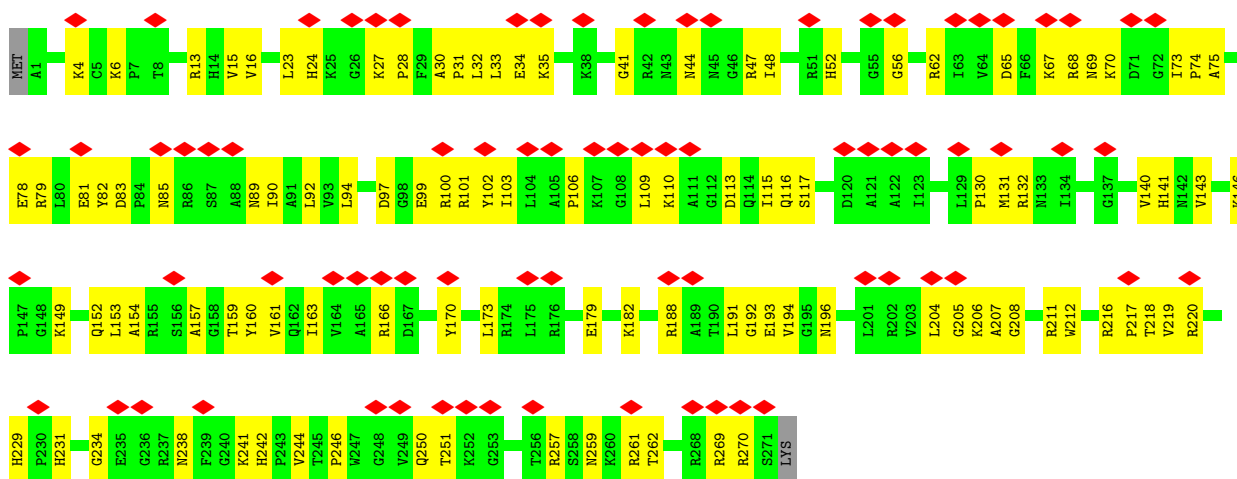
• Molecule 9: 5S ribosomal RNA

Chain B: 38% 48% 14%



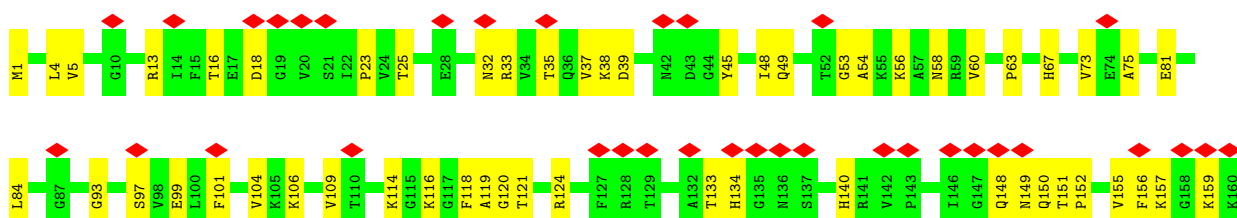
• Molecule 10: 50S ribosomal protein L2

Chain C: 29% 60% 40%



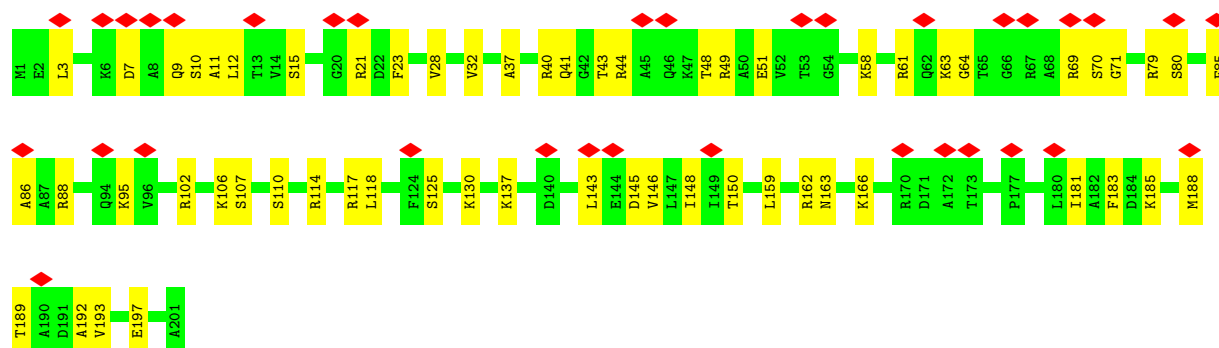
• Molecule 11: 50S ribosomal protein L3

Chain D: 25% 68% 32%

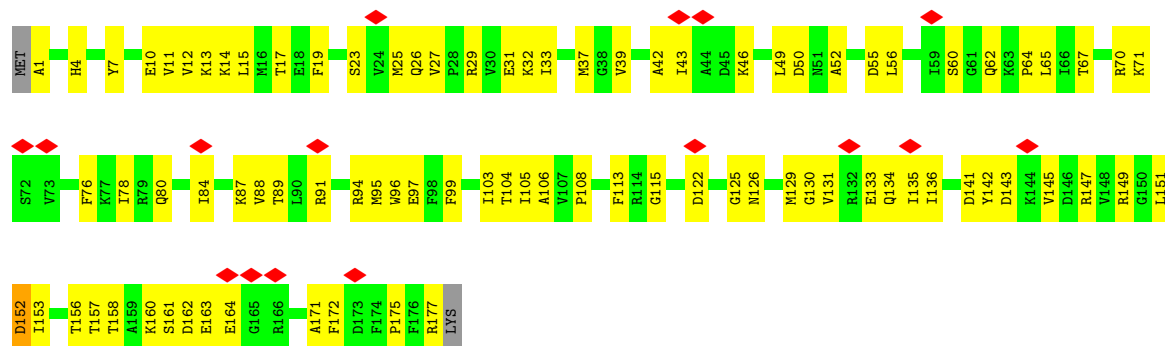




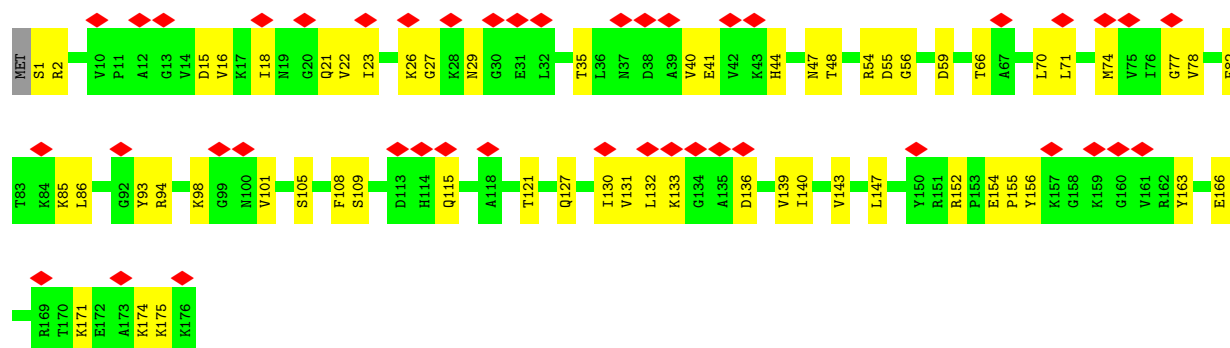
- Molecule 12: 50S ribosomal protein L4



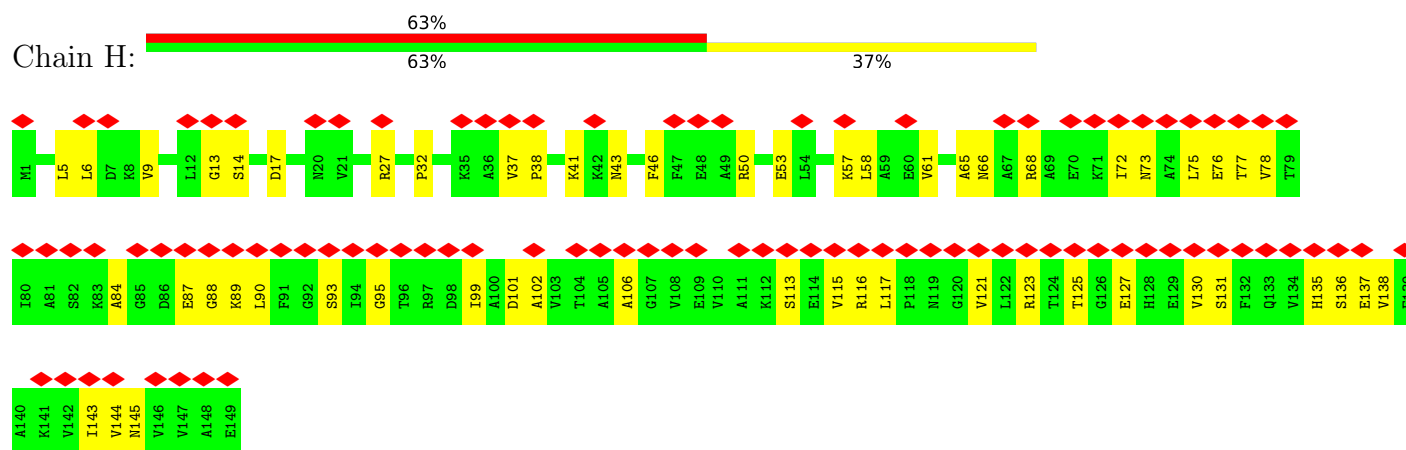
- Molecule 13: 50S ribosomal protein L5



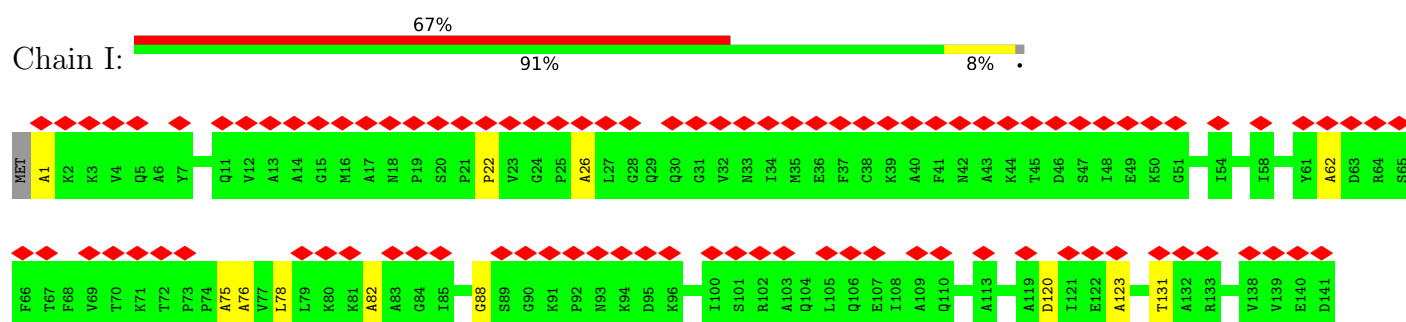
- Molecule 14: 50S ribosomal protein L6



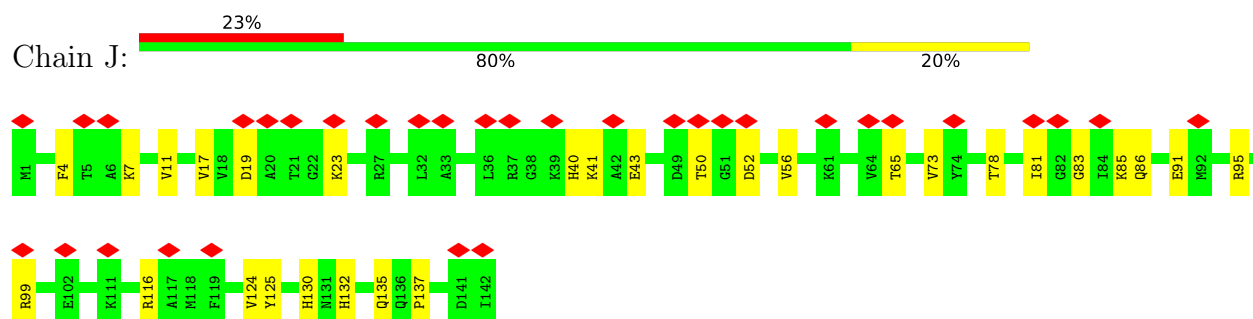
- Molecule 15: 50S ribosomal protein L9



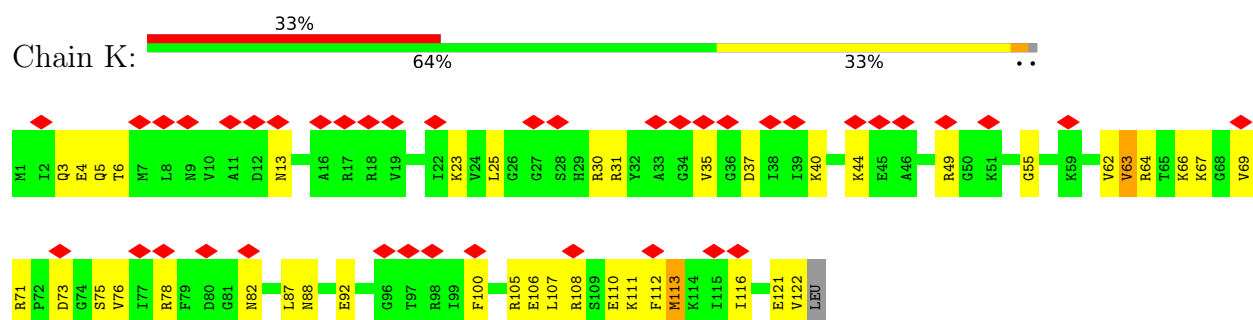
- Molecule 16: Ribosomal protein L11



- Molecule 17: 50S ribosomal protein L13

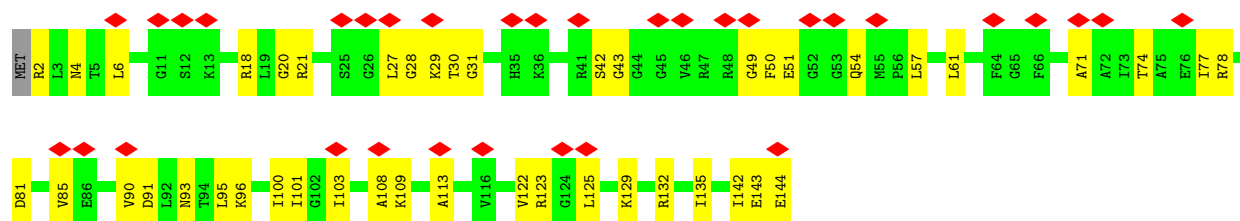


- Molecule 18: 50S ribosomal protein L14

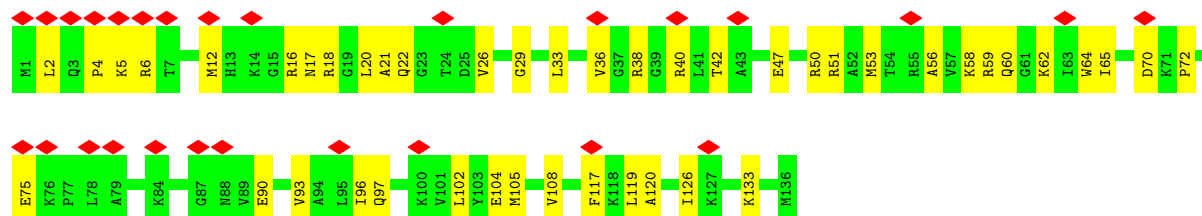


- Molecule 19: 50S ribosomal protein L15

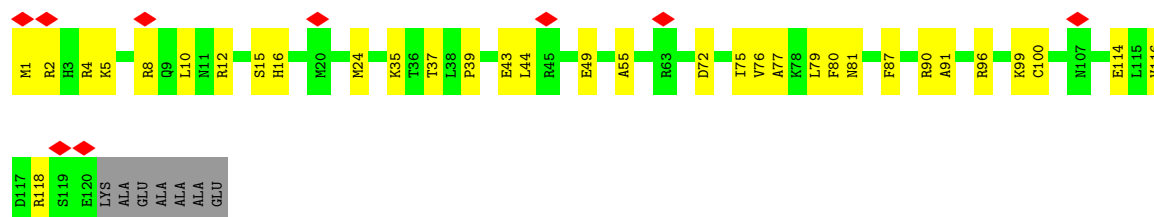




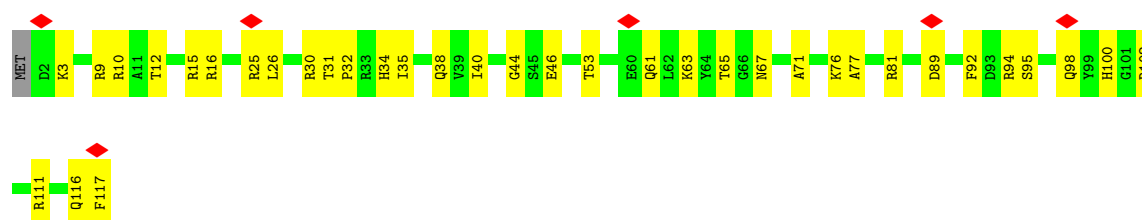
- Molecule 20: 50S ribosomal protein L16



