



# wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 03:33 am BST

PDB ID : 7PJS / pdb\_00007pjs  
EMDB ID : EMD-13458  
Title : Structure of the 70S ribosome with tRNAs in the classical pre-translocation state and apramycin (C)  
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.  
Deposited on : 2021-08-24  
Resolution : 2.35 Å (reported)  
Based on initial models : 4AQY, 6YSS, 5LZD

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

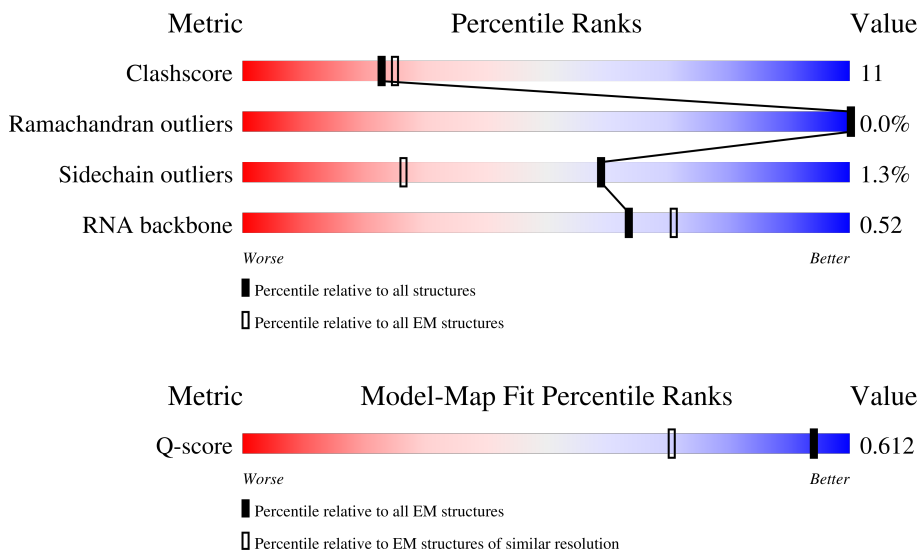
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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

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

The reported resolution of this entry is 2.35 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	4607 ( 1.85 - 2.85 )

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  $\geq 3$ , 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	
2	1	55	













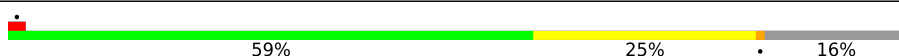
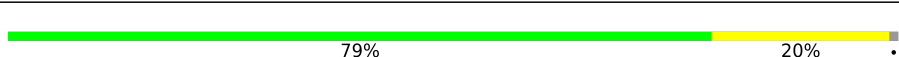
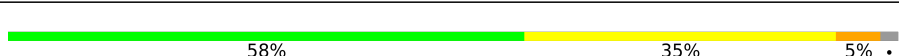

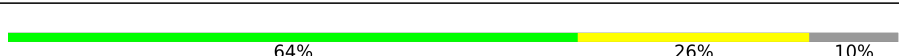
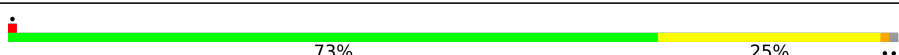
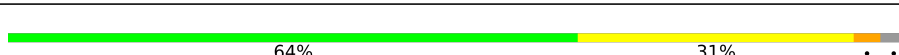
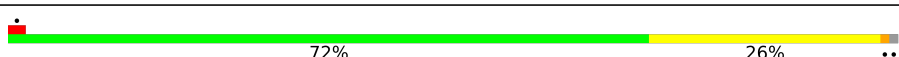
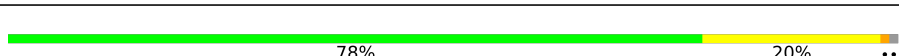



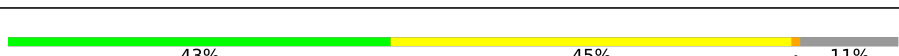
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Mol	Chain	Length	Quality of chain
3	2	46	85% 15%
4	3	65	88% 11%
5	4	38	74% 26%
6	5	165	79% 77% 21%
7	6	70	10% 47% 46% 6%
8	A	2903	49% 42% 9%
9	B	120	57% 32% 12%
10	C	273	75% 24%
11	D	209	80% 20%
12	E	201	88% 12%
13	F	179	61% 37%
14	G	177	67% 32%
15	H	149	48% 57% 42%
16	I	142	96% 94% 5%
17	J	142	82% 18%
18	K	123	71% 28%
19	L	144	84% 15%
20	M	136	71% 29%
21	N	127	76% 18% 6%
22	O	117	78% 21%
23	P	115	70% 29%
24	Q	118	82% 17%
25	R	103	76% 23%
26	S	110	82% 18%
27	T	100	72% 20% 7%







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Mol	Chain	Length	Quality of chain
28	U	104	 72% 26%
29	V	94	 70% 30%
30	W	85	 75% 13% 12%
31	X	78	 77% 22%
32	Y	63	 75% 25%
33	Z	59	 81% 17%
34	a	1542	 44% 45% 10%
35	b	240	 5% 62% 28% 9%
36	c	233	 65% 24% 12%
37	d	206	 71% 28%
38	e	167	 72% 22% 6%
39	f	135	 53% 21% 26%
40	g	179	 59% 25% 16%
41	h	130	 79% 20%
42	i	130	 58% 35% 5%
43	j	103	 66% 29% 5%
44	k	129	 64% 26% 10%
45	l	124	 73% 25% ..
46	m	118	 64% 31% ..
47	n	102	 72% 26% ..
48	o	89	 78% 20% ..
49	p	82	 76% 22%
50	q	84	 75% 19% 5%
51	r	75	 68% 19% 13%
52	s	92	 43% 45% 11%

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Mol	Chain	Length	Quality of chain
53	t	87	 76% 21% ..
54	u	71	 61% 31% 8%
55	v	77	 44% 42% 13% .
56	w	76	 34% 46% 18% .
57	y	2	 50% 50%
58	z	33	 15% 15% . 67%

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 147741 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
			Total	C	N	O	S		
1	0	56	444	269	94	80	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	A	2903	62338	27816	11471	20148	2903	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 16 is a protein called 50S ribosomal protein L11.

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

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

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

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

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

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

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

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

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

- 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	S	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	S	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 50S 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 50S ribosomal protein L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

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

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

- Molecule 39 is a protein called 30S ribosomal protein S6.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

- 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	
			Total	C	N	O	P			S
55	v	77	1642	733	297	534	77	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	y	2	21	15	2	3	1	0	0

- Molecule 58 is a RNA chain called mRNA.

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

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	0	1	Total 1	Mg 1	0
59	A	258	Total 258	Mg 258	0
59	B	4	Total 4	Mg 4	0
59	C	2	Total 2	Mg 2	0
59	D	1	Total 1	Mg 1	0
59	N	1	Total 1	Mg 1	0
59	O	1	Total 1	Mg 1	0
59	P	1	Total 1	Mg 1	0
59	a	92	Total 92	Mg 92	0

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Mol	Chain	Residues	Atoms		AltConf
59	m	1	Total	Mg	0
			1	1	
59	n	1	Total	Mg	0
			1	1	

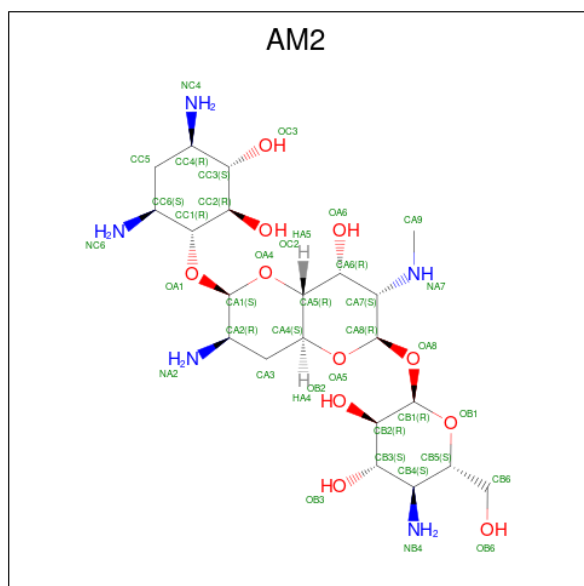
- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	4	1	Total	Zn	0
			1	1	
60	6	1	Total	Zn	0
			1	1	

- Molecule 61 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
61	A	1	Total	Na	0
			1	1	
61	B	1	Total	Na	0
			1	1	

- Molecule 62 is APRAMYCIN (CCD ID: AM2) (formula: C<sub>21</sub>H<sub>41</sub>N<sub>5</sub>O<sub>11</sub>).



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

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

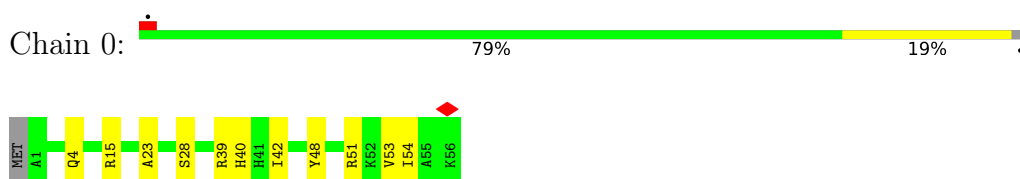
- Molecule 63 is water.

Mol	Chain	Residues	Atoms		AltConf
63	A	5	Total 5	O 5	0
63	a	15	Total 15	O 15	0
63	z	2	Total 2	O 2	0

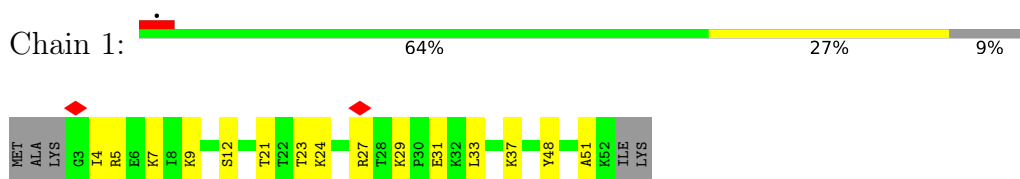
### 3 Residue-property plots [i](#)

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.

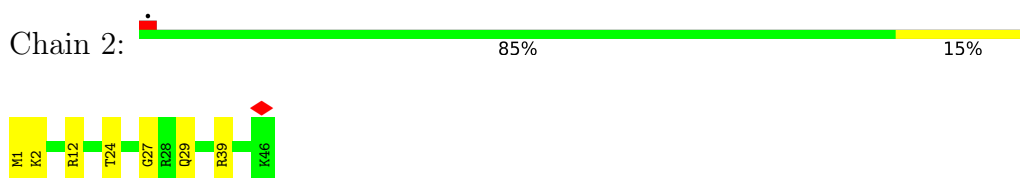
- Molecule 1: 50S ribosomal protein L32



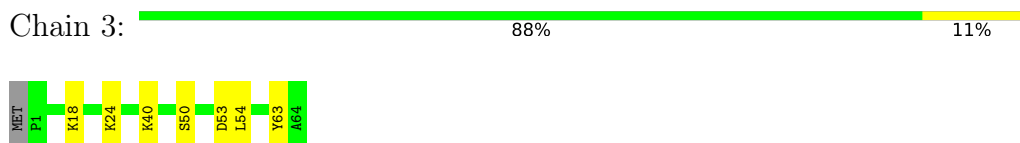
- Molecule 2: 50S ribosomal protein L33



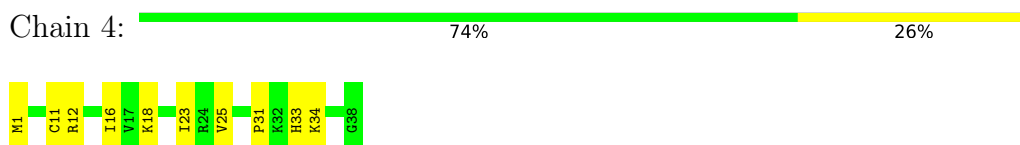
- Molecule 3: 50S ribosomal protein L34



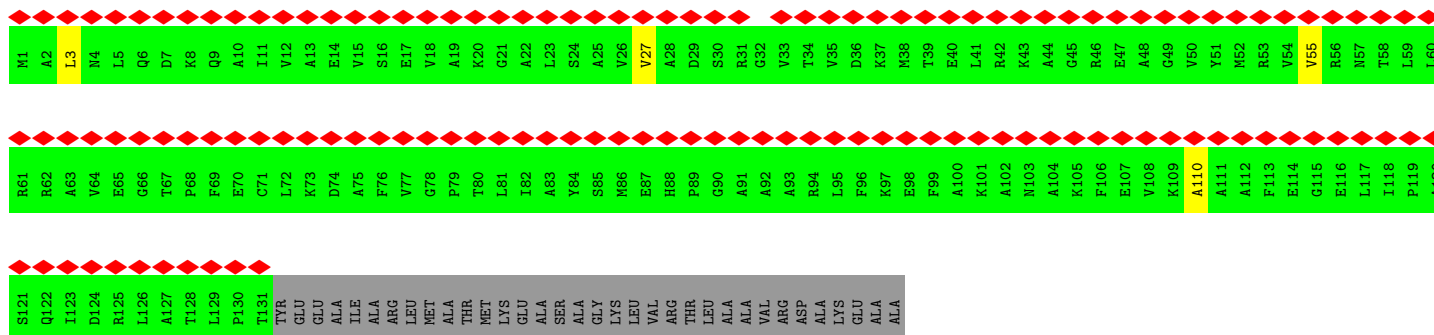
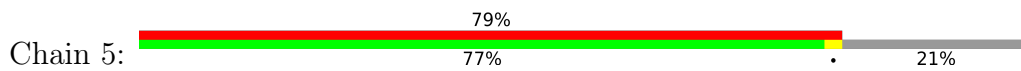
- Molecule 4: 50S ribosomal protein L35



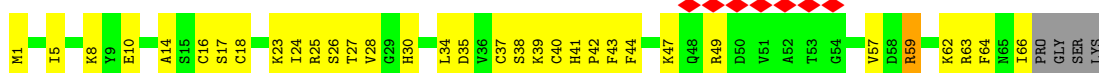
- Molecule 5: 50S ribosomal protein L36



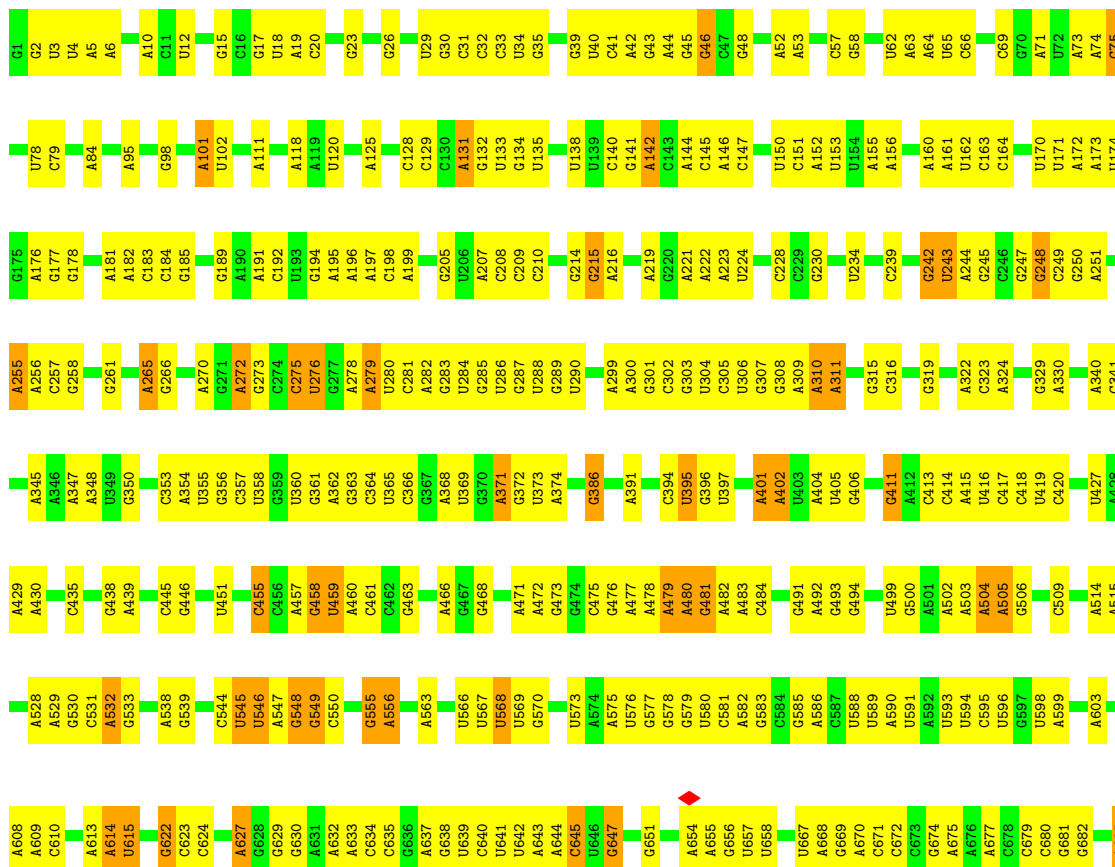
- Molecule 6: 50S ribosomal protein L10



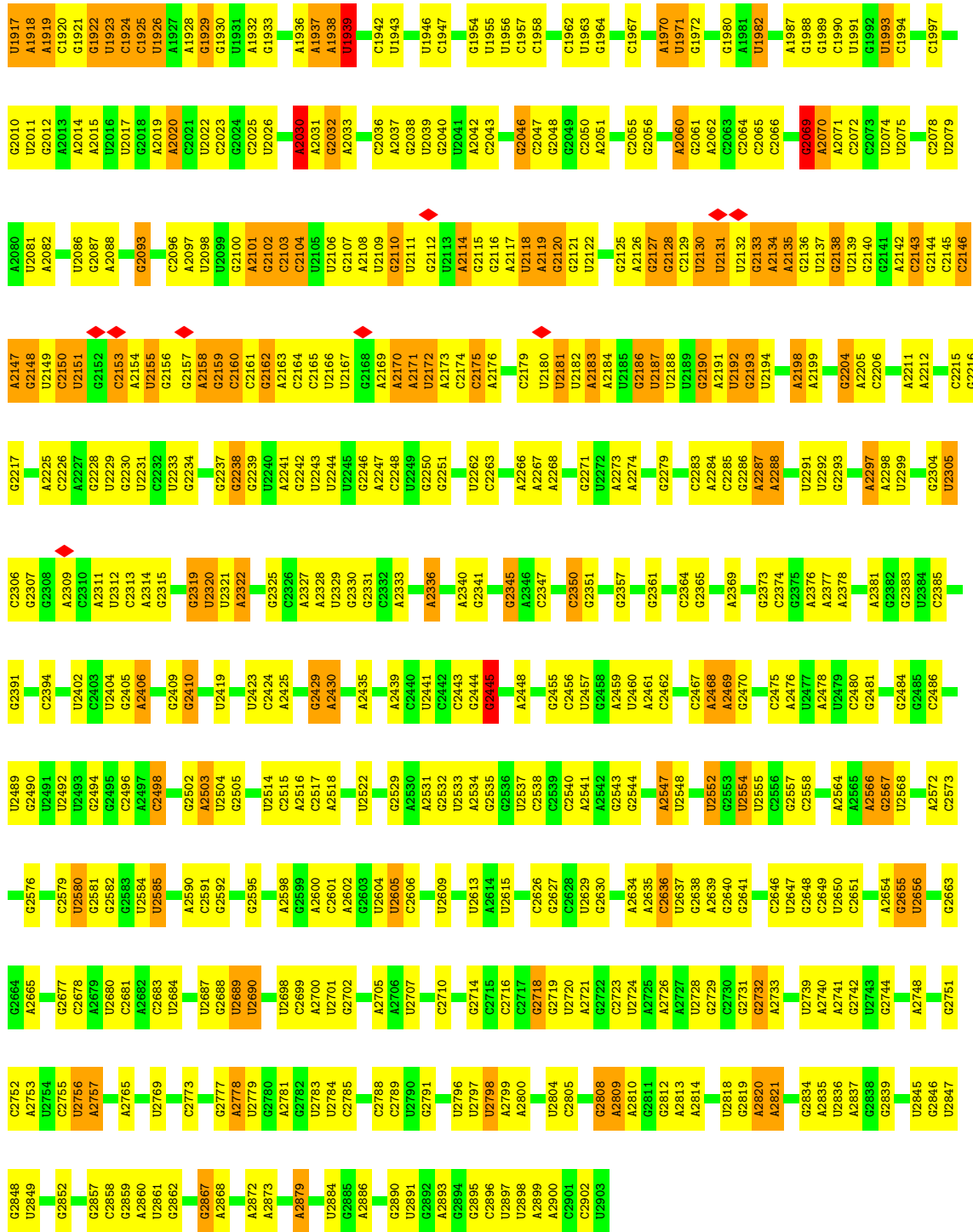
• Molecule 7: 50S ribosomal protein L31



• Molecule 8: 23S ribosomal RNA



U1818	A1819	U1820	G1826	U1827	G1828	A1829	C1830	G1831	C1832	G1835	C1838	G1842	G1843	G1844	G1847	A1848	A1853	A1854	U1855	U1856	C1857	A1858	A1866	C1867	C1868	G1869	C1874	G1875	G1884	A1885	A1889	A1890	A1901	C1902	G1903	C1904	C1905	G1906	G1907	C1908	C1909	G1910	U1911	A1912	A1913	3TD1915	A1916								
A1717	U1720	G1721	A1722	C1726	C1727	C1728	U1729	U1730	G1731	C1732	G1738	A1744	A1745	A1746	U1747	C1748	G1753	C1760	C1764	A1773	U1779	U1782	A1783	A1784	A1785	A1786	C1790	A1791	G1792	C1793	A1794	C1795	U1796	G1797	G1798	G1799	C1800	A1801	A1802	A1803	G1807	A1808	A1809	A1810	C1816	G1817									
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A1618	A1626	G1631	A1632	G1633	U1634	U1635	A1636	A1637	A1641	A1642	C1646	A1647	A1648	U1649	A1650	G1651	G1652	G1653	A1654	A1655	C1656	A1657	G1658	G1659	A1672	G1673	G1674	U1680	G1681	G1682	U1683	G1684	U1688	C1693	C1694	G1697	G1698	A1698	G1699	A1700	G1703	C1704	U1709	U1710	A1711	G1715	U1716								
G1443	G1444	G1445	C1446	C1447	C1451	G1452	A1453	U1460	C1461	G1464	G1465	A1469	A1470	G1475	G1478	G1482	U1483	U1484	U1485	U1486	U1487	A1490	G1492	A1493	A1494	A1495	A1496	U1497	C1498	A1504	A1505	U1506	C1507	A1508	A1509	G1510	U1513	G1514	A1515	G1521	G1522	U1523	G1524	A1528	A1532										
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A1175	U1176	G1177	C1178	G1179	U1180	U1181	A1182	U1183	U1184	G1187	G1197	U1198	U1199	C1200	U1203	A1204	A1205	G1206	G1212	U1219	G1220	U1224	G1225	G1226	G1227	U1231	G1232	G1233	U1234	G1235	G1236	A1247	G1248	U1249	G1250	C1251	A1253	A1254	U1255	G1256	A1262	U1263	A1264	G1265	G1266	A1269	C1270	G1271							
A1088	A1089	A1090	G1091	C1092	U1093	U1094	A1095	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	A1110	A1111	G1112	G1115	G1120	C1123	G1124	G1125	A1126	U1130	G1131	U1132	A1133	A1134	C1135	U1141	A1142	G1149	C1150	G1153	C1154	A1155	A1156	G1168	A1169	C1170	G1171	A1172	U1173	U1174					
G1022	U1023	G1026	A1027	A1028	A1029	C1030	G1031	A1032	U1033	G1036	G1037	G1038	A1039	A1040	G1041	C1044	C1045	A1046	G1047	A1048	C1053	A1054	G1055	A1056	A1057	U1058	C1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	C1071	C1072	A1073	G1074	C1075	C1076	A1077	U1078	C1079	U1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087
U847	C848	A849	U850	G851	C852	C853	G856	G857	G858	G859	A863	G864	U871	A1040	U872	C876	A877	A878	G879	G880	G881	G882	G883	U884	C885	G886	G887	C888	C889	C890	G891	A892	C893	U894	U895	A896	C897	C898	A899	A900	C903	G907	C968	A909	A910	A911	C912	U913	G914	C915	G916	A917	A918	U846	
U866	C867	U868	A869	G890	A893	G894	G897	G784	A785	G786	U703	G704	U709	U710	G711	U714	A715	A716	C717	U720	A721	A722	C723	G726	A727	G728	G729	A730	A734	A739	C740	U741	A742	A743	U744	G745	U746	C747	A748	A749	A753	U754	U755	G760	A761	U762	A763	A764							