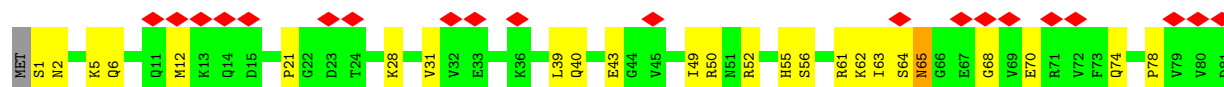
- Molecule 21: 50S ribosomal protein L17

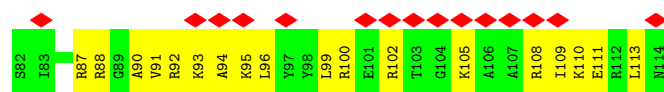


- Molecule 22: 50S ribosomal protein L18



- Molecule 23: 50S ribosomal protein L19

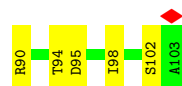
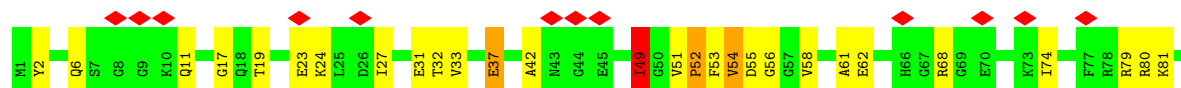




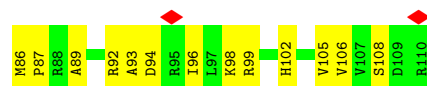
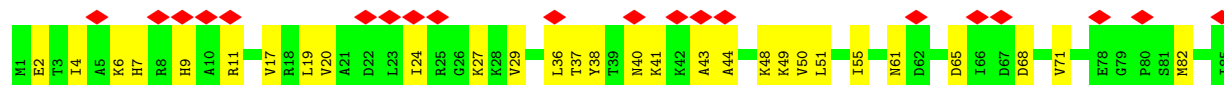
- Molecule 24: 50S ribosomal protein L20



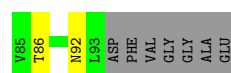
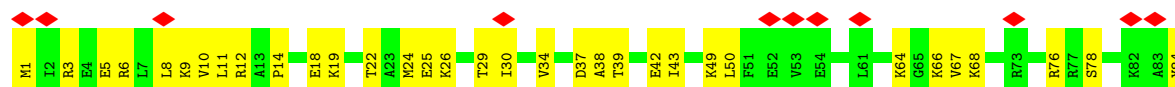
- Molecule 25: 50S ribosomal protein L21



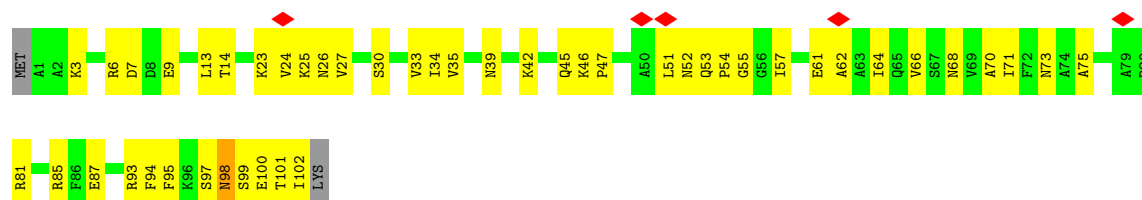
- Molecule 26: Ribosomal protein L22



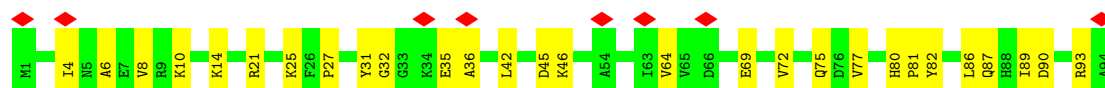
- Molecule 27: 50S ribosomal protein L23



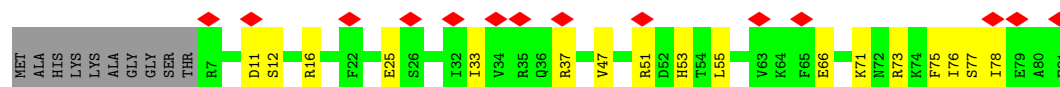
- Molecule 28: Ribosomal protein L24



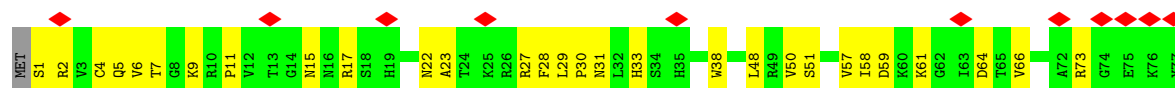
- Molecule 29: 50S ribosomal protein L25



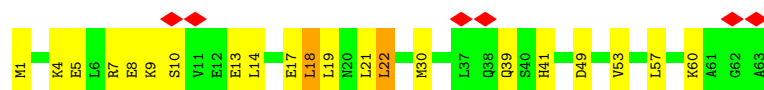
- Molecule 30: 50S ribosomal protein L27



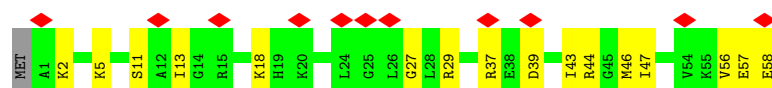
- Molecule 31: 50S ribosomal protein L28



- Molecule 32: 50S ribosomal protein L29

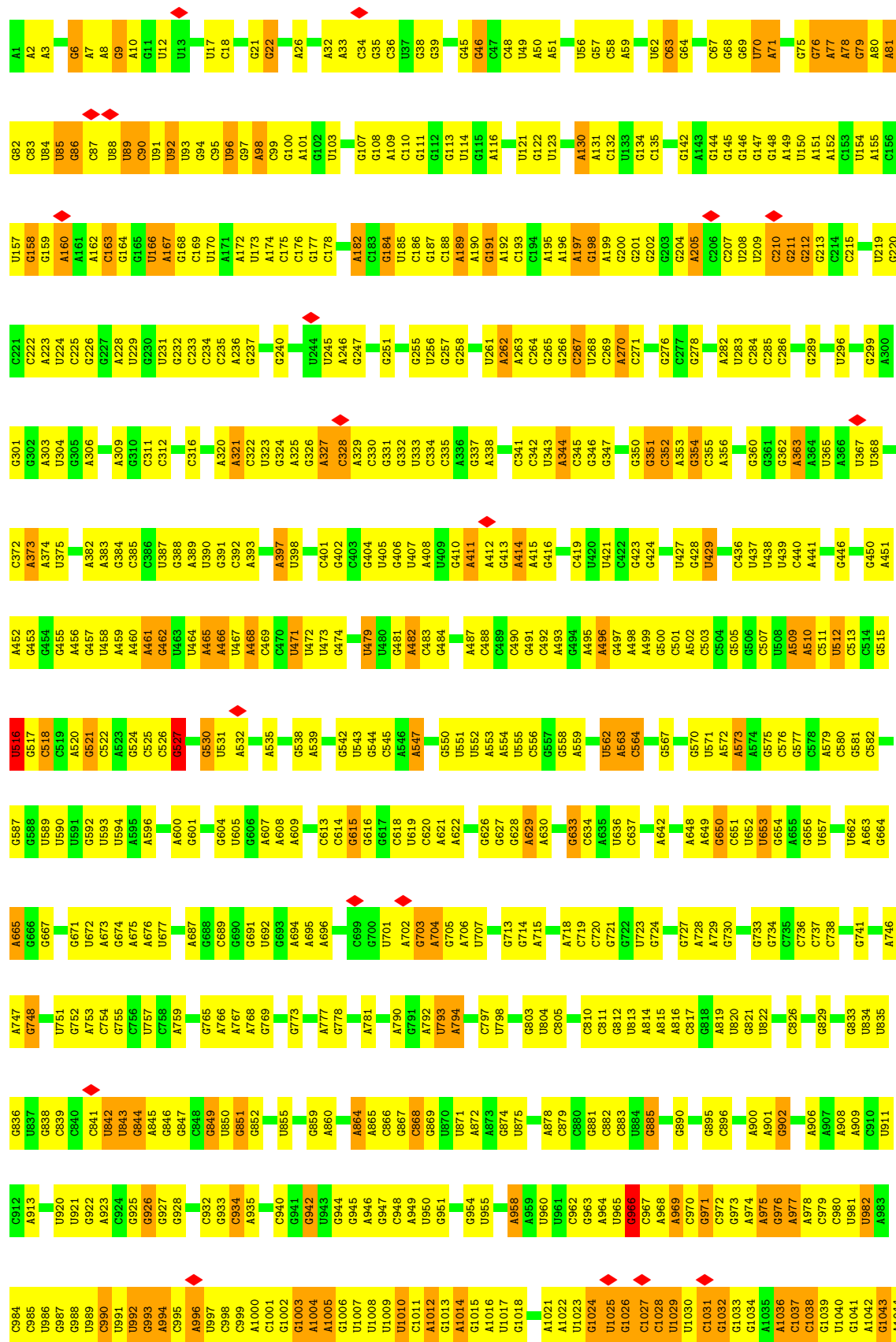


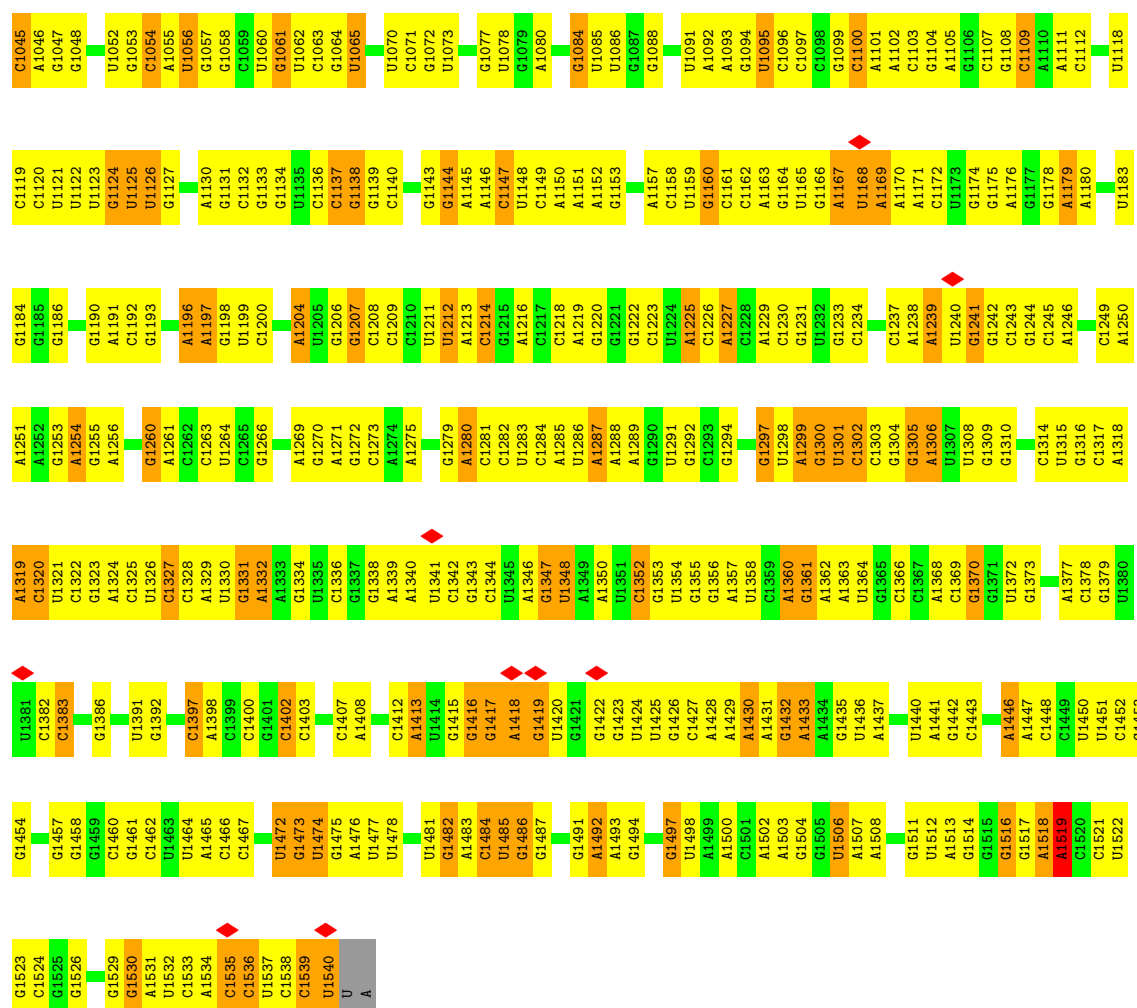
- Molecule 33: 50S ribosomal protein L30