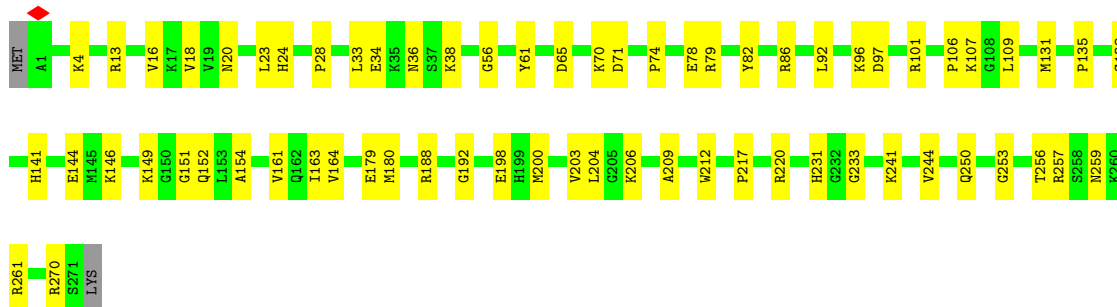


• Molecule 9: 5S ribosomal RNA

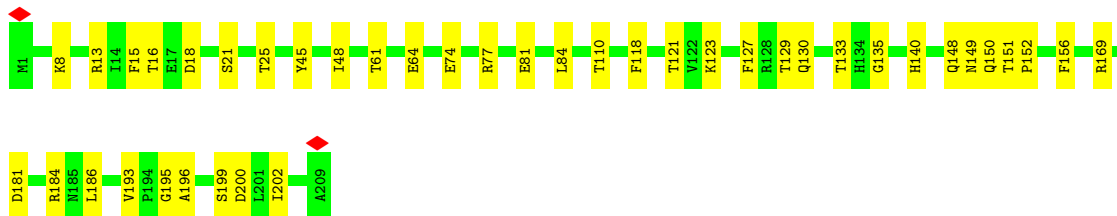
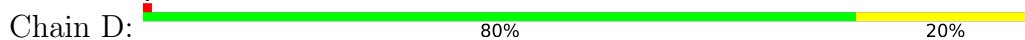




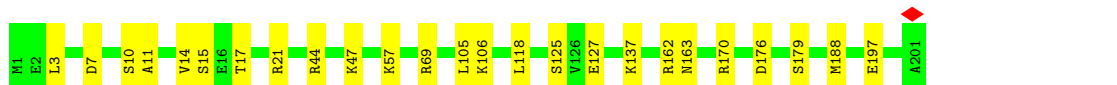
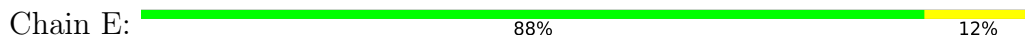
• Molecule 10: 50S ribosomal protein L2



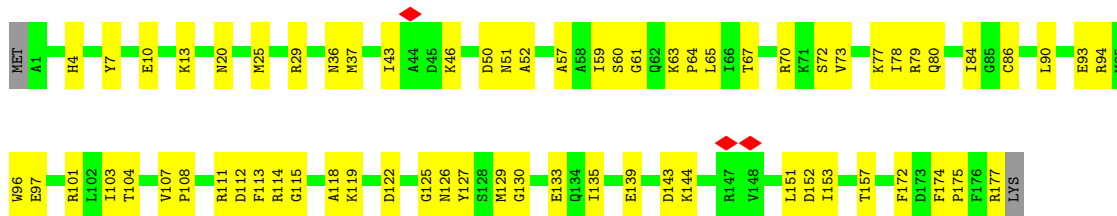
• Molecule 11: 50S ribosomal protein L3



• Molecule 12: 50S ribosomal protein L4

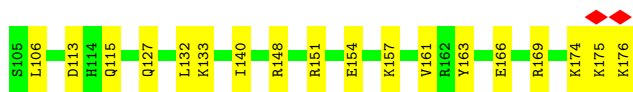


• Molecule 13: 50S ribosomal protein L5

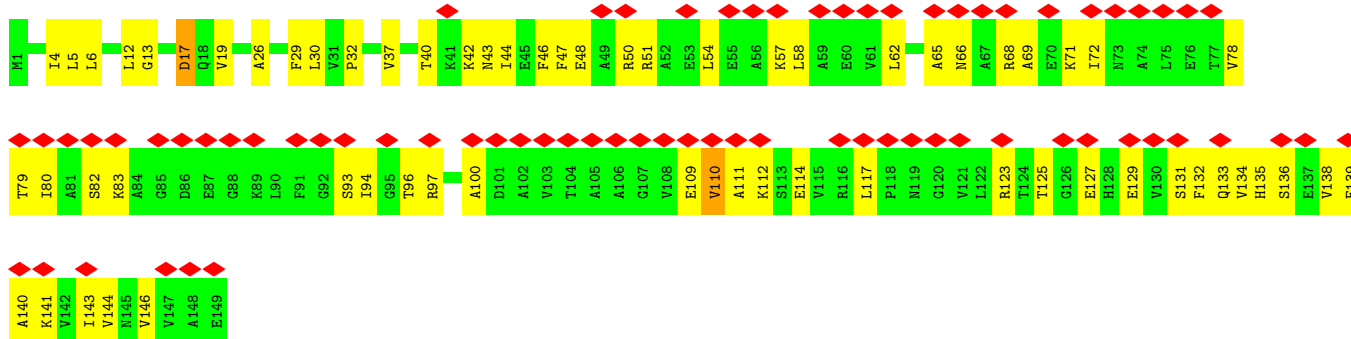


• Molecule 14: 50S ribosomal protein L6

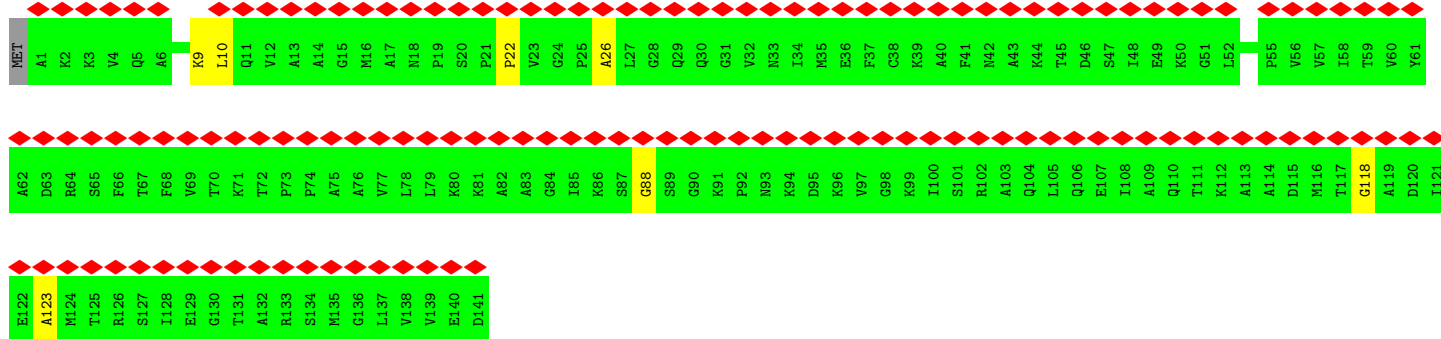
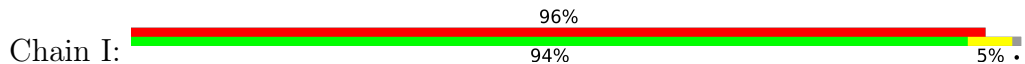




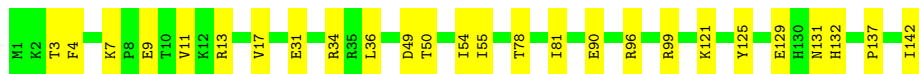
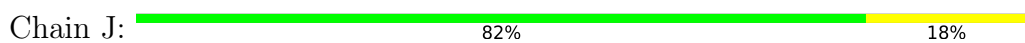
• Molecule 15: 50S ribosomal protein L9



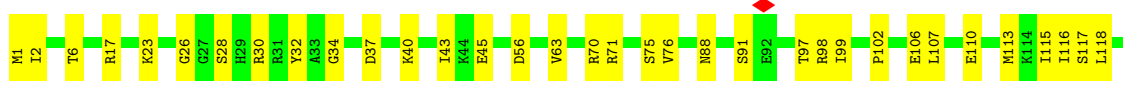
• Molecule 16: 50S ribosomal protein L11



• Molecule 17: 50S ribosomal protein L13

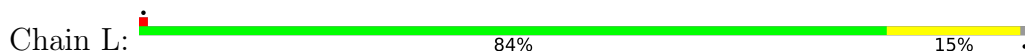


• Molecule 18: 50S ribosomal protein L14

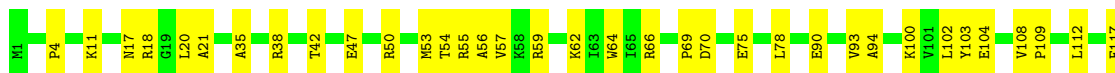




• Molecule 19: 50S ribosomal protein L15



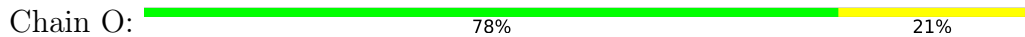
• Molecule 20: 50S ribosomal protein L16



• Molecule 21: 50S ribosomal protein L17



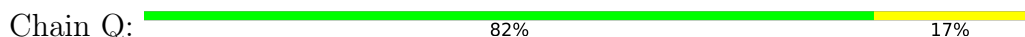
• Molecule 22: 50S ribosomal protein L18



• Molecule 23: 50S ribosomal protein L19

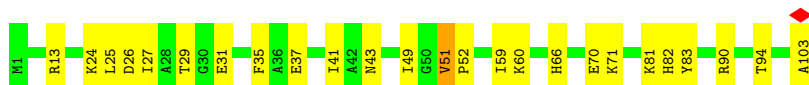
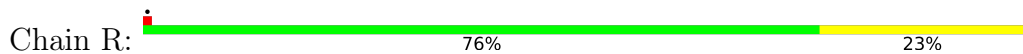


• Molecule 24: 50S ribosomal protein L20

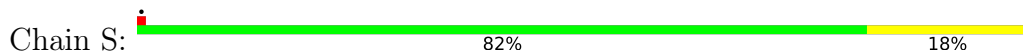




- Molecule 25: 50S ribosomal protein L21



- Molecule 26: 50S ribosomal protein L22



- Molecule 27: 50S ribosomal protein L23



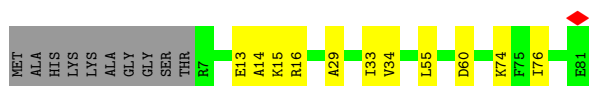
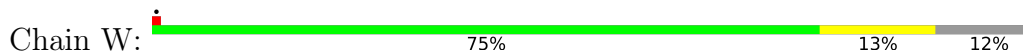
- Molecule 28: 50S ribosomal protein L24



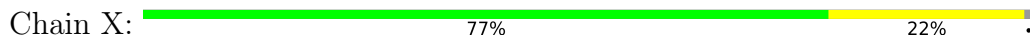
- Molecule 29: 50S ribosomal protein L25



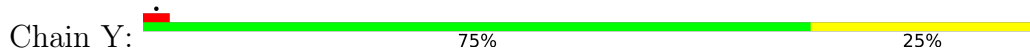
- Molecule 30: 50S ribosomal protein L27



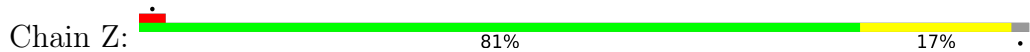
- Molecule 31: 50S ribosomal protein L28



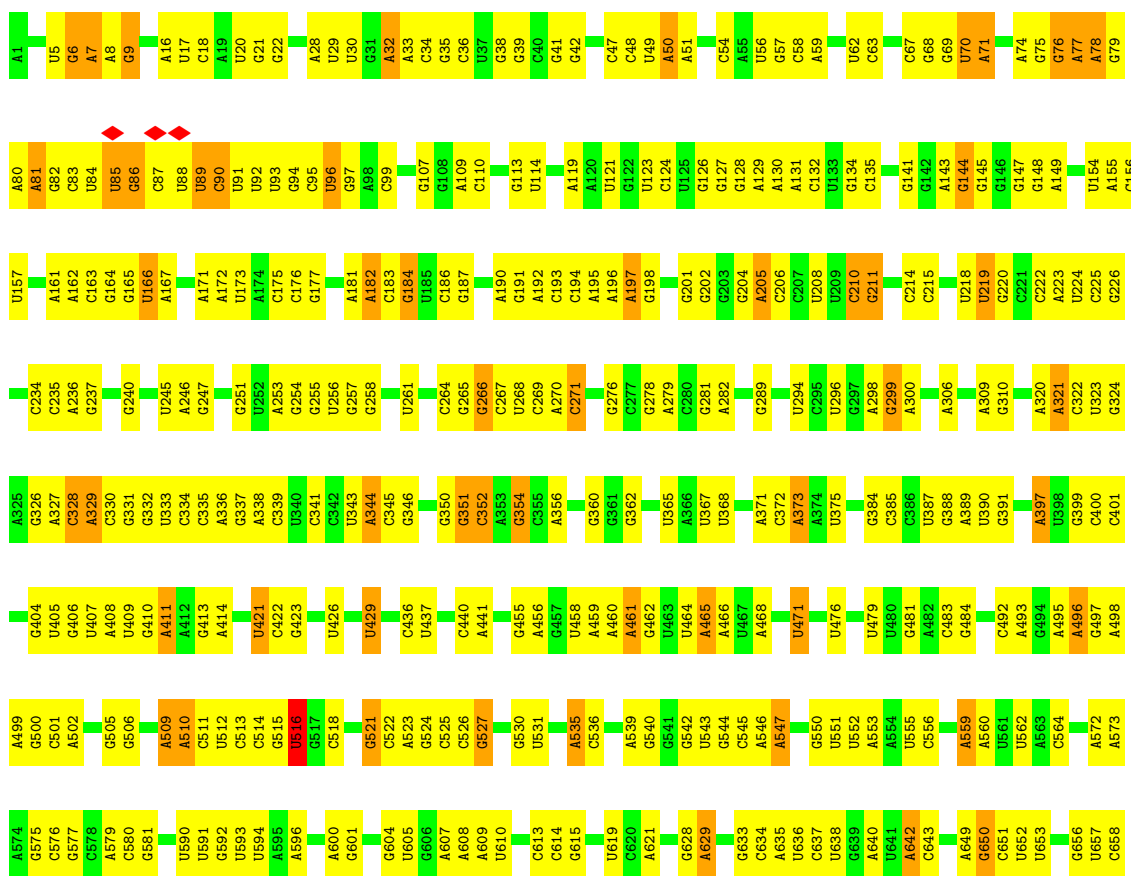
• Molecule 32: 50S ribosomal protein L29