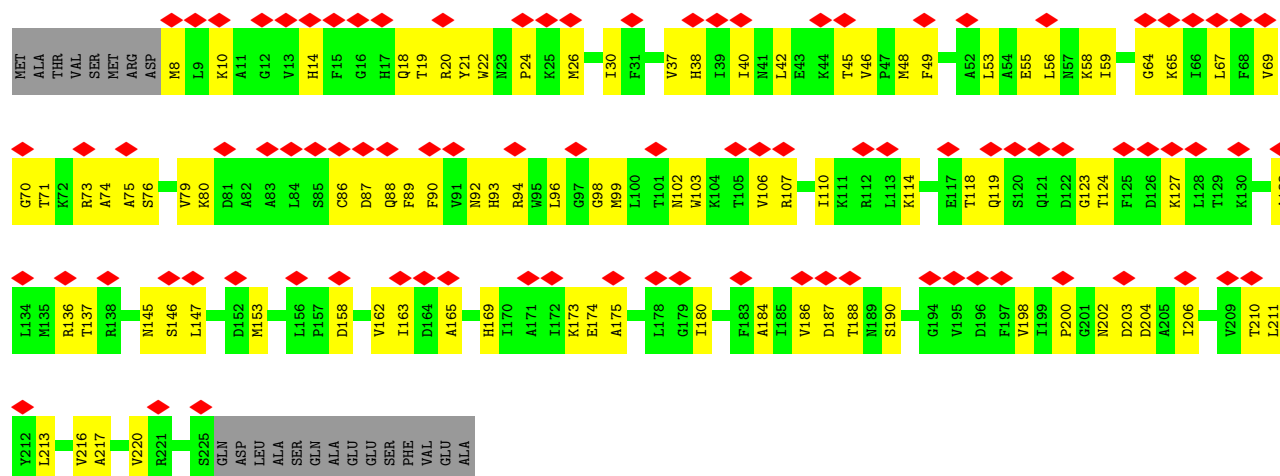
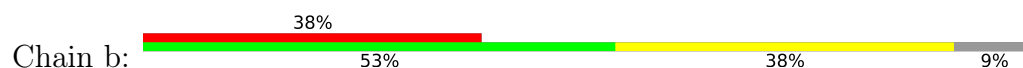
- Molecule 34: 16S ribosomal RNA



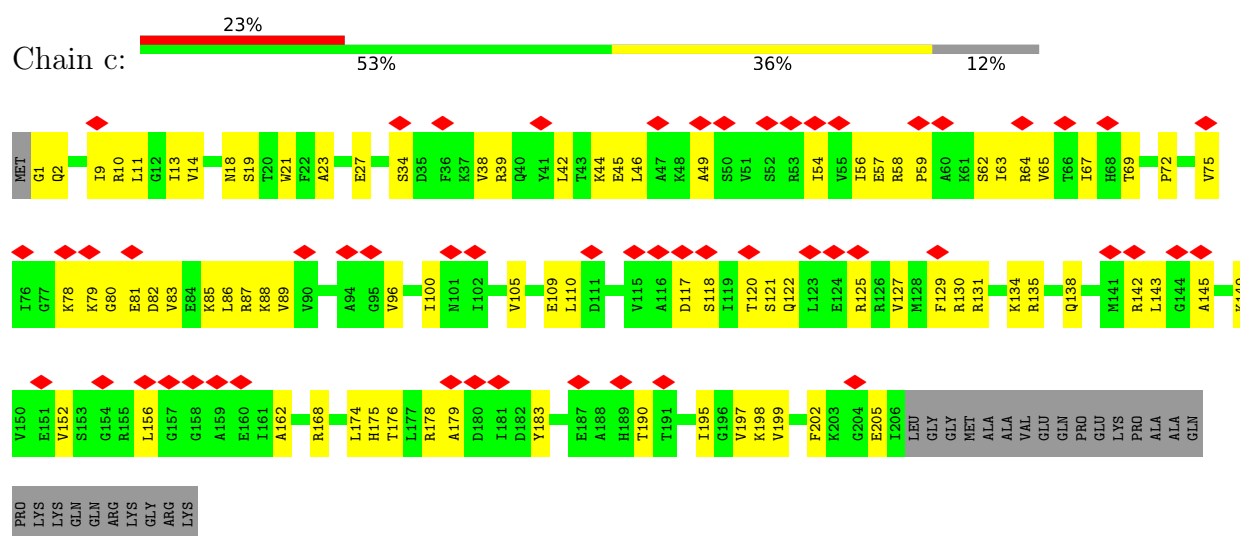




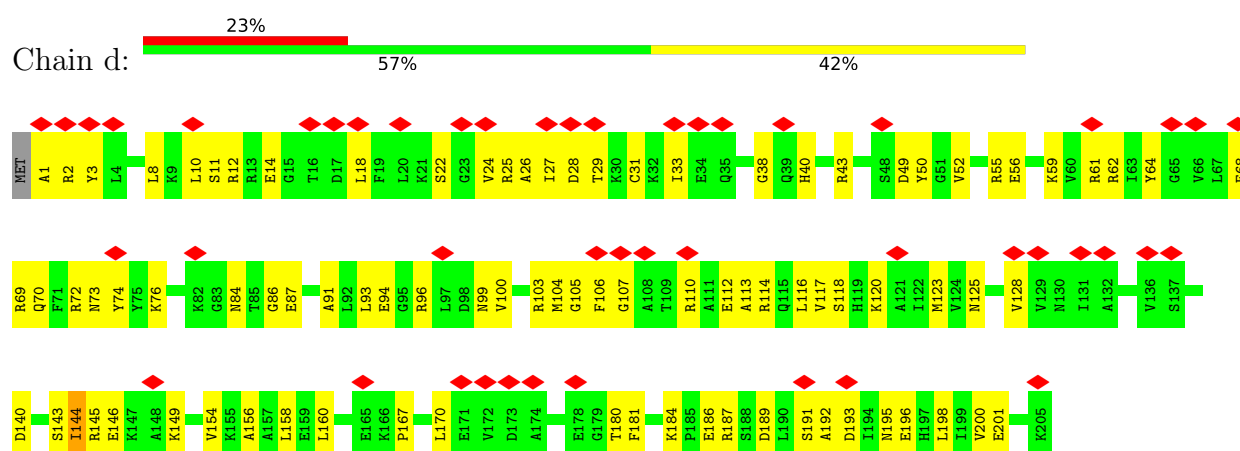
• Molecule 35: 30S ribosomal protein S2



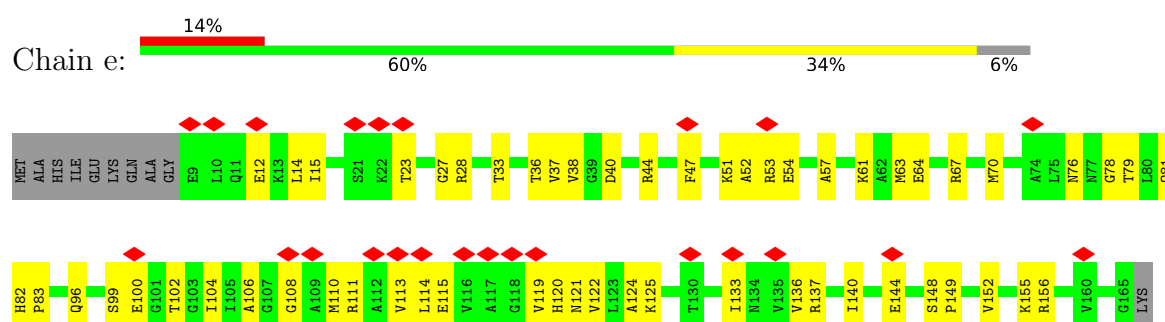
• Molecule 36: 30S ribosomal protein S3



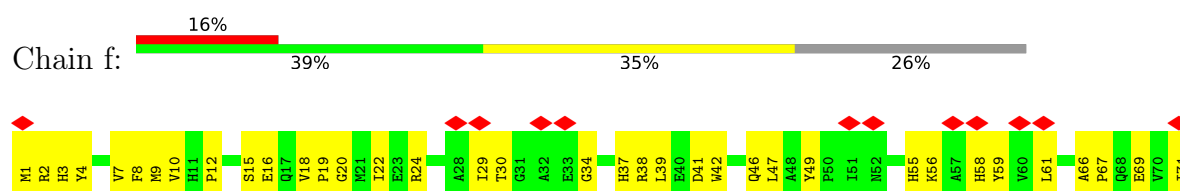
• Molecule 37: Ribosomal protein S4

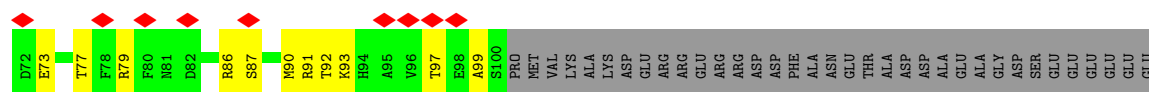


• Molecule 38: 30S ribosomal protein S5

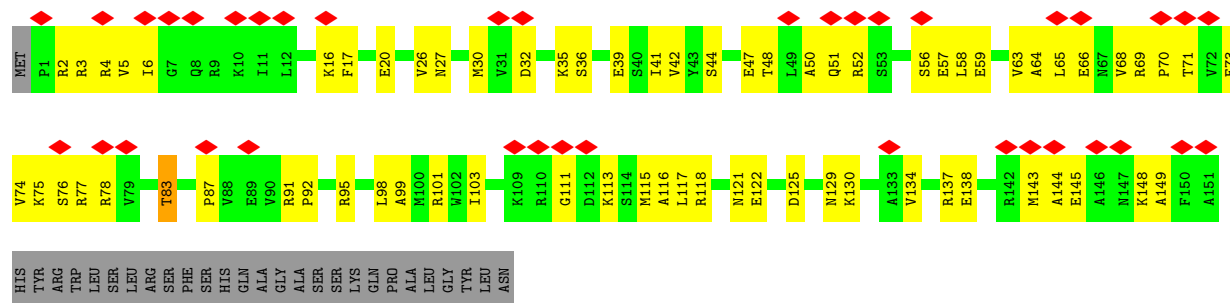


• Molecule 39: 30S ribosomal protein S6, fully modified isoform

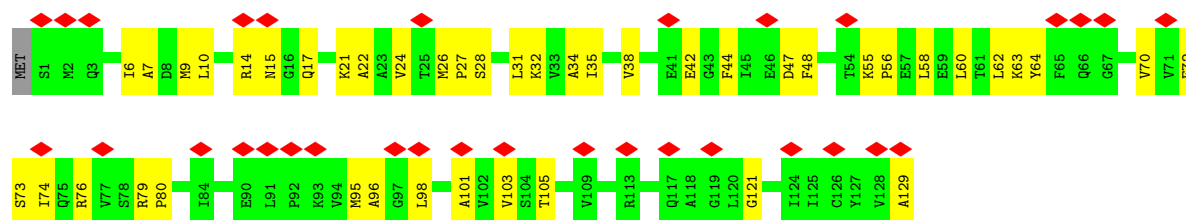




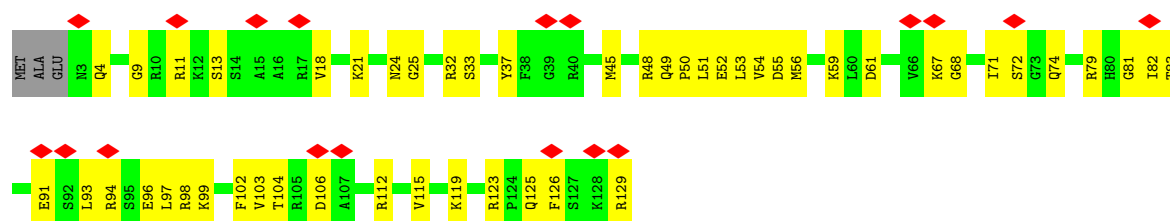
• Molecule 40: 30S ribosomal protein S7



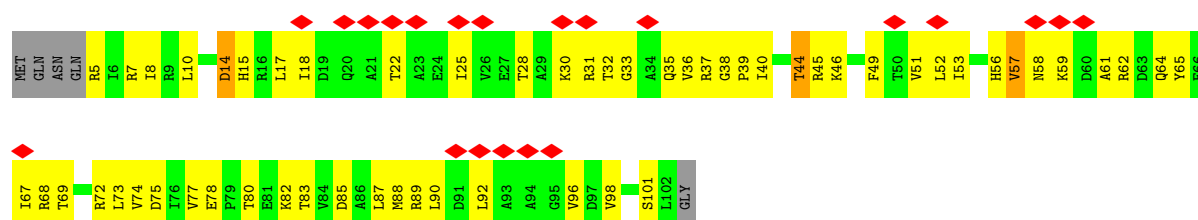
• Molecule 41: 30S ribosomal protein S8



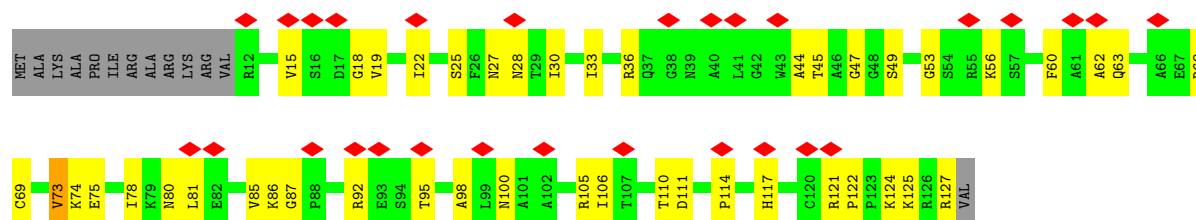
• Molecule 42: 30S ribosomal protein S9



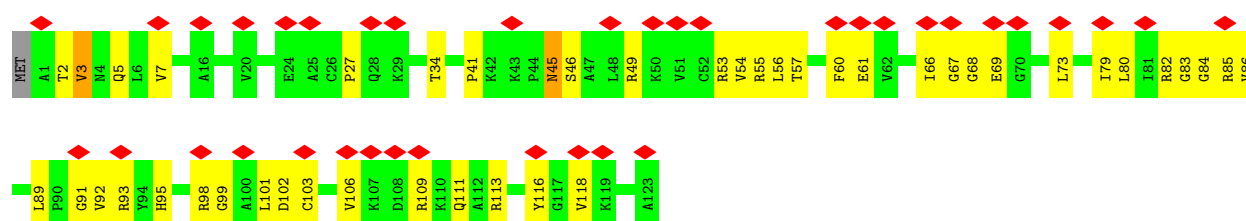
• Molecule 43: 30S ribosomal protein S10



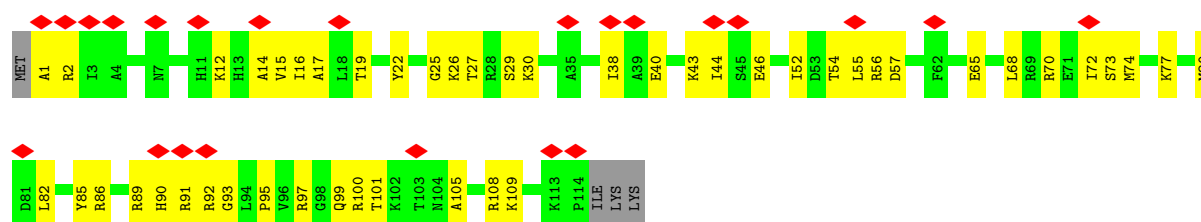
- Molecule 44: 30S ribosomal protein S11