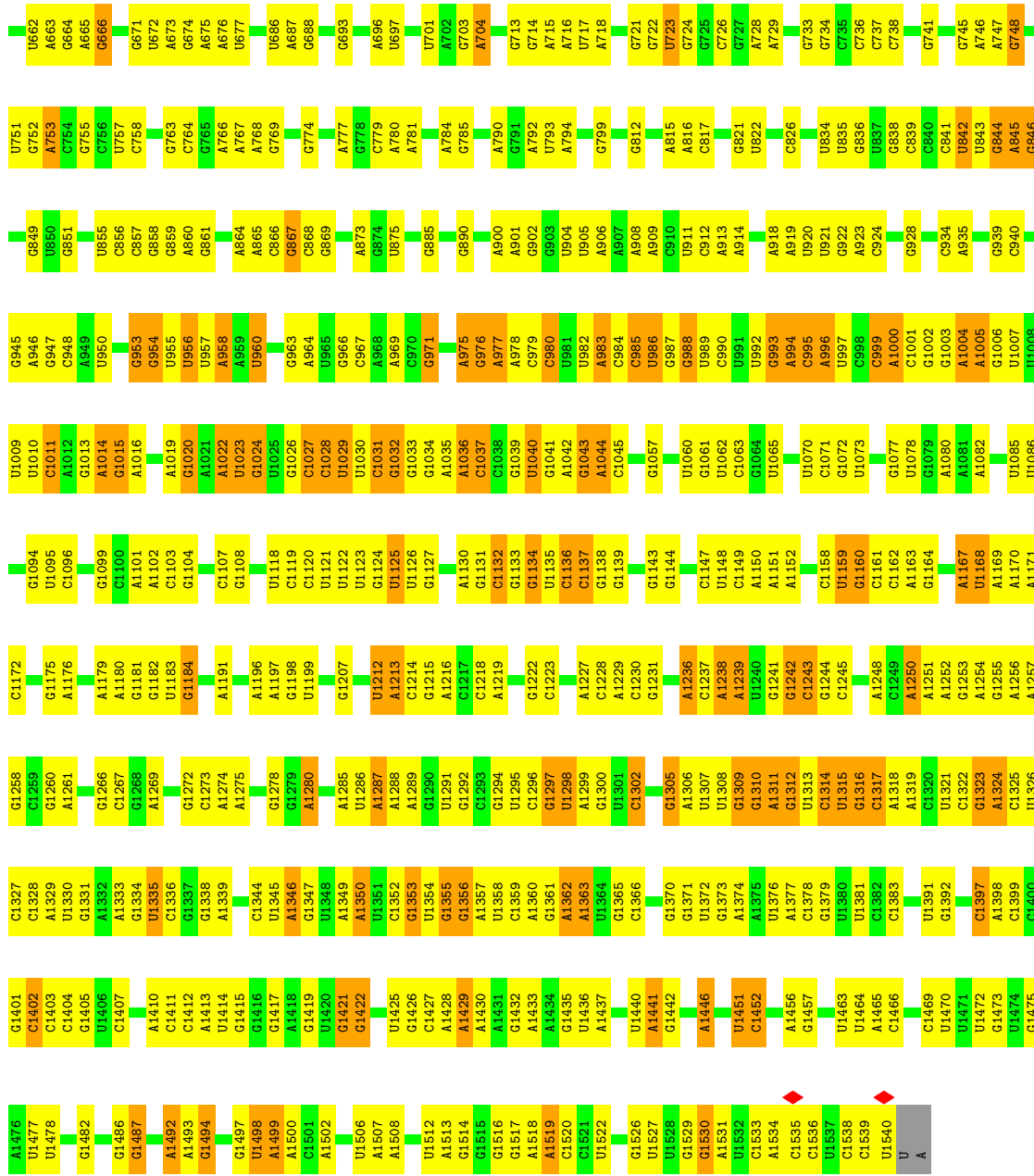


• Molecule 33: 50S ribosomal protein L30



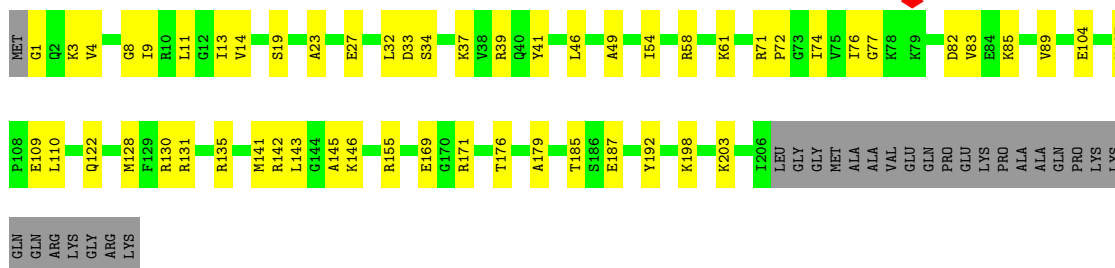
• Molecule 34: 16S ribosomal RNA





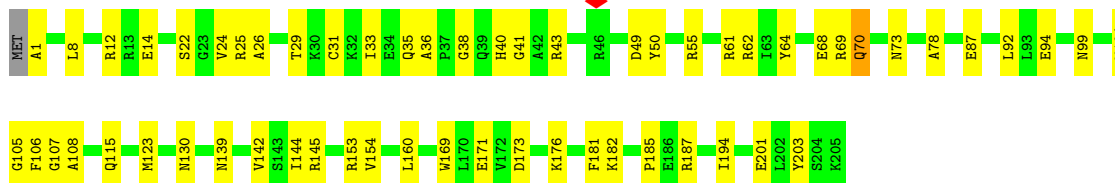
- Molecule 36: 30S ribosomal protein S3

Chain c:  65% 24% 12%



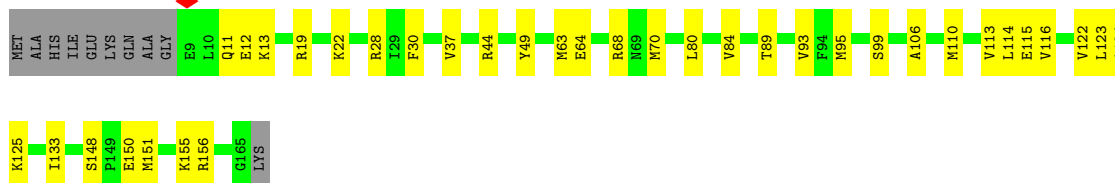
- Molecule 37: 30S ribosomal protein S4

Chain d:  71% 28%



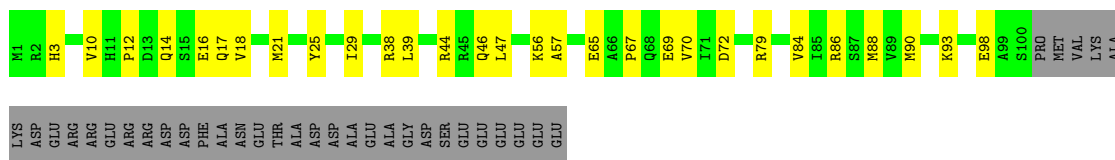
- Molecule 38: 30S ribosomal protein S5

Chain e:  72% 22% 6%



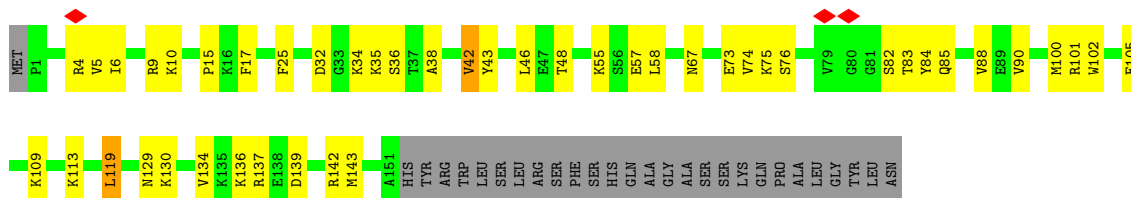
- Molecule 39: 30S ribosomal protein S6

Chain f:  53% 21% 26%

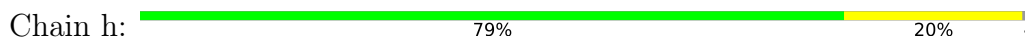


- Molecule 40: 30S ribosomal protein S7

Chain g:  59% 25% 16%



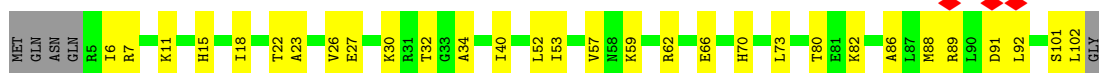
• Molecule 41: 30S ribosomal protein S8



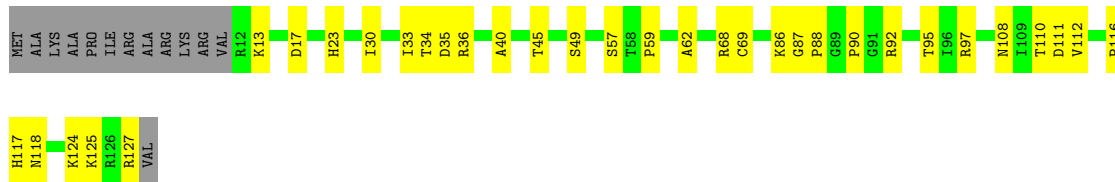
• Molecule 42: 30S ribosomal protein S9



• Molecule 43: 30S ribosomal protein S10



• Molecule 44: 30S ribosomal protein S11



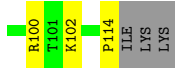
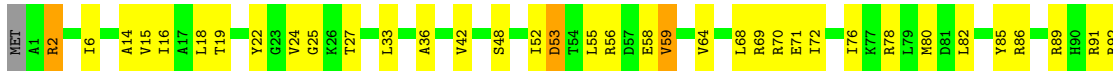
• Molecule 45: 30S ribosomal protein S12





- Molecule 46: 30S ribosomal protein S13

Chain m: 64% 31%



- Molecule 47: 30S ribosomal protein S14

Chain n: 72% 26%



- Molecule 48: 30S ribosomal protein S15

Chain o: 78% 20%



- Molecule 49: 30S ribosomal protein S16

Chain p: 76% 22%



- Molecule 50: 30S ribosomal protein S17

Chain q: 75% 19% 5%

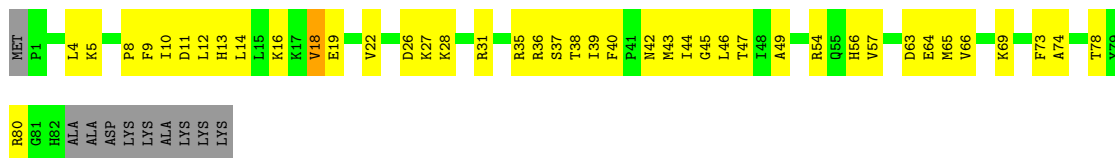


- Molecule 51: 30S ribosomal protein S18

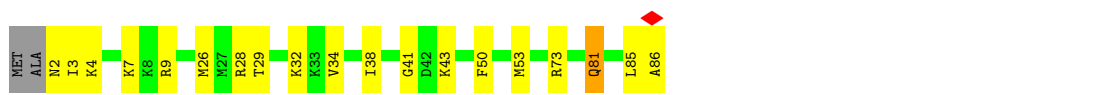
Chain r: 68% 19% 13%



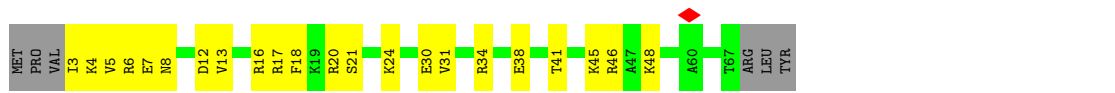
• Molecule 52: 30S ribosomal protein S19



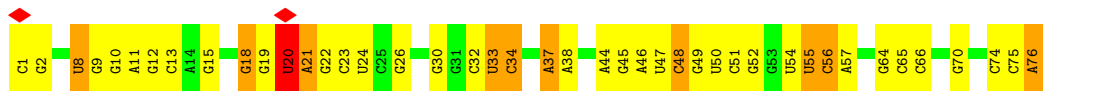
• Molecule 53: 30S ribosomal protein S20



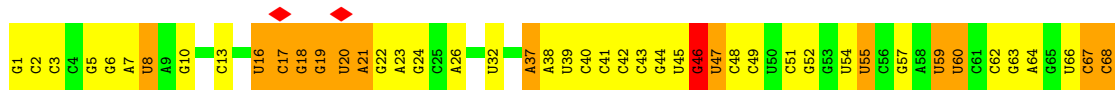
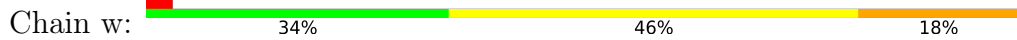
• Molecule 54: 30S ribosomal protein S21



• Molecule 55: P-site tRNA(fMet)



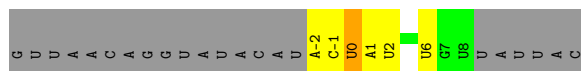
• Molecule 56: P-site fMet-Phe-tRNA(Phe)



• Molecule 57: Dipeptide (FME-PHE)



● Molecule 58: mRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	537761	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	21.985	Depositor
Minimum map value	-5.122	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6525, 0.6525, 0.6525	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.23	0/450	0.38	0/599
2	1	0.19	0/416	0.31	0/554
3	2	0.23	0/380	0.29	0/498
4	3	0.22	0/513	0.29	0/676
5	4	0.22	0/303	0.42	0/397
6	5	0.08	0/646	0.27	0/898
7	6	0.21	0/531	0.59	0/709
8	A	0.28	0/69266	0.30	0/108055
9	B	0.23	0/2873	0.28	0/4478
10	C	0.24	0/2121	0.35	0/2852
11	D	0.23	0/1586	0.34	0/2134
12	E	0.21	0/1571	0.29	0/2113
13	F	0.20	0/1434	0.41	0/1926
14	G	0.16	0/1343	0.32	0/1816
15	H	0.21	0/1122	0.57	0/1515
16	I	0.08	0/692	0.25	0/960
17	J	0.22	0/1152	0.30	0/1551
18	K	0.23	0/947	0.36	0/1268
19	L	0.23	0/1054	0.37	0/1403
20	M	0.23	0/1093	0.31	0/1460
21	N	0.22	0/973	0.33	0/1301
22	O	0.20	0/902	0.38	0/1209
23	P	0.23	0/929	0.30	0/1242
24	Q	0.22	0/960	0.26	0/1278
25	R	0.25	0/829	0.40	0/1107
26	S	0.22	0/864	0.30	0/1156
27	T	0.21	0/744	0.35	0/994
28	U	0.20	0/787	0.36	0/1051
29	V	0.21	0/766	0.38	0/1025
30	W	0.22	0/582	0.30	0/769
31	X	0.25	0/635	0.34	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Y	0.21	0/510	0.40	0/677
33	Z	0.21	0/453	0.28	0/605
34	a	0.25	0/36725	0.32	0/57285
35	b	0.17	0/1735	0.40	0/2338
36	c	0.21	0/1651	0.34	0/2225
37	d	0.18	0/1665	0.34	0/2227
38	e	0.22	0/1154	0.34	0/1554
39	f	0.20	0/835	0.42	0/1128
40	g	0.18	0/1195	0.40	0/1602
41	h	0.18	0/989	0.27	0/1326
42	i	0.21	0/1034	0.42	0/1375
43	j	0.23	0/796	0.54	0/1077
44	k	0.21	0/885	0.40	0/1195
45	l	0.24	0/969	0.41	0/1300
46	m	0.20	0/892	0.41	0/1193
47	n	0.20	0/811	0.31	0/1081
48	o	0.18	0/722	0.30	0/964
49	p	0.20	0/659	0.35	0/884
50	q	0.21	0/657	0.38	0/881
51	r	0.20	0/544	0.35	0/731
52	s	0.23	0/675	0.43	0/908
53	t	0.17	0/671	0.28	0/888
54	u	0.20	0/512	0.37	0/683
55	v	0.23	0/1745	0.29	0/2716
56	w	0.24	1/1650 (0.1%)	0.28	0/2569
57	y	0.20	0/11	0.17	0/13
58	z	0.25	0/255	0.73	2/394 (0.5%)
All	All	0.25	1/158864 (0.0%)	0.32	2/237661 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	46	G7M	O3'-P	5.18	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	z	-1	C	OP2-P-O3'	-8.79	81.61	108.00
58	z	-1	C	OP1-P-O3'	-8.78	81.67	108.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	8	0
2	1	409	0	440	15	0
3	2	377	0	418	6	0
4	3	504	0	574	7	0
5	4	302	0	340	8	0
6	5	647	0	336	3	0
7	6	522	0	521	37	0
8	A	62338	0	31372	1050	0
9	B	2570	0	1301	33	0
10	C	2082	0	2157	52	0
11	D	1565	0	1616	35	0
12	E	1552	0	1619	21	0
13	F	1410	0	1447	59	0
14	G	1323	0	1374	39	0
15	H	1111	0	1148	48	0
16	I	693	0	347	8	0
17	J	1129	0	1162	26	0
18	K	938	0	1012	29	0
19	L	1045	0	1117	18	0
20	M	1074	0	1157	31	0
21	N	960	0	1000	17	0
22	O	892	0	923	22	0
23	P	917	0	965	27	0
24	Q	947	0	1022	18	0
25	R	816	0	839	18	0
26	S	857	0	922	13	0
27	T	738	0	807	17	0
28	U	779	0	834	21	0
29	V	753	0	780	23	0
30	W	575	0	592	10	0
31	X	625	0	655	14	0
32	Y	509	0	543	19	0
33	Z	449	0	491	7	0
34	a	33050	0	16654	628	0
35	b	1704	0	1732	51	0
36	c	1624	0	1699	37	0
37	d	1643	0	1710	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	e	1141	0	1170	27	0
39	f	817	0	808	21	0
40	g	1181	0	1240	38	0
41	h	979	0	1034	18	0
42	i	1022	0	1070	44	0
43	j	786	0	828	27	0
44	k	869	0	878	28	0
45	l	955	0	1019	29	0
46	m	883	0	944	34	0
47	n	799	0	841	24	0
48	o	714	0	737	15	0
49	p	649	0	666	15	0
50	q	648	0	691	15	0
51	r	535	0	552	11	0
52	s	658	0	685	33	0
53	t	665	0	714	17	0
54	u	506	0	502	23	0
55	v	1642	0	839	26	0
56	w	1631	0	836	40	0
57	y	21	0	19	1	0
58	z	230	0	116	4	0
59	0	1	0	0	0	0
59	A	258	0	0	0	0
59	B	4	0	0	0	0
59	C	2	0	0	0	0
59	D	1	0	0	0	0
59	N	1	0	0	0	0
59	O	1	0	0	0	0
59	P	1	0	0	0	0
59	a	92	0	0	0	0
59	m	1	0	0	0	0
59	n	1	0	0	0	0
60	4	1	0	0	0	0
60	6	1	0	0	0	0
61	A	1	0	0	0	0
61	B	1	0	0	0	0
62	a	148	0	164	3	0
63	A	5	0	0	0	0
63	a	15	0	0	2	0
63	z	2	0	0	0	0
All	All	147741	0	98440	2674	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 11.