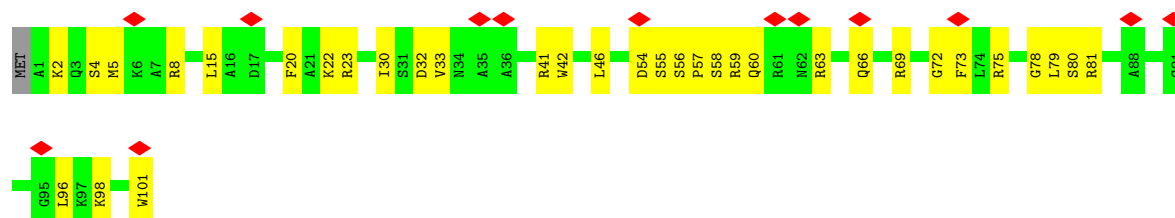
- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13

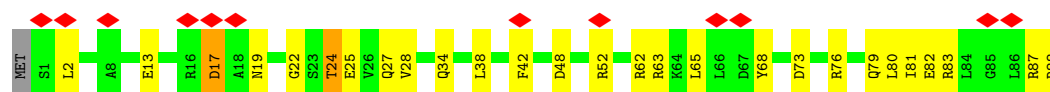


- Molecule 47: 30S ribosomal protein S14

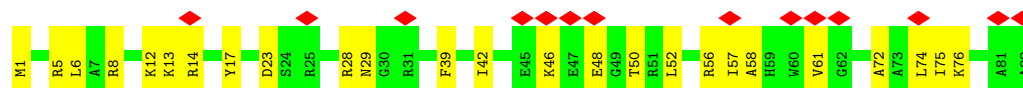


- Molecule 48: 30S ribosomal protein S15

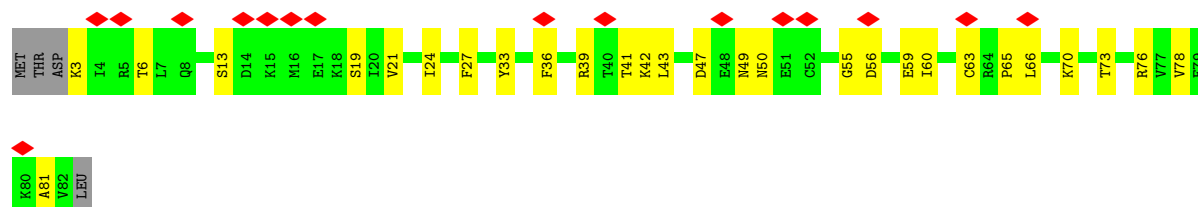




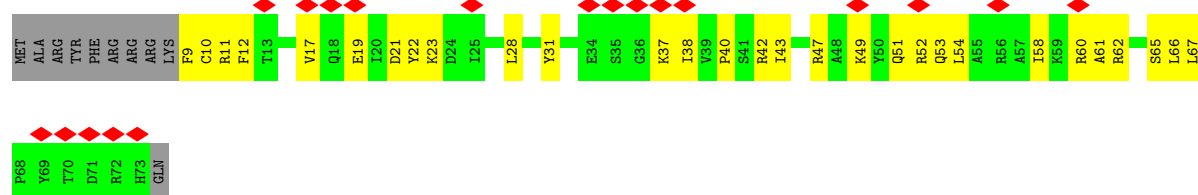
- Molecule 49: 30S ribosomal protein S16



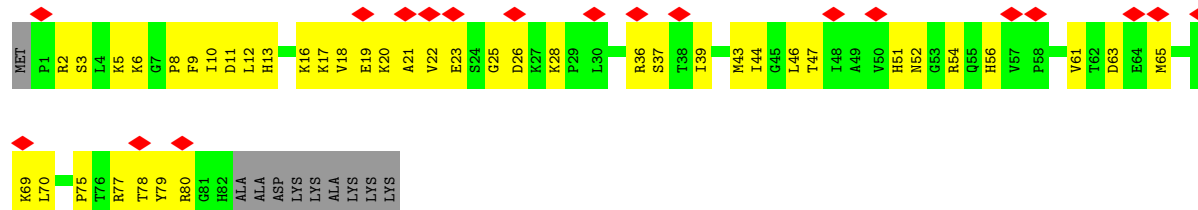
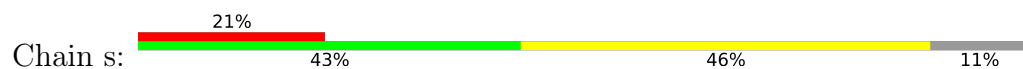
- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18

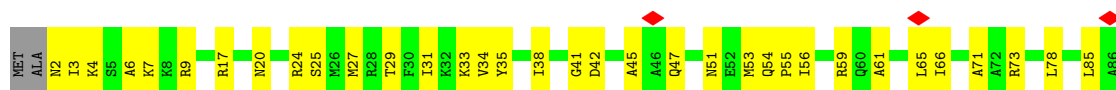


- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20

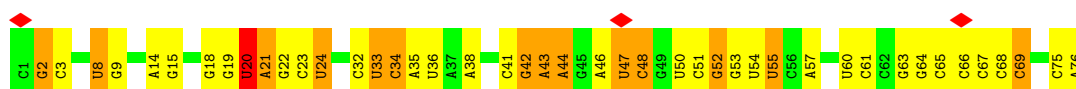




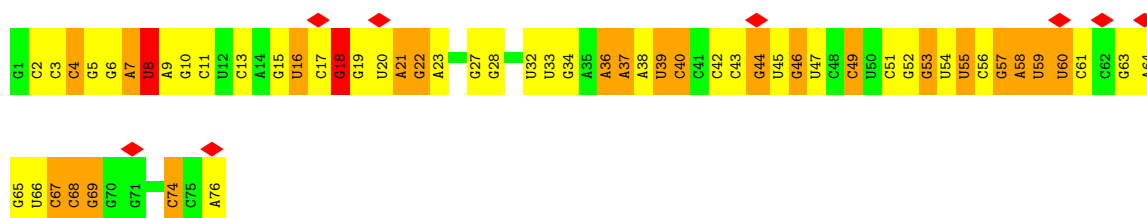
- Molecule 54: 30S ribosomal protein S21



- Molecule 55: P-site tRNA(fMet)



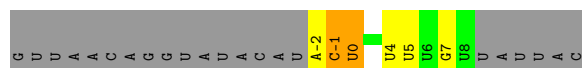
- Molecule 56: P-site fMet-Phe-tRNA(Phe)



- Molecule 57: Dipeptide (FME-PHE)



- Molecule 58: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1737	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	7.499	Depositor
Minimum map value	-4.218	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.837	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, G7M, 5MU, 3TD, 2MA, AM2, 1MG, 5MC, MA6, OMC, 4SU, UR3, 2MG, H2U, 4OC, 6MZ, OMU, FME, PSU, MIA, ZN

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	0.44	0/450	0.42	0/599
2	1	0.34	0/416	0.41	0/554
3	2	0.50	0/380	0.48	0/498
4	3	0.51	0/513	0.67	0/676
5	4	0.41	0/303	0.54	0/397
6	5	0.19	0/646	0.51	0/898
7	6	0.25	0/531	0.62	1/709 (0.1%)
8	A	0.49	1/69266 (0.0%)	0.41	1/108055 (0.0%)
9	B	0.40	0/2873	0.38	0/4478
10	C	0.47	0/2121	0.54	0/2852
11	D	0.43	0/1586	0.45	0/2134
12	E	0.41	0/1571	0.42	0/2113
13	F	0.29	0/1434	0.45	0/1926
14	G	0.31	0/1343	0.42	0/1816
15	H	0.23	0/1122	0.52	0/1515
16	I	0.19	0/692	0.50	0/960
17	J	0.42	0/1152	0.45	0/1551
18	K	0.53	0/947	0.66	1/1268 (0.1%)
19	L	0.45	0/1054	0.53	0/1403
20	M	0.42	0/1093	0.47	0/1460
21	N	0.44	0/973	0.54	0/1301
22	O	0.33	0/902	0.49	0/1209
23	P	0.42	0/929	0.45	0/1242
24	Q	0.53	0/960	0.50	0/1278
25	R	0.49	0/829	0.62	2/1107 (0.2%)
26	S	0.42	0/864	0.46	0/1156
27	T	0.38	0/744	0.47	0/994
28	U	0.36	0/787	0.45	0/1051
29	V	0.37	0/766	0.41	0/1025
30	W	0.43	0/582	0.44	0/769
31	X	0.44	0/635	0.48	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.41	0/510	0.71	1/677 (0.1%)
33	Z	0.40	0/453	0.43	0/605
34	a	0.41	2/36725 (0.0%)	0.40	2/57285 (0.0%)
35	b	0.26	0/1735	0.45	0/2338
36	c	0.32	0/1651	0.45	0/2225
37	d	0.32	0/1665	0.57	0/2227
38	e	0.35	0/1154	0.47	0/1554
39	f	0.31	0/835	0.49	0/1128
40	g	0.33	0/1195	0.59	0/1602
41	h	0.36	0/989	0.43	0/1326
42	i	0.29	0/1034	0.45	0/1375
43	j	0.42	0/796	0.65	1/1077 (0.1%)
44	k	0.34	0/885	0.53	1/1195 (0.1%)
45	l	0.50	0/969	0.68	1/1300 (0.1%)
46	m	0.29	0/892	0.51	0/1193
47	n	0.30	0/811	0.47	0/1081
48	o	0.35	0/722	0.46	0/964
49	p	0.37	0/659	0.47	0/884
50	q	0.39	0/657	0.51	0/881
51	r	0.33	0/544	0.50	0/731
52	s	0.31	0/675	0.57	0/908
53	t	0.33	0/671	0.44	0/888
54	u	0.44	0/512	0.72	0/683
55	v	0.35	0/1745	0.44	0/2716
56	w	0.33	0/1650	0.44	1/2569 (0.0%)
57	y	0.33	0/10	0.36	0/12
58	z	0.43	0/255	0.46	0/394
All	All	0.44	3/158863 (0.0%)	0.44	12/237660 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	527	G7M	O3'-P	8.74	1.65	1.56
8	A	874	G	O3'-P	7.23	1.72	1.61
34	a	1053	G	O3'-P	-5.94	1.52	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	527	G7M	P-O3'-C3'	12.41	134.59	119.70
43	j	44	THR	CB-CA-C	6.26	122.88	110.42
32	Y	19	LEU	N-CA-C	-6.18	104.55	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	63	VAL	N-CA-C	-5.75	108.25	113.71
56	w	18	G	C2'-C3'-O3'	5.70	118.05	109.50

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	444	0	461	21	0
2	1	409	0	440	14	0
3	2	377	0	418	14	0
4	3	504	0	574	19	0
5	4	302	0	340	11	0
6	5	647	0	336	8	0
7	6	522	0	521	43	0
8	A	62339	0	31373	1371	0
9	B	2570	0	1301	64	0
10	C	2082	0	2157	90	0
11	D	1565	0	1616	52	0
12	E	1552	0	1618	48	0
13	F	1410	0	1447	76	0
14	G	1323	0	1374	39	0
15	H	1111	0	1148	43	0
16	I	693	0	347	11	0
17	J	1129	0	1162	23	0
18	K	938	0	1012	41	0
19	L	1045	0	1117	41	0
20	M	1074	0	1157	36	0
21	N	960	0	1000	27	0
22	O	892	0	923	31	0
23	P	917	0	965	38	0
24	Q	947	0	1022	31	0
25	R	816	0	839	25	0
26	S	857	0	922	34	0
27	T	738	0	807	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	U	779	0	834	34	0
29	V	753	0	780	23	0
30	W	575	0	592	13	0
31	X	625	0	655	24	0
32	Y	509	0	543	17	0
33	Z	449	0	491	9	0
34	a	33050	0	16654	883	0
35	b	1704	0	1732	67	0
36	c	1624	0	1699	69	0
37	d	1643	0	1710	79	0
38	e	1141	0	1170	42	0
39	f	817	0	808	49	0
40	g	1181	0	1240	58	0
41	h	979	0	1034	35	0
42	i	1022	0	1070	42	0
43	j	786	0	828	48	0
44	k	869	0	878	34	0
45	l	955	0	1019	36	0
46	m	883	0	944	44	0
47	n	799	0	841	34	0
48	o	714	0	737	18	0
49	p	649	0	666	20	0
50	q	648	0	691	21	0
51	r	535	0	552	23	0
52	s	658	0	685	54	0
53	t	665	0	714	28	0
54	u	506	0	502	13	0
55	v	1642	0	840	32	0
56	w	1631	0	838	73	0
57	y	20	0	19	15	0
58	z	230	0	116	4	0
59	4	1	0	0	0	0
59	6	1	0	0	0	0
60	a	37	0	41	17	0
All	All	147243	0	98320	3680	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 15.

The worst 5 of 3680 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)
8:A:2451:A:C1'	56:w:76:A:H2'	1.62	1.28
8:A:1915:3TD:C1'	8:A:1915:3TD:O4'	1.67	1.25
8:A:2451:A:H1'	56:w:76:A:C2'	1.67	1.24
8:A:279:A:C8	8:A:361:G:N2	2.12	1.17
8:A:1056:G:N2	8:A:1103:A:C5	2.15	1.14

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
2	1	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
3	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
4	3	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
5	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
6	5	129/165 (78%)	96 (74%)	33 (26%)	0	100	100
7	6	64/70 (91%)	53 (83%)	11 (17%)	0	100	100
10	C	269/273 (98%)	239 (89%)	30 (11%)	0	100	100
11	D	207/209 (99%)	182 (88%)	25 (12%)	0	100	100
12	E	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
13	F	175/179 (98%)	150 (86%)	25 (14%)	0	100	100
14	G	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
15	H	147/149 (99%)	116 (79%)	31 (21%)	0	100	100
16	I	139/142 (98%)	101 (73%)	38 (27%)	0	100	100
17	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	K	120/123 (98%)	102 (85%)	18 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	L	141/144 (98%)	117 (83%)	24 (17%)	0	100	100
20	M	134/136 (98%)	119 (89%)	14 (10%)	1 (1%)	18	56
21	N	118/127 (93%)	107 (91%)	11 (9%)	0	100	100
22	O	114/117 (97%)	103 (90%)	11 (10%)	0	100	100
23	P	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
24	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
25	R	101/103 (98%)	82 (81%)	18 (18%)	1 (1%)	12	49
26	S	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
27	T	91/100 (91%)	80 (88%)	11 (12%)	0	100	100
28	U	100/104 (96%)	86 (86%)	13 (13%)	1 (1%)	12	49
29	V	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
30	W	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
31	X	75/78 (96%)	68 (91%)	7 (9%)	0	100	100
32	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
33	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
35	b	216/240 (90%)	187 (87%)	28 (13%)	1 (0%)	24	63
36	c	204/233 (88%)	192 (94%)	12 (6%)	0	100	100
37	d	203/206 (98%)	170 (84%)	32 (16%)	1 (0%)	24	63
38	e	155/167 (93%)	135 (87%)	20 (13%)	0	100	100
39	f	98/135 (73%)	86 (88%)	12 (12%)	0	100	100
40	g	149/179 (83%)	140 (94%)	9 (6%)	0	100	100
41	h	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
42	i	125/130 (96%)	102 (82%)	23 (18%)	0	100	100
43	j	96/103 (93%)	78 (81%)	16 (17%)	2 (2%)	5	30
44	k	114/129 (88%)	95 (83%)	19 (17%)	0	100	100
45	l	121/124 (98%)	106 (88%)	14 (12%)	1 (1%)	16	54
46	m	112/118 (95%)	96 (86%)	16 (14%)	0	100	100
47	n	99/102 (97%)	90 (91%)	9 (9%)	0	100	100
48	o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
49	p	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
50	q	78/84 (93%)	68 (87%)	10 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	r	63/75 (84%)	51 (81%)	12 (19%)	0	100	100
52	s	80/92 (87%)	68 (85%)	12 (15%)	0	100	100
53	t	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
54	u	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	7	38
All	All	5850/6220 (94%)	5143 (88%)	698 (12%)	9 (0%)	44	78

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
54	u	9	GLU
20	M	59	ARG
28	U	98	ASN
35	b	20	ARG
43	j	58	ASN

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	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/52 (98%)	49 (96%)	2 (4%)	28	49
5	4	34/34 (100%)	34 (100%)	0	100	100
7	6	59/62 (95%)	58 (98%)	1 (2%)	53	69
10	C	216/218 (99%)	216 (100%)	0	100	100
11	D	164/164 (100%)	163 (99%)	1 (1%)	78	83
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	147 (99%)	1 (1%)	76	81
14	G	137/138 (99%)	137 (100%)	0	100	100
15	H	114/114 (100%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	J	116/116 (100%)	116 (100%)	0	100	100
18	K	103/104 (99%)	100 (97%)	3 (3%)	37	58
19	L	102/103 (99%)	102 (100%)	0	100	100
20	M	109/109 (100%)	109 (100%)	0	100	100
21	N	100/103 (97%)	100 (100%)	0	100	100
22	O	86/87 (99%)	86 (100%)	0	100	100
23	P	99/100 (99%)	98 (99%)	1 (1%)	68	78
24	Q	89/90 (99%)	88 (99%)	1 (1%)	65	76
25	R	84/84 (100%)	82 (98%)	2 (2%)	43	64
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	80 (100%)	0	100	100
28	U	83/85 (98%)	83 (100%)	0	100	100
29	V	78/78 (100%)	78 (100%)	0	100	100
30	W	57/63 (90%)	57 (100%)	0	100	100
31	X	67/68 (98%)	67 (100%)	0	100	100
32	Y	55/55 (100%)	53 (96%)	2 (4%)	31	52
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	180 (100%)	0	100	100
36	c	170/190 (90%)	170 (100%)	0	100	100
37	d	172/173 (99%)	172 (100%)	0	100	100
38	e	114/126 (90%)	114 (100%)	0	100	100
39	f	87/116 (75%)	87 (100%)	0	100	100
40	g	124/147 (84%)	122 (98%)	2 (2%)	55	70
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	105/107 (98%)	105 (100%)	0	100	100
43	j	86/90 (96%)	84 (98%)	2 (2%)	44	64
44	k	89/99 (90%)	89 (100%)	0	100	100
45	l	103/104 (99%)	102 (99%)	1 (1%)	68	78
46	m	92/96 (96%)	92 (100%)	0	100	100
47	n	79/84 (94%)	79 (100%)	0	100	100
48	o	76/77 (99%)	74 (97%)	2 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/78 (95%)	74 (100%)	0	100	100
51	r	56/65 (86%)	56 (100%)	0	100	100
52	s	72/79 (91%)	72 (100%)	0	100	100
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	46 (100%)	0	100	100
57	y	1/1 (100%)	1 (100%)	0	100	100
All	All	4627/4830 (96%)	4606 (100%)	21 (0%)	78	83

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	g	20	GLU
43	j	44	THR
48	o	24	THR
45	l	86	VAL
43	j	14	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
41	h	66	GLN
52	s	51	HIS
43	j	56	HIS
46	m	13	HIS
22	O	29	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1539/1542 (99%)	358 (23%)	0
55	v	76/77 (98%)	21 (27%)	0
56	w	75/76 (98%)	28 (37%)	0
58	z	10/33 (30%)	4 (40%)	0
8	A	2902/2903 (99%)	684 (23%)	51 (1%)
9	B	119/120 (99%)	31 (26%)	4 (3%)
All	All	4721/4751 (99%)	1126 (23%)	55 (1%)

5 of 1126 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	15	G
8	A	23	G
8	A	34	U
8	A	42	A

5 of 55 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1730	C
8	A	2154	A
9	B	66	A
8	A	2796	U
8	A	1907	G

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

46 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	$\# Z > 2$
56	4SU	w	8	56	18,21,22	3.45	7 (38%)	26,30,33	2.20	4 (15%)
8	PSU	A	746	8	18,21,22	1.07	2 (11%)	22,30,33	1.81	4 (18%)
8	PSU	A	2457	8	18,21,22	1.06	3 (16%)	22,30,33	1.81	4 (18%)
8	5MC	A	1962	8	18,22,23	3.52	7 (38%)	26,32,35	1.08	2 (7%)
8	OMU	A	2552	8	19,22,23	2.76	7 (36%)	26,31,34	1.83	5 (19%)
8	2MG	A	1835	8	23,26,27	2.88	6 (26%)	32,38,41	2.15	10 (31%)
55	PSU	v	55	55	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
8	6MZ	A	2030	8	22,25,26	3.00	6 (27%)	30,36,39	4.59	14 (46%)
34	2MG	a	1207	34	23,26,27	2.86	8 (34%)	32,38,41	2.28	11 (34%)
56	PSU	w	32	56	18,21,22	1.39	2 (11%)	22,30,33	1.93	4 (18%)
8	PSU	A	1911	8	18,21,22	1.40	2 (11%)	22,30,33	2.03	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	3TD	A	1915	8	22,23,23	6.55	11 (50%)	29,35,35	3.49	10 (34%)
8	PSU	A	2580	8	18,21,22	1.11	3 (16%)	22,30,33	1.94	6 (27%)
56	PSU	w	55	56	18,21,22	1.36	3 (16%)	22,30,33	2.13	5 (22%)
8	OMG	A	2251	8,56	23,26,27	1.23	3 (13%)	33,38,41	1.99	7 (21%)
8	PSU	A	2604	8	18,21,22	1.06	2 (11%)	22,30,33	2.01	5 (22%)
8	G7M	A	2069	8	23,26,27	2.55	7 (30%)	35,39,42	2.28	10 (28%)
55	4SU	v	8	55	18,21,22	3.58	7 (38%)	26,30,33	2.26	5 (19%)
34	5MC	a	967	34	18,22,23	3.62	7 (38%)	26,32,35	1.00	1 (3%)
34	PSU	a	516	34	18,21,22	0.90	1 (5%)	22,30,33	1.66	5 (22%)
8	OMC	A	2498	8	19,22,23	2.79	7 (36%)	26,31,34	0.81	0
8	PSU	A	2504	8	18,21,22	1.05	1 (5%)	22,30,33	1.92	4 (18%)
8	PSU	A	955	8	18,21,22	1.07	2 (11%)	22,30,33	1.87	4 (18%)
34	UR3	a	1498	34	19,22,23	2.44	6 (31%)	26,32,35	1.30	1 (3%)
8	5MC	A	747	8	18,22,23	3.58	7 (38%)	26,32,35	1.20	2 (7%)
8	PSU	A	1917	8	18,21,22	1.36	3 (16%)	22,30,33	1.99	5 (22%)
56	G7M	w	46	56	23,26,27	2.65	8 (34%)	35,39,42	2.25	10 (28%)
34	G7M	a	527	34	23,26,27	3.95	16 (69%)	35,39,42	3.26	15 (42%)
34	MA6	a	1519	34	23,26,27	1.51	5 (21%)	34,38,41	2.76	11 (32%)
34	MA6	a	1518	34	23,26,27	1.48	5 (21%)	34,38,41	2.79	11 (32%)
55	5MU	v	54	55	19,22,23	4.66	7 (36%)	28,32,35	3.69	9 (32%)
56	5MU	w	54	56	19,22,23	1.33	5 (26%)	28,32,35	2.18	8 (28%)
34	5MC	a	1407	34	18,22,23	3.57	7 (38%)	26,32,35	1.03	1 (3%)
8	2MA	A	2503	8	22,25,26	3.60	10 (45%)	33,37,40	2.21	9 (27%)
56	MIA	w	37	56	28,31,32	2.38	6 (21%)	40,44,47	2.68	15 (37%)
8	2MG	A	2445	8	23,26,27	2.80	9 (39%)	32,38,41	2.36	12 (37%)
8	1MG	A	745	8	22,26,27	2.56	6 (27%)	33,39,42	2.07	8 (24%)
8	6MZ	A	1618	8	22,25,26	2.93	6 (27%)	30,36,39	4.42	13 (43%)
34	2MG	a	966	34	23,26,27	2.95	7 (30%)	32,38,41	2.30	9 (28%)
57	FME	y	101	57	8,9,10	0.60	0	7,9,11	1.29	1 (14%)
8	5MU	A	1939	8	19,22,23	4.61	7 (36%)	28,32,35	3.82	10 (35%)
34	2MG	a	1516	34	23,26,27	2.87	9 (39%)	32,38,41	2.33	11 (34%)
55	H2U	v	20	55	18,21,22	3.01	5 (27%)	21,30,33	1.94	5 (23%)
8	PSU	A	2605	8	18,21,22	1.11	2 (11%)	22,30,33	1.88	2 (9%)
34	4OC	a	1402	34	20,23,24	2.86	8 (40%)	26,32,35	0.93	2 (7%)
56	PSU	w	39	56	18,21,22	1.44	3 (16%)	22,30,33	1.97	5 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
8	PSU	A	746	8	-	3/7/25/26	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	1/7/25/26	0/2/2/2
8	OMU	A	2552	8	-	3/9/27/28	0/2/2/2
8	2MG	A	1835	8	-	2/9/27/28	0/3/3/3
55	PSU	v	55	55	-	3/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	2/9/27/28	0/3/3/3
34	2MG	a	1207	34	-	0/9/27/28	0/3/3/3
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
8	3TD	A	1915	8	-	9/10/26/26	0/2/2/2
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
56	PSU	w	55	56	-	2/7/25/26	0/2/2/2
8	OMG	A	2251	8,56	-	1/9/27/28	0/3/3/3
8	PSU	A	2604	8	-	1/7/25/26	0/2/2/2
8	G7M	A	2069	8	-	1/7/25/26	0/3/3/3
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
8	OMC	A	2498	8	-	2/9/27/28	0/2/2/2
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
8	5MC	A	747	8	-	2/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
56	G7M	w	46	56	-	3/7/25/26	0/3/3/3
34	G7M	a	527	34	-	1/7/25/26	0/3/3/3
34	MA6	a	1519	34	-	3/11/29/30	0/3/3/3
34	MA6	a	1518	34	-	0/11/29/30	0/3/3/3
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
8	2MA	A	2503	8	-	1/7/25/26	0/3/3/3
56	MIA	w	37	56	-	5/15/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2MG	A	2445	8	-	2/9/27/28	0/3/3/3
8	1MG	A	745	8	-	0/7/25/26	0/3/3/3
8	6MZ	A	1618	8	-	0/9/27/28	0/3/3/3
34	2MG	a	966	34	-	2/9/27/28	0/3/3/3
57	FME	y	101	57	-	4/7/9/11	-
8	5MU	A	1939	8	-	4/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	1/9/29/30	0/2/2/2
56	PSU	w	39	56	-	2/7/25/26	0/2/2/2

The worst 5 of 252 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	O4'-C1'	16.96	1.67	1.43
8	A	1915	3TD	C2'-C1'	-15.15	1.34	1.53
8	A	1915	3TD	C6-C5	13.18	1.50	1.35
8	A	2030	6MZ	C6-N6	11.77	1.46	1.34
8	A	1618	6MZ	C6-N6	11.63	1.46	1.34

The worst 5 of 303 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2030	6MZ	C4-N9-C8	14.29	121.22	105.73
8	A	1618	6MZ	C4-N9-C8	13.38	120.22	105.73
8	A	1939	5MU	C5-C4-N3	12.04	125.59	115.31
55	v	54	5MU	C5-C4-N3	11.82	125.40	115.31
8	A	2030	6MZ	N9-C8-N7	-11.34	98.41	113.91

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	20	H2U	O4'-C1'-N1-C6
55	v	20	H2U	C2'-C1'-N1-C2
55	v	20	H2U	C2'-C1'-N1-C6
55	v	55	PSU	O4'-C1'-C5-C6
8	A	746	PSU	C2'-C1'-C5-C4

There are no ring outliers.

25 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	w	8	4SU	1	0
8	A	746	PSU	1	0
8	A	2552	OMU	3	0
8	A	2030	6MZ	2	0
34	a	1207	2MG	1	0
8	A	1915	3TD	2	0
56	w	55	PSU	2	0
8	A	2251	OMG	1	0
55	v	8	4SU	1	0
34	a	516	PSU	2	0
8	A	2498	OMC	2	0
8	A	747	5MC	1	0
34	a	527	G7M	2	0
34	a	1519	MA6	2	0
34	a	1518	MA6	1	0
56	w	37	MIA	3	0
8	A	2445	2MG	1	0
8	A	745	1MG	1	0
34	a	966	2MG	1	0
57	y	101	FME	15	0
8	A	1939	5MU	1	0
34	a	1516	2MG	1	0
55	v	20	H2U	3	0
34	a	1402	4OC	1	0
56	w	39	PSU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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	$\# Z > 2$
60	AM2	a	2001	-	40,40,40	1.63	10 (25%)	53,60,60	1.26	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	AM2	a	2001	-	-	3/12/84/84	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	a	2001	AM2	OA4-CA1	4.20	1.52	1.41
60	a	2001	AM2	CB3-CB4	-3.50	1.49	1.53
60	a	2001	AM2	OB1-CB1	3.29	1.50	1.41
60	a	2001	AM2	OA5-CA8	3.25	1.50	1.41
60	a	2001	AM2	OA5-CA4	2.82	1.51	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	a	2001	AM2	CA9-NA7-CA7	-4.89	107.26	114.38
60	a	2001	AM2	OA5-CA4-CA5	2.11	114.19	109.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

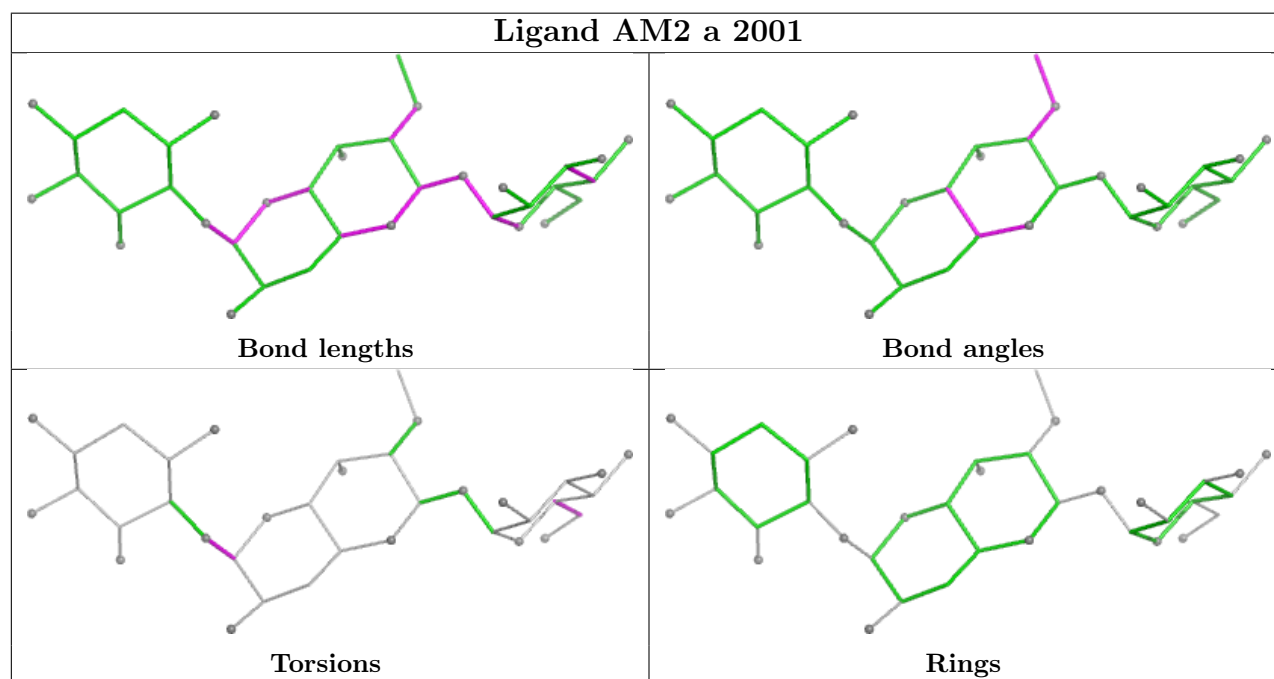
Mol	Chain	Res	Type	Atoms
60	a	2001	AM2	OB1-CB5-CB6-OB6
60	a	2001	AM2	CB4-CB5-CB6-OB6
60	a	2001	AM2	OA4-CA1-OA1-CC1

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	a	2001	AM2	17	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.