The worst 5 of 2674 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)
43:j:88:MET:HE3	43:j:89:ARG:H	1.20	1.02
34:a:1310:G:H1	34:a:1327:C:H5	1.15	0.92
8:A:1478:G:H1	8:A:1513:U:H3	1.17	0.91
8:A:881:G:H1	8:A:895:U:H3	1.15	0.90
56:w:5:G:N2	56:w:68:C:O2	2.04	0.89

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	54/57 (95%)	54 (100%)	0	0	100	100
2	1	48/55 (87%)	48 (100%)	0	0	100	100
3	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
4	3	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
5	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
6	5	129/165 (78%)	116 (90%)	13 (10%)	0	100	100
7	6	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
10	C	269/273 (98%)	256 (95%)	13 (5%)	0	100	100
11	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
12	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
13	F	175/179 (98%)	161 (92%)	14 (8%)	0	100	100
14	G	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
15	H	147/149 (99%)	128 (87%)	19 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	I	139/142 (98%)	130 (94%)	9 (6%)	0	100	100
17	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
18	K	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
19	L	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
20	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
21	N	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
22	O	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
23	P	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
24	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
25	R	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	12	12
26	S	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
27	T	91/100 (91%)	91 (100%)	0	0	100	100
28	U	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
29	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
30	W	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
31	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
32	Y	61/63 (97%)	61 (100%)	0	0	100	100
33	Z	56/59 (95%)	56 (100%)	0	0	100	100
35	b	216/240 (90%)	203 (94%)	13 (6%)	0	100	100
36	c	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
37	d	203/206 (98%)	190 (94%)	13 (6%)	0	100	100
38	e	155/167 (93%)	152 (98%)	3 (2%)	0	100	100
39	f	98/135 (73%)	94 (96%)	4 (4%)	0	100	100
40	g	149/179 (83%)	145 (97%)	4 (3%)	0	100	100
41	h	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
42	i	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
43	j	96/103 (93%)	85 (88%)	11 (12%)	0	100	100
44	k	114/129 (88%)	106 (93%)	8 (7%)	0	100	100
45	l	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
46	m	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
47	n	99/102 (97%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
49	p	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
50	q	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
51	r	63/75 (84%)	61 (97%)	2 (3%)	0	100	100
52	s	80/92 (87%)	79 (99%)	1 (1%)	0	100	100
53	t	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
54	u	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
All	All	5850/6220 (94%)	5602 (96%)	247 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	R	51	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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%)	50 (98%)	1 (2%)	48	63
5	4	34/34 (100%)	34 (100%)	0	100	100
7	6	59/62 (95%)	56 (95%)	3 (5%)	21	26
10	C	216/218 (99%)	216 (100%)	0	100	100
11	D	164/164 (100%)	164 (100%)	0	100	100
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	146 (99%)	2 (1%)	59	73
14	G	137/138 (99%)	136 (99%)	1 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	H	114/114 (100%)	110 (96%)	4 (4%)	32	42
17	J	116/116 (100%)	115 (99%)	1 (1%)	70	82
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	102 (100%)	0	100	100
20	M	109/109 (100%)	108 (99%)	1 (1%)	70	82
21	N	100/103 (97%)	99 (99%)	1 (1%)	68	81
22	O	86/87 (99%)	86 (100%)	0	100	100
23	P	99/100 (99%)	98 (99%)	1 (1%)	68	81
24	Q	89/90 (99%)	89 (100%)	0	100	100
25	R	84/84 (100%)	82 (98%)	2 (2%)	43	57
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	79 (99%)	1 (1%)	61	76
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%)	55 (100%)	0	100	100
33	Z	48/49 (98%)	47 (98%)	1 (2%)	47	61
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%)	171 (99%)	1 (1%)	78	87
38	e	114/126 (90%)	114 (100%)	0	100	100
39	f	87/116 (75%)	86 (99%)	1 (1%)	65	79
40	g	124/147 (84%)	119 (96%)	5 (4%)	28	37
41	h	104/105 (99%)	102 (98%)	2 (2%)	50	65
42	i	105/107 (98%)	94 (90%)	11 (10%)	6	6
43	j	86/90 (96%)	86 (100%)	0	100	100
44	k	89/99 (90%)	89 (100%)	0	100	100
45	l	103/104 (99%)	102 (99%)	1 (1%)	68	81
46	m	92/96 (96%)	86 (94%)	6 (6%)	15	18
47	n	79/84 (94%)	78 (99%)	1 (1%)	61	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	o	76/77 (99%)	74 (97%)	2 (3%)	40	54
49	p	65/65 (100%)	63 (97%)	2 (3%)	35	47
50	q	74/78 (95%)	73 (99%)	1 (1%)	59	73
51	r	56/65 (86%)	56 (100%)	0	100	100
52	s	72/79 (91%)	67 (93%)	5 (7%)	14	16
53	t	65/66 (98%)	64 (98%)	1 (2%)	57	72
54	u	46/61 (75%)	45 (98%)	1 (2%)	45	59
57	y	1/1 (100%)	1 (100%)	0	100	100
All	All	4627/4830 (96%)	4568 (99%)	59 (1%)	59	76

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	i	13	SER
52	s	78	THR
42	i	79	ARG
52	s	57	VAL
49	p	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
32	Y	36	GLN
38	e	77	ASN
53	t	60	GLN
32	Y	39	GLN
36	c	99	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1539/1542 (99%)	314 (20%)	0
55	v	76/77 (98%)	18 (23%)	0
56	w	75/76 (98%)	18 (24%)	0
58	z	10/33 (30%)	1 (10%)	0
8	A	2902/2903 (99%)	518 (17%)	37 (1%)
9	B	119/120 (99%)	23 (19%)	4 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4721/4751 (99%)	892 (18%)	41 (0%)

5 of 892 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	35	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	2158	A
8	A	2796	U
8	A	2192	U
8	A	2468	A
9	B	36	C

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

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
34	MA6	a	1518	34	23,26,27	1.45	4 (17%)	34,38,41	2.75	12 (35%)
34	2MG	a	1207	34	23,26,27	2.93	8 (34%)	32,38,41	2.22	11 (34%)
8	OMC	A	2498	8,59	19,22,23	2.86	7 (36%)	26,31,34	0.75	0
8	PSU	A	955	8	18,21,22	1.03	1 (5%)	22,30,33	1.86	5 (22%)
8	PSU	A	1917	8	18,21,22	1.03	1 (5%)	22,30,33	1.75	5 (22%)
8	2MG	A	2445	8	23,26,27	2.88	9 (39%)	32,38,41	2.22	12 (37%)
8	PSU	A	2457	8	18,21,22	1.06	1 (5%)	22,30,33	1.86	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	5MU	w	54	56	19,22,23	4.79	7 (36%)	28,32,35	3.65	9 (32%)
56	G7M	w	46	56	23,26,27	2.62	8 (34%)	35,39,42	2.24	10 (28%)
8	6MZ	A	1618	8	22,25,26	2.98	5 (22%)	30,36,39	4.28	13 (43%)
56	PSU	w	32	56	18,21,22	1.02	1 (5%)	22,30,33	1.70	4 (18%)
34	MA6	a	1519	34	23,26,27	1.45	5 (21%)	34,38,41	2.78	12 (35%)
56	PSU	w	55	56	18,21,22	1.06	1 (5%)	22,30,33	1.97	5 (22%)
8	PSU	A	746	8,59	18,21,22	1.05	1 (5%)	22,30,33	1.71	4 (18%)
55	H2U	v	20	55	18,21,22	3.08	5 (27%)	21,30,33	1.98	5 (23%)
34	4OC	a	1402	34	20,23,24	2.97	8 (40%)	26,32,35	0.90	1 (3%)
8	PSU	A	2605	8	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
8	OMU	A	2552	8,59	19,22,23	2.89	8 (42%)	26,31,34	1.76	5 (19%)
55	4SU	v	8	55	18,21,22	3.59	7 (38%)	26,30,33	2.22	4 (15%)
34	2MG	a	966	34	23,26,27	2.92	8 (34%)	32,38,41	2.24	11 (34%)
34	5MC	a	967	34	18,22,23	3.68	7 (38%)	26,32,35	1.00	2 (7%)
34	UR3	a	1498	34	19,22,23	2.68	7 (36%)	26,32,35	1.37	3 (11%)
34	2MG	a	1516	34	23,26,27	2.90	8 (34%)	32,38,41	2.28	12 (37%)
8	2MG	A	1835	8	23,26,27	2.92	8 (34%)	32,38,41	2.25	11 (34%)
8	5MC	A	1962	8	18,22,23	3.65	7 (38%)	26,32,35	1.04	2 (7%)
56	4SU	w	8	56	18,21,22	3.56	7 (38%)	26,30,33	2.20	4 (15%)
34	G7M	a	527	34	23,26,27	2.60	8 (34%)	35,39,42	2.29	10 (28%)
8	1MG	A	745	8	22,26,27	2.64	5 (22%)	33,39,42	2.01	8 (24%)
8	2MA	A	2503	8,59	22,25,26	3.76	8 (36%)	33,37,40	2.24	7 (21%)
56	MIA	w	37	56	28,31,32	2.54	6 (21%)	40,44,47	3.05	16 (40%)
8	OMG	A	2251	8,59,55	23,26,27	2.38	9 (39%)	33,38,41	1.83	8 (24%)
55	PSU	v	55	55	18,21,22	1.06	1 (5%)	22,30,33	1.68	4 (18%)
8	5MU	A	1939	8	19,22,23	4.76	7 (36%)	28,32,35	3.79	10 (35%)
8	PSU	A	1911	8	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
8	PSU	A	2580	8	18,21,22	1.10	2 (11%)	22,30,33	1.90	6 (27%)
34	PSU	a	516	34,59	18,21,22	0.98	1 (5%)	22,30,33	1.70	5 (22%)
8	6MZ	A	2030	8	22,25,26	2.89	5 (22%)	30,36,39	4.36	14 (46%)
55	5MU	v	54	55	19,22,23	4.81	7 (36%)	28,32,35	3.66	9 (32%)
8	PSU	A	2604	8	18,21,22	1.01	1 (5%)	22,30,33	1.85	4 (18%)
56	PSU	w	39	56	18,21,22	1.09	1 (5%)	22,30,33	1.71	3 (13%)
8	5MC	A	747	8	18,22,23	3.65	7 (38%)	26,32,35	1.09	2 (7%)
8	G7M	A	2069	8	23,26,27	2.56	8 (34%)	35,39,42	2.38	11 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PSU	A	2504	8	18,21,22	1.09	1 (5%)	22,30,33	1.78	4 (18%)
57	FME	y	101	57	8,9,10	0.88	0	7,9,11	1.81	2 (28%)
8	3TD	A	1915	8	18,22,23	4.25	5 (27%)	22,32,35	1.65	2 (9%)
34	5MC	a	1407	34	18,22,23	3.69	7 (38%)	26,32,35	1.03	2 (7%)