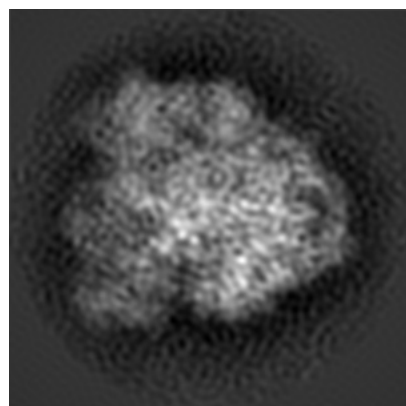
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13460. These allow visual inspection of the internal detail of the map and identification of artifacts.

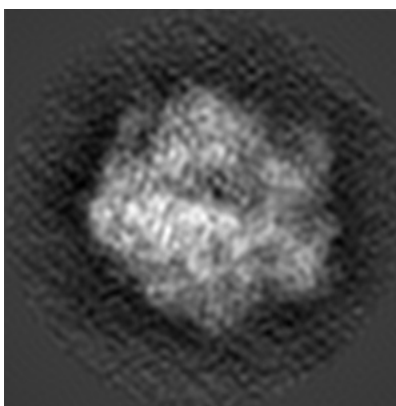
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

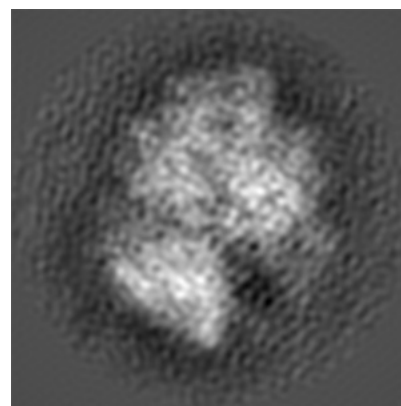
6.1.1 Primary map



X

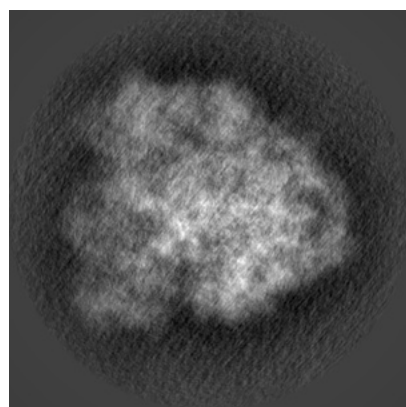


Y

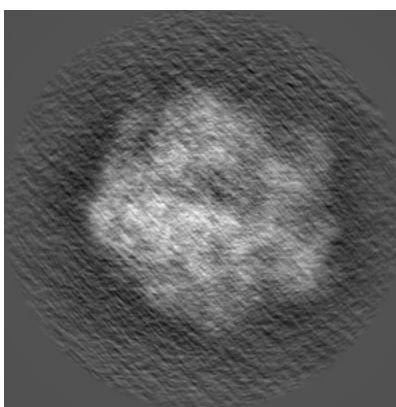


Z

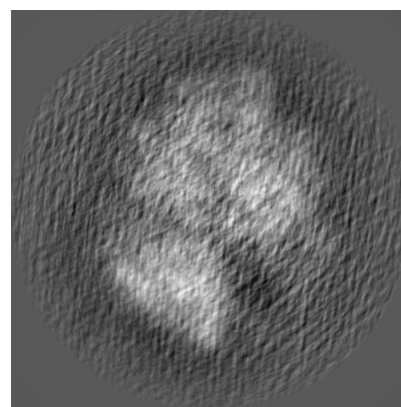
6.1.2 Raw map



X



Y

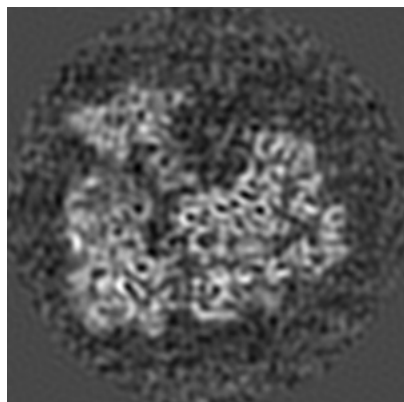


Z

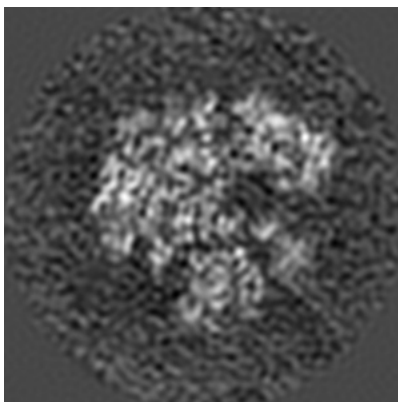
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

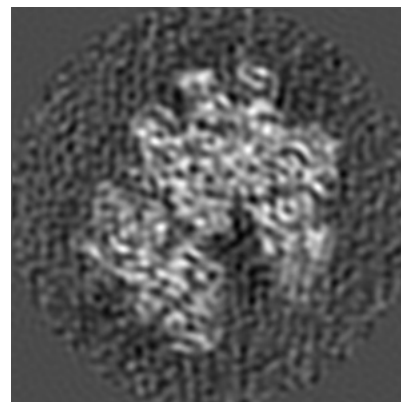
6.2.1 Primary map



X Index: 144

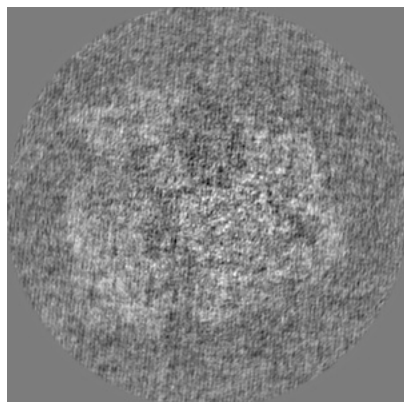


Y Index: 144

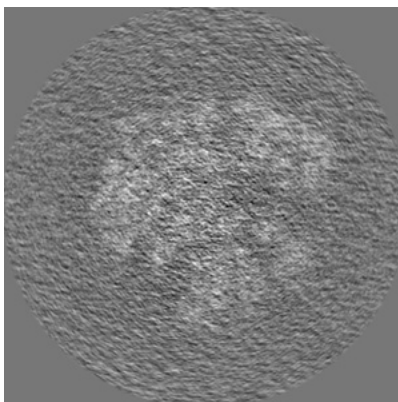


Z Index: 144

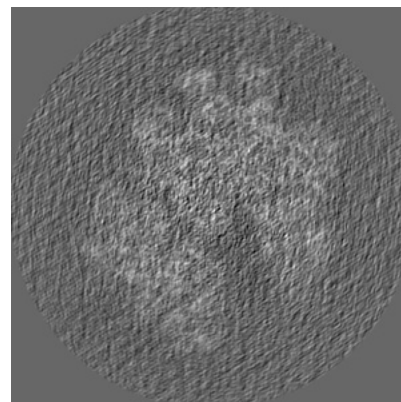
6.2.2 Raw map



X Index: 144



Y Index: 144

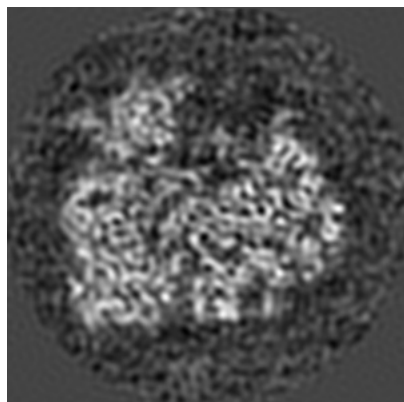


Z Index: 144

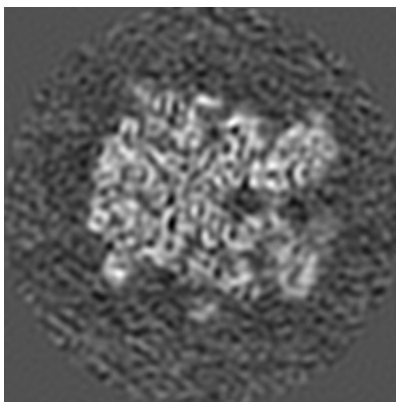
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

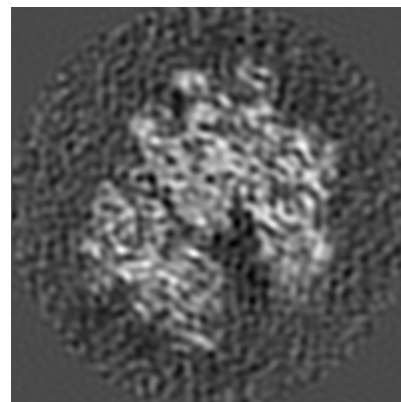
6.3.1 Primary map



X Index: 139

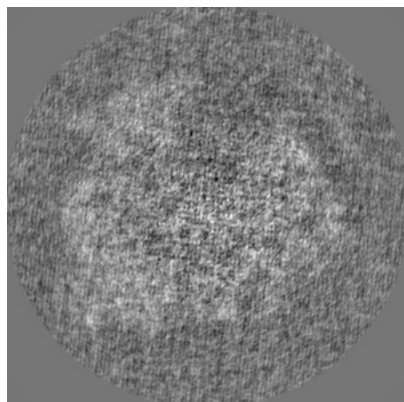


Y Index: 158

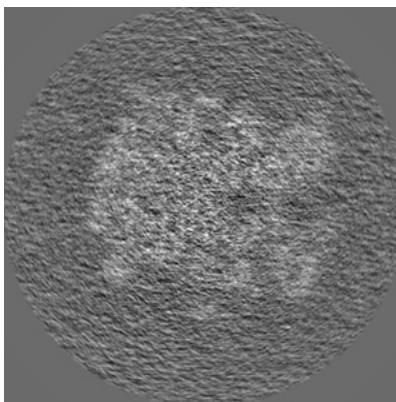


Z Index: 146

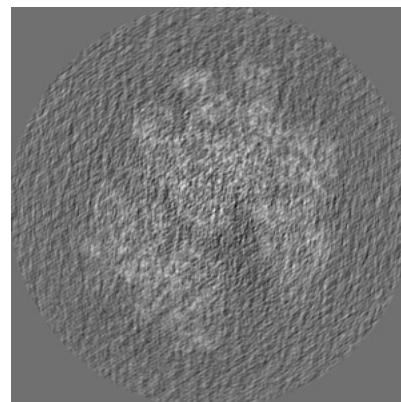
6.3.2 Raw map



X Index: 140



Y Index: 158

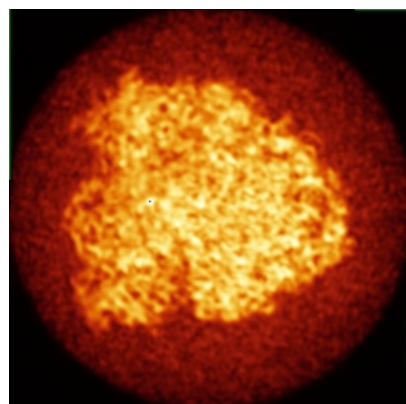


Z Index: 145

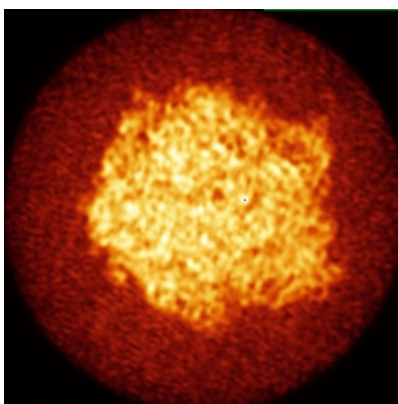
The images above show the largest variance slices of the map in three orthogonal directions.

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

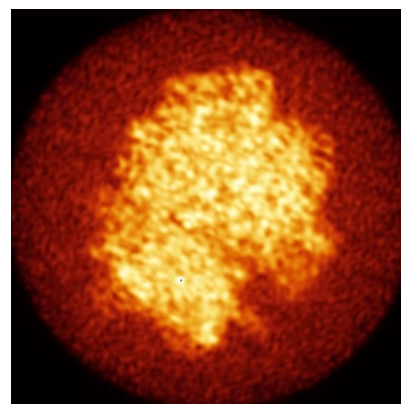
6.4.1 Primary map



X

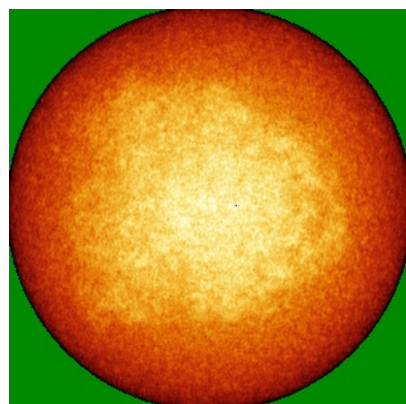


Y

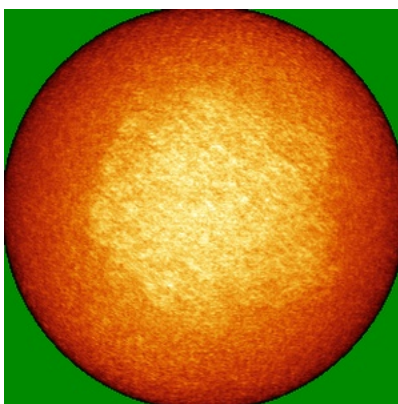


Z

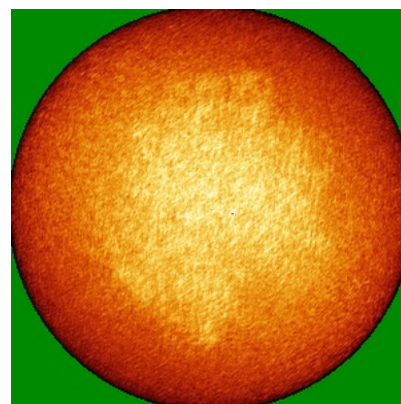
6.4.2 Raw map



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.

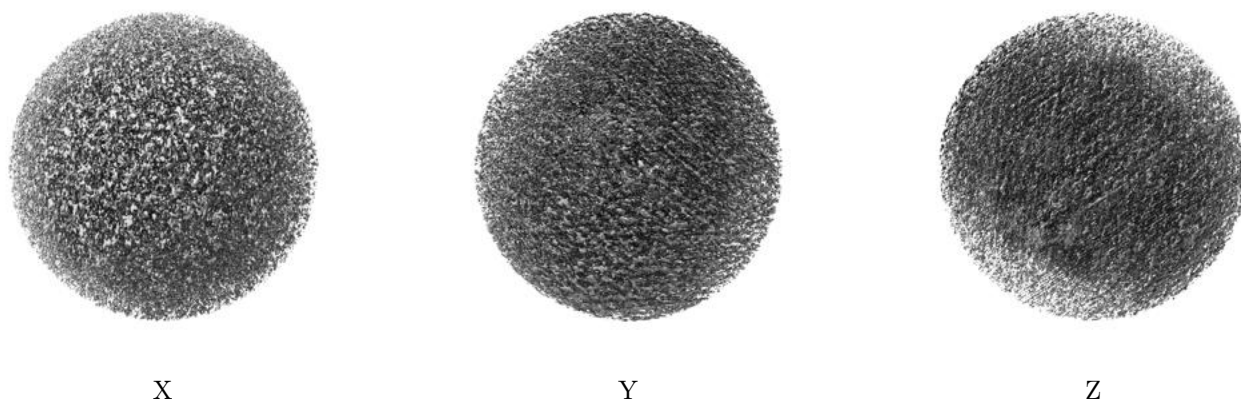
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

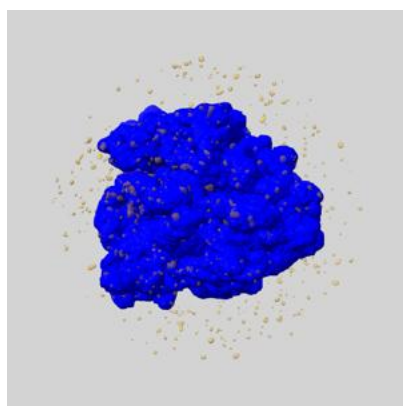
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

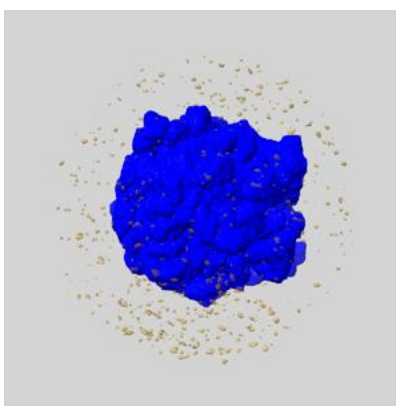
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

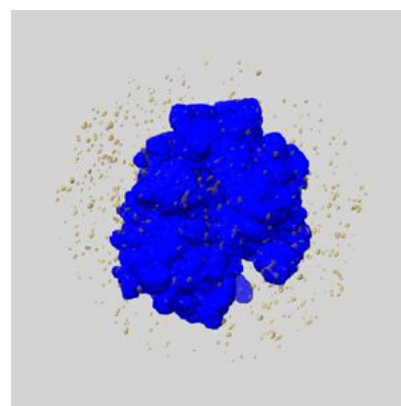
6.6.1 emd_13460_msk_1.map [i](#)



X



Y

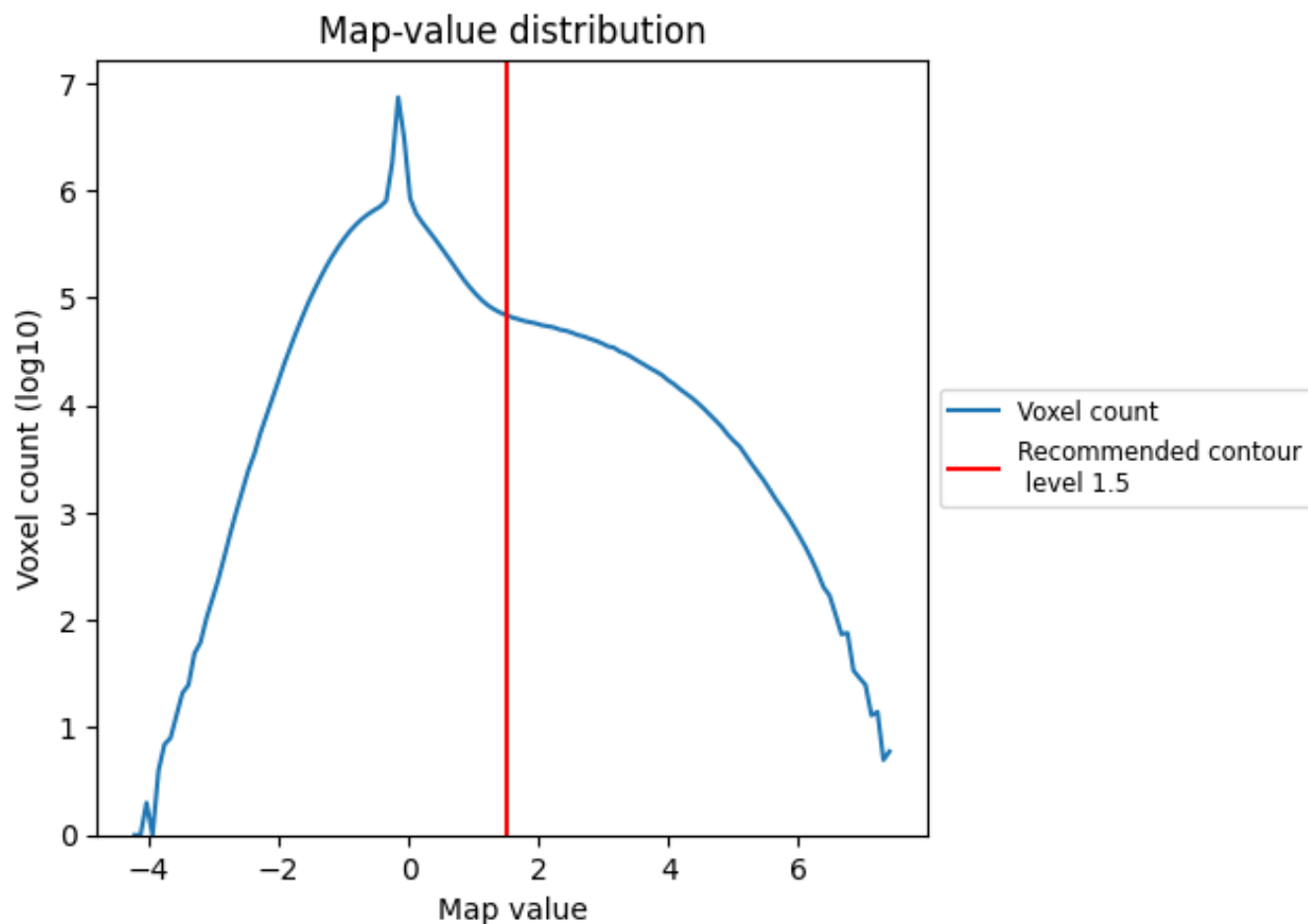


Z

7 Map analysis [i](#)

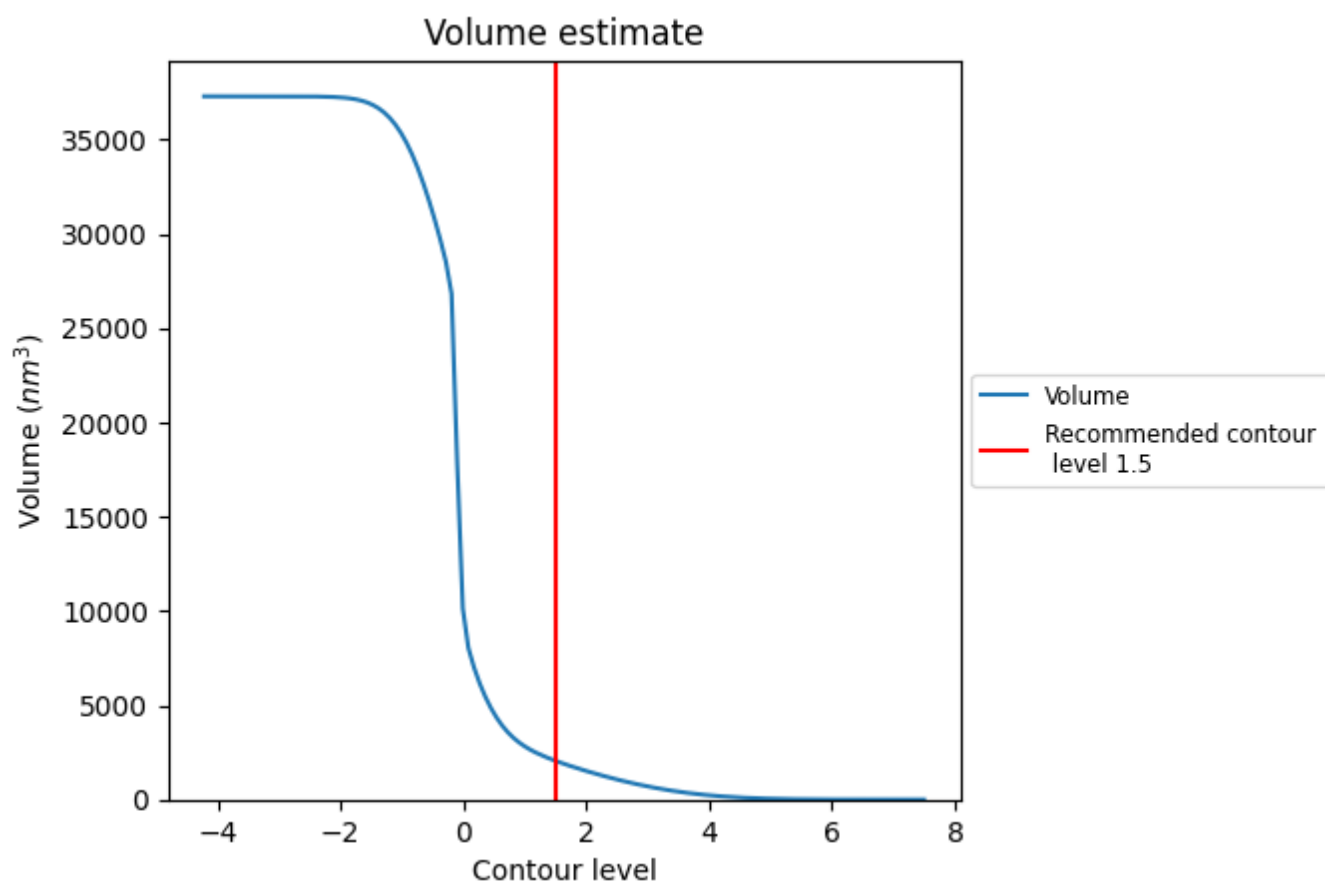
This section contains the results of statistical analysis of the map.

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.

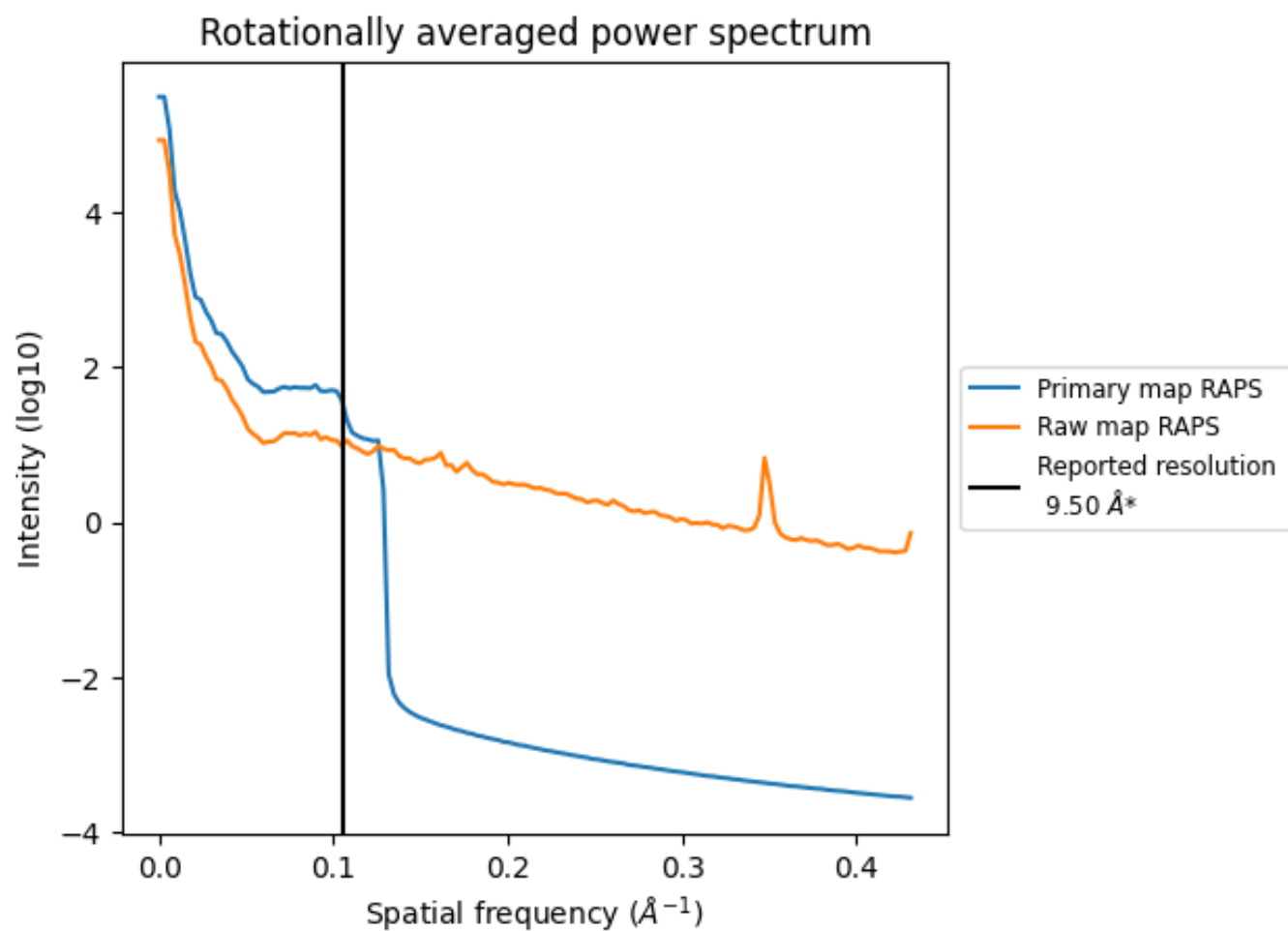
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2056 nm³; this corresponds to an approximate mass of 1857 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 ⓘ