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
34	MA6	a	1518	34	-	0/11/29/30	0/3/3/3
34	2MG	a	1207	34	-	0/9/27/28	0/3/3/3
8	OMC	A	2498	8,59	-	2/9/27/28	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	1/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/9/27/28	0/3/3/3
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
56	G7M	w	46	56	-	0/7/25/26	0/3/3/3
8	6MZ	A	1618	8	-	0/9/27/28	0/3/3/3
56	PSU	w	32	56	-	3/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	1/11/29/30	0/3/3/3
56	PSU	w	55	56	-	1/7/25/26	0/2/2/2
8	PSU	A	746	8,59	-	2/7/25/26	0/2/2/2
55	H2U	v	20	55	-	3/7/38/39	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
8	OMU	A	2552	8,59	-	3/9/27/28	0/2/2/2
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
34	2MG	a	966	34	-	0/9/27/28	0/3/3/3
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
8	2MG	A	1835	8	-	2/9/27/28	0/3/3/3
8	5MC	A	1962	8	-	2/7/25/26	0/2/2/2
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
34	G7M	a	527	34	-	1/7/25/26	0/3/3/3
8	1MG	A	745	8	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2MA	A	2503	8,59	-	2/7/25/26	0/3/3/3
56	MIA	w	37	56	-	2/15/33/34	0/3/3/3
8	OMG	A	2251	8,59,55	-	1/9/27/28	0/3/3/3
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	2/7/25/26	0/2/2/2
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
34	PSU	a	516	34,59	-	0/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	2/9/27/28	0/3/3/3
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2
8	5MC	A	747	8	-	0/7/25/26	0/2/2/2
8	G7M	A	2069	8	-	1/7/25/26	0/3/3/3
8	PSU	A	2504	8	-	2/7/25/26	0/2/2/2
57	FME	y	101	57	-	5/7/9/11	-
8	3TD	A	1915	8	-	3/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2

The worst 5 of 230 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C6-C5	12.88	1.50	1.35
8	A	1618	6MZ	C6-N6	12.29	1.47	1.34
8	A	2503	2MA	C4-N3	11.97	1.49	1.34
8	A	2030	6MZ	C6-N6	11.67	1.46	1.34
55	v	54	5MU	C2-N1	11.06	1.56	1.38

The worst 5 of 302 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2030	6MZ	C4-N9-C8	13.24	120.08	105.73
8	A	1618	6MZ	C4-N9-C8	13.13	119.95	105.73
8	A	1939	5MU	C5-C4-N3	12.47	125.95	115.31
55	v	54	5MU	C5-C4-N3	12.28	125.80	115.31
56	w	54	5MU	C5-C4-N3	12.28	125.79	115.31

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	20	H2U	O4'-C4'-C5'-O5'
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
8	A	746	PSU	C2'-C1'-C5-C4
8	A	1915	3TD	C2'-C1'-C5-C4

There are no ring outliers.

20 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2445	2MG	1	0
56	w	46	G7M	4	0
56	w	55	PSU	1	0
55	v	20	H2U	3	0
34	a	1402	4OC	2	0
8	A	2605	PSU	1	0
8	A	2552	OMU	2	0
55	v	8	4SU	1	0
34	a	1498	UR3	2	0
56	w	8	4SU	1	0
34	a	527	G7M	1	0
56	w	37	MIA	2	0
55	v	55	PSU	1	0
8	A	1939	5MU	1	0
8	A	2580	PSU	1	0
34	a	516	PSU	2	0
8	A	2030	6MZ	1	0
8	A	2069	G7M	1	0
57	y	101	FME	1	0
8	A	1915	3TD	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 371 ligands modelled in this entry, 367 are monoatomic - leaving 4 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
62	AM2	a	1682	-	40,40,40	1.61	9 (22%)	53,60,60	1.05	3 (5%)
62	AM2	a	1684	-	40,40,40	1.62	8 (20%)	53,60,60	1.10	3 (5%)
62	AM2	a	1689	-	40,40,40	1.64	8 (20%)	53,60,60	1.09	4 (7%)
62	AM2	a	1685	-	40,40,40	1.67	7 (17%)	53,60,60	1.08	5 (9%)

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
62	AM2	a	1682	-	-	1/12/84/84	0/4/4/4
62	AM2	a	1684	-	-	4/12/84/84	0/4/4/4
62	AM2	a	1689	-	-	3/12/84/84	0/4/4/4
62	AM2	a	1685	-	-	4/12/84/84	0/4/4/4

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	a	1685	AM2	OA4-CA1	4.60	1.53	1.41
62	a	1689	AM2	OA4-CA1	4.58	1.53	1.41
62	a	1684	AM2	OA4-CA1	4.49	1.53	1.41
62	a	1682	AM2	OA4-CA1	4.32	1.52	1.41
62	a	1685	AM2	OA4-CA5	3.77	1.49	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	a	1684	AM2	CA9-NA7-CA7	-3.48	109.32	114.38
62	a	1682	AM2	CA9-NA7-CA7	-3.46	109.35	114.38
62	a	1684	AM2	CA1-OA1-CC1	-3.28	109.83	117.96
62	a	1689	AM2	CA9-NA7-CA7	-3.19	109.74	114.38
62	a	1689	AM2	CA1-OA1-CC1	-3.08	110.35	117.96

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

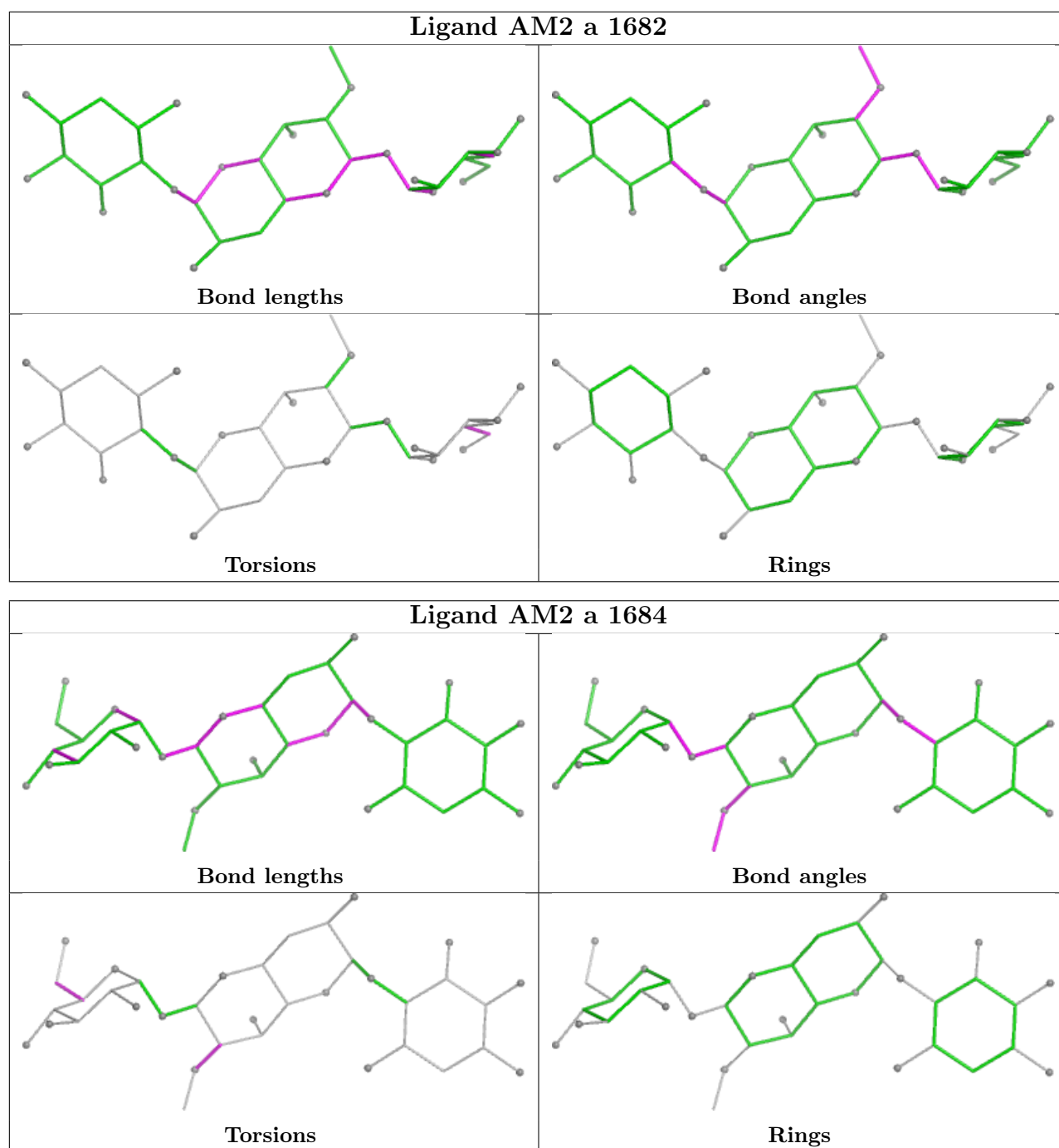
Mol	Chain	Res	Type	Atoms
62	a	1684	AM2	CA6-CA7-NA7-CA9
62	a	1684	AM2	CA8-CA7-NA7-CA9
62	a	1685	AM2	CA8-CA7-NA7-CA9
62	a	1684	AM2	OB1-CB5-CB6-OB6
62	a	1684	AM2	CB4-CB5-CB6-OB6

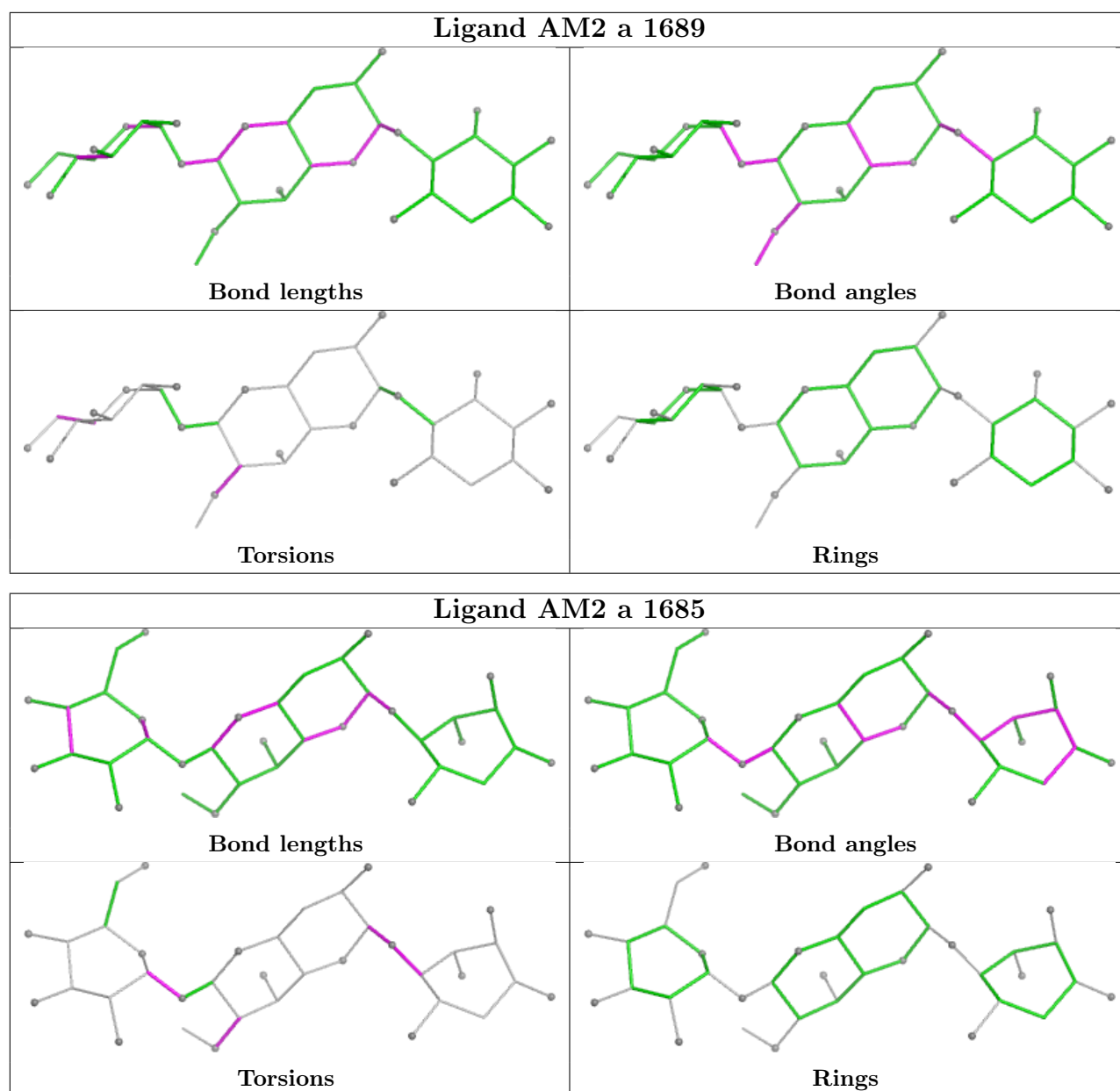
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	a	1682	AM2	1	0
62	a	1684	AM2	1	0
62	a	1685	AM2	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.