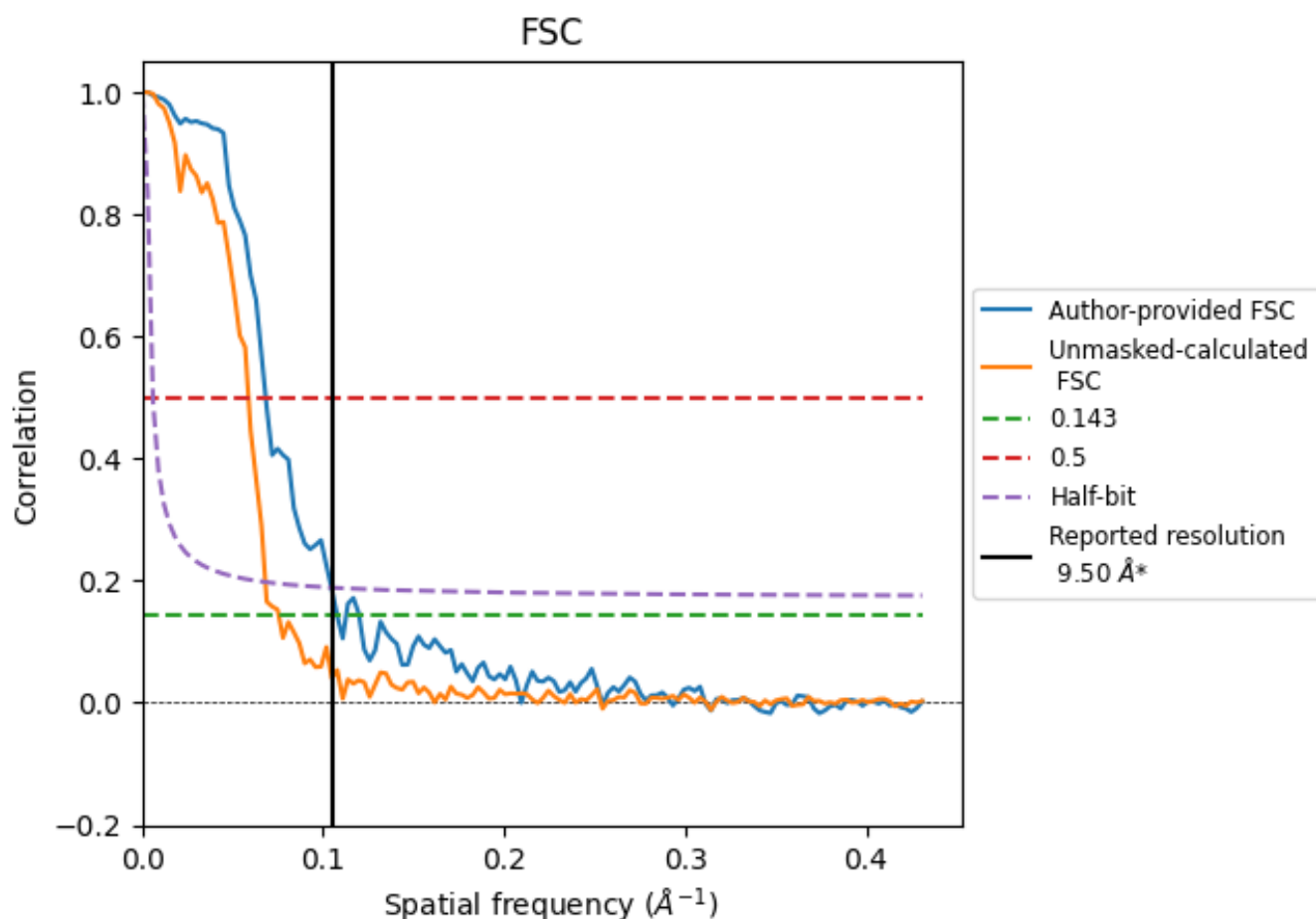


*Reported resolution corresponds to spatial frequency of 0.105 Å⁻¹

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 $0.105 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

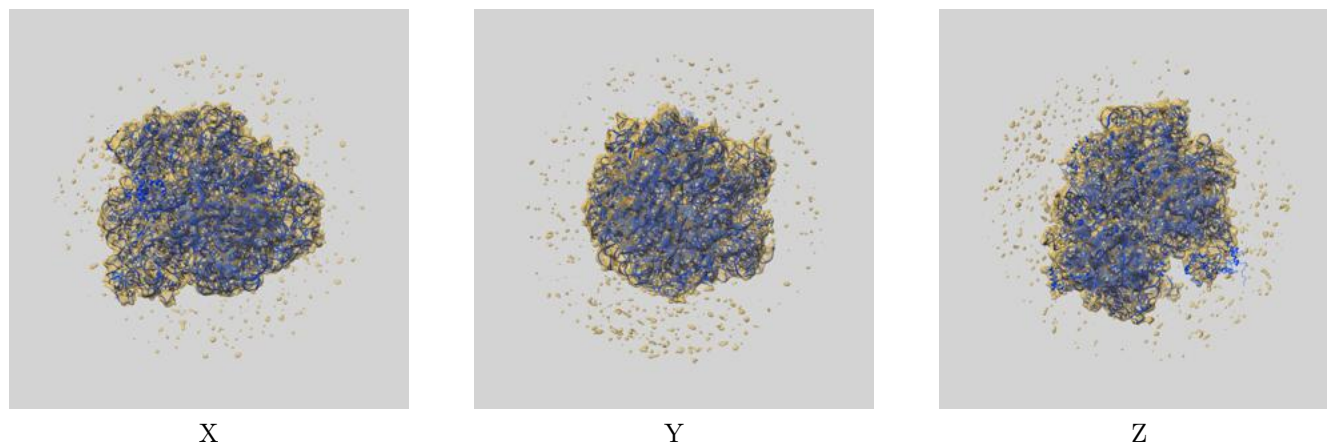
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.50	-	-
Author-provided FSC curve	9.29	14.64	9.56
Unmasked-calculated*	13.26	17.04	14.68

*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 13.26 differs from the reported value 9.5 by more than 10 %

9 Map-model fit [i](#)

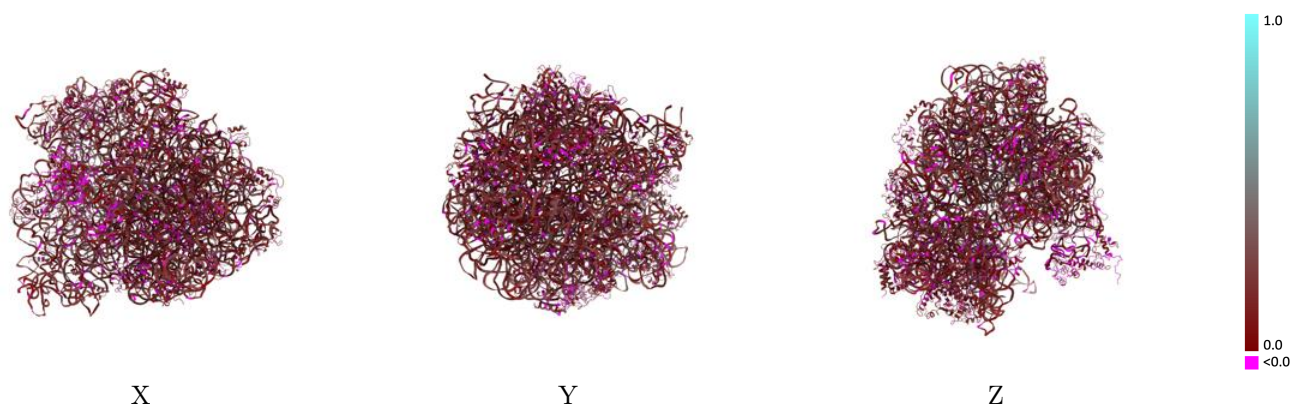
This section contains information regarding the fit between EMDB map EMD-13460 and PDB model 7PJU. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



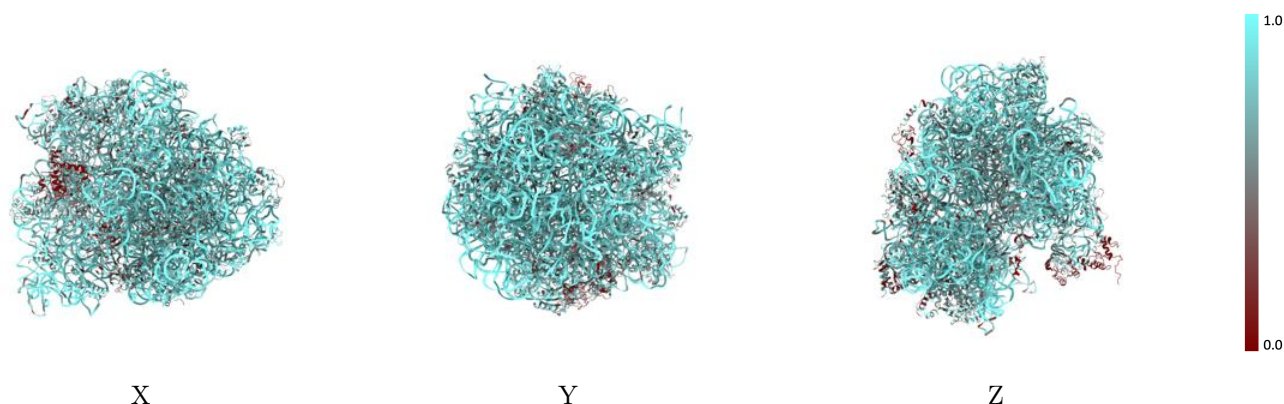
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



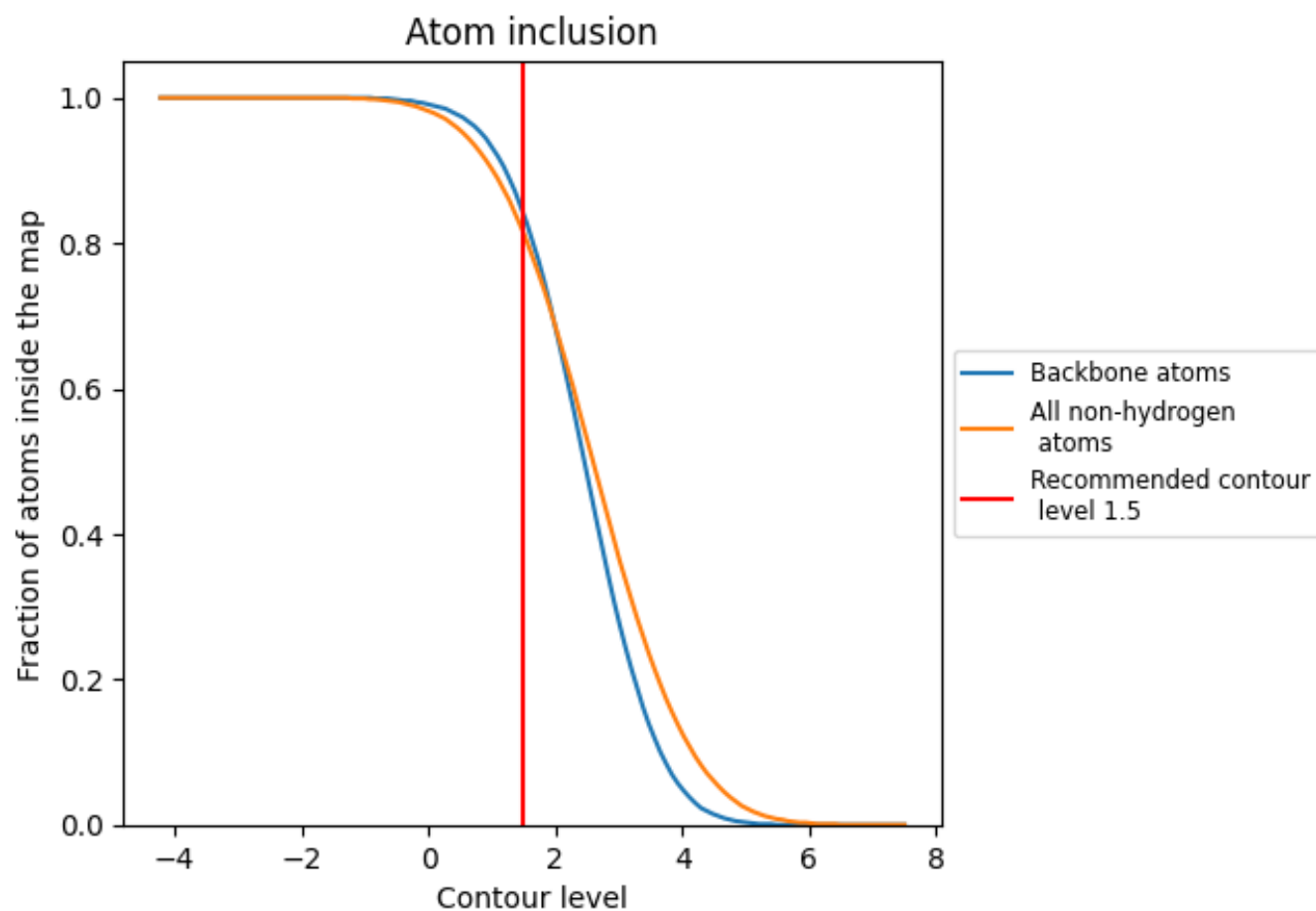
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 81% 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	 0.8140	 0.1430
0	 0.5650	 0.0650
1	 0.6260	 0.1320
2	 0.6450	 0.0900
3	 0.5700	 0.0710
4	 0.7340	 0.0710
5	 0.1210	 0.0200
6	 0.5190	 0.0750
A	 0.9040	 0.1600
B	 0.9440	 0.1790
C	 0.5710	 0.1070
D	 0.6130	 0.0920
E	 0.6680	 0.1090
F	 0.7140	 0.1240
G	 0.6820	 0.1040
H	 0.3030	 0.1040
I	 0.3160	 0.0210
J	 0.6400	 0.1050
K	 0.5200	 0.1080
L	 0.6270	 0.0920
M	 0.6250	 0.1010
N	 0.7040	 0.0910
O	 0.7900	 0.1170
P	 0.5700	 0.1070
Q	 0.6950	 0.0970
R	 0.7250	 0.1160
S	 0.6360	 0.1030
T	 0.6800	 0.1170
U	 0.7930	 0.1360
V	 0.7590	 0.1240
W	 0.6740	 0.0710
X	 0.6120	 0.1240
Y	 0.7490	 0.1330
Z	 0.6410	 0.1250
a	 0.9010	 0.1560



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Chain	Atom inclusion	Q-score
b	 0.4750	 0.1300
c	 0.6320	 0.1230
d	 0.6260	 0.1120
e	 0.6910	 0.1360
f	 0.6260	 0.1350
g	 0.5370	 0.1150
h	 0.6060	 0.1010
i	 0.7110	 0.0960
j	 0.6430	 0.1090
k	 0.5920	 0.1280
l	 0.5790	 0.1210
m	 0.6560	 0.1260
n	 0.7170	 0.0990
o	 0.6710	 0.0990
p	 0.6540	 0.0940
q	 0.6300	 0.0910
r	 0.5780	 0.0860
s	 0.6790	 0.0980
t	 0.7220	 0.1400
u	 0.5440	 0.1240
v	 0.8240	 0.1760
w	 0.7150	 0.1440
y	 0.4000	 0.0600
z	 0.7870	 0.1390