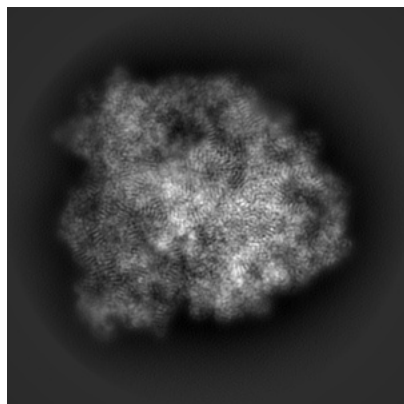
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13458. These allow visual inspection of the internal detail of the map and identification of artifacts.

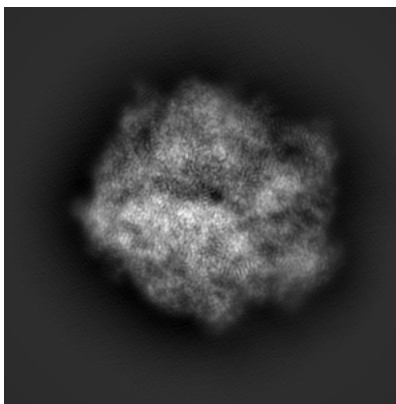
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

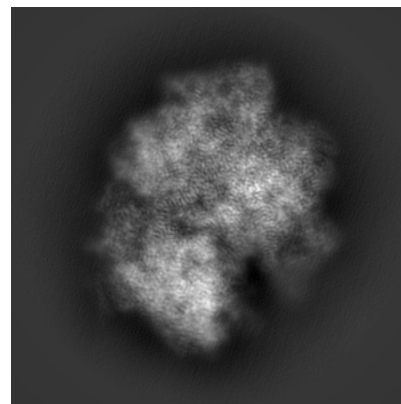
#### 6.1.1 Primary map



X

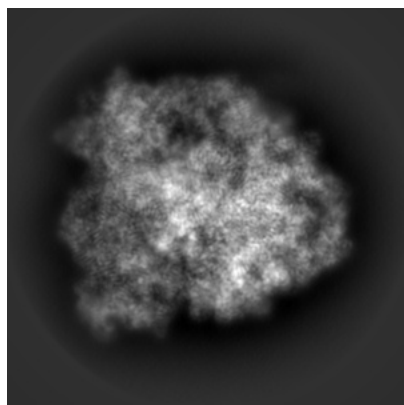


Y

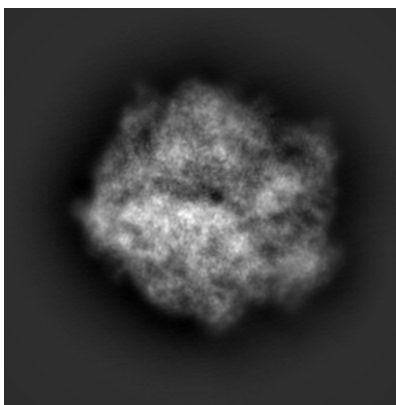


Z

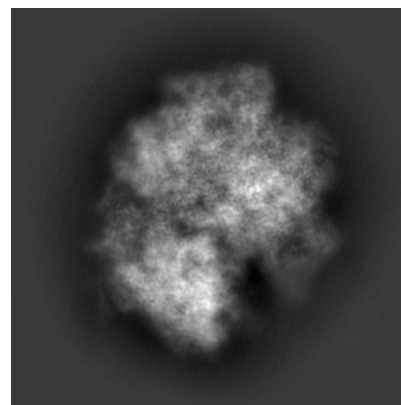
#### 6.1.2 Raw map



X



Y

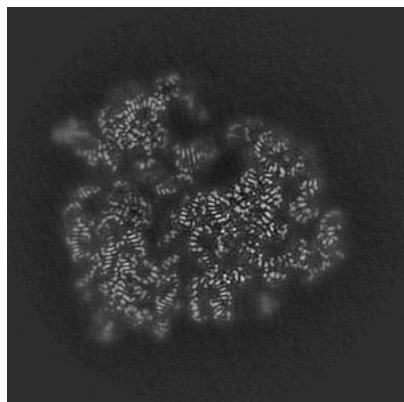


Z

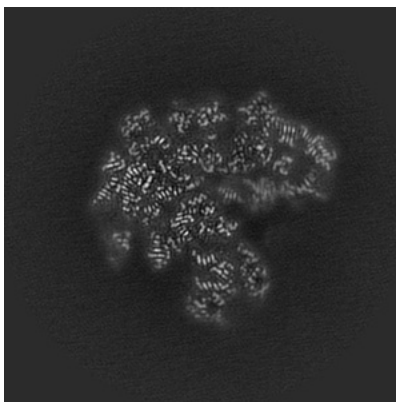
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

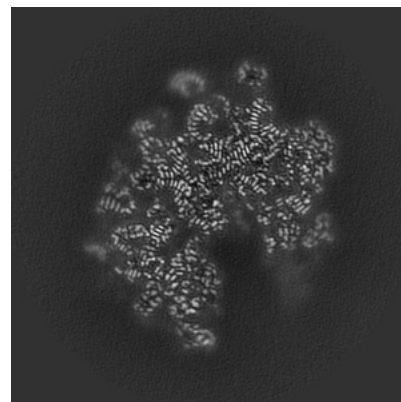
### 6.2.1 Primary map



X Index: 256

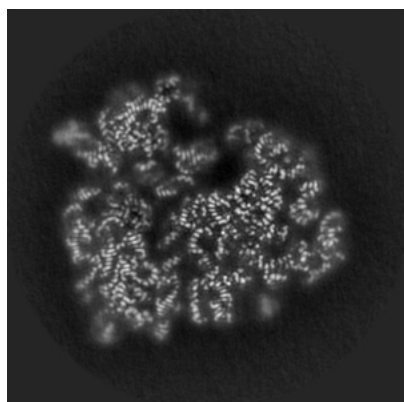


Y Index: 256

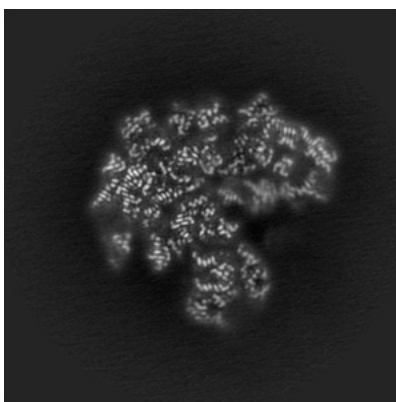


Z Index: 256

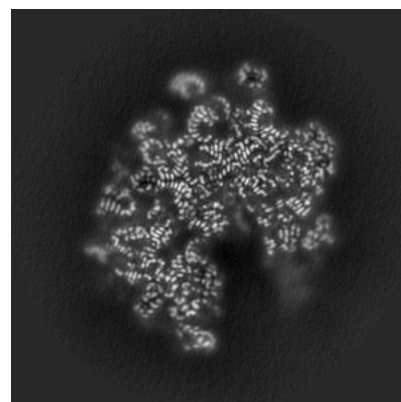
### 6.2.2 Raw map



X Index: 144



Y Index: 144

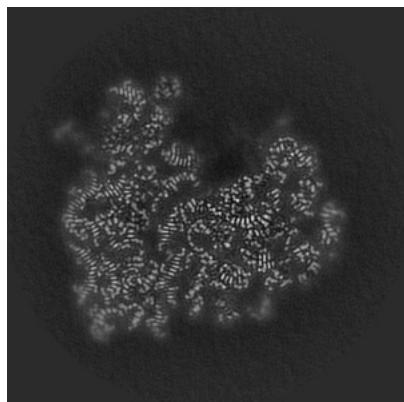


Z Index: 144

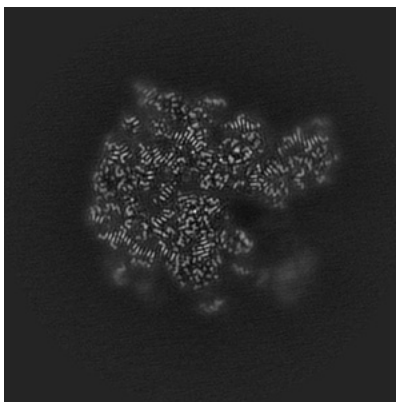
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

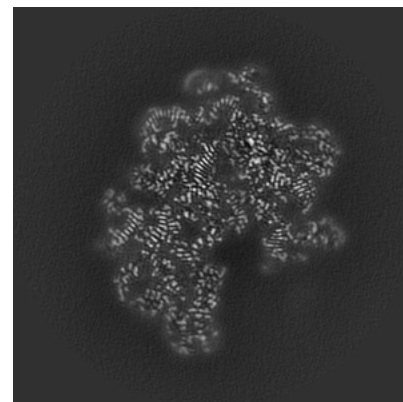
### 6.3.1 Primary map



X Index: 246

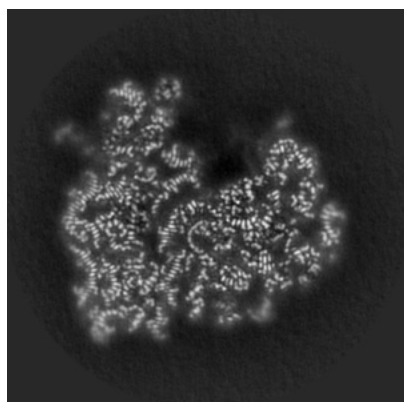


Y Index: 285

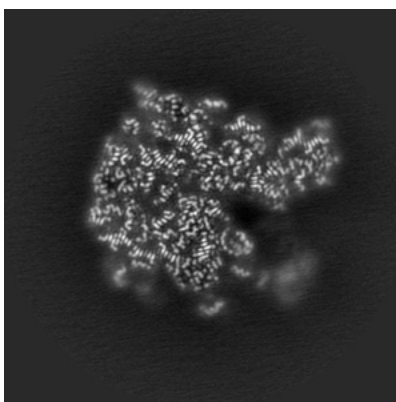


Z Index: 242

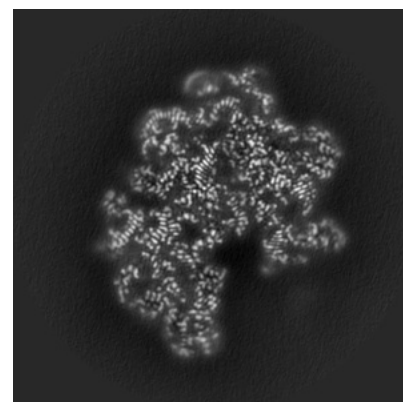
### 6.3.2 Raw map



X Index: 138



Y Index: 160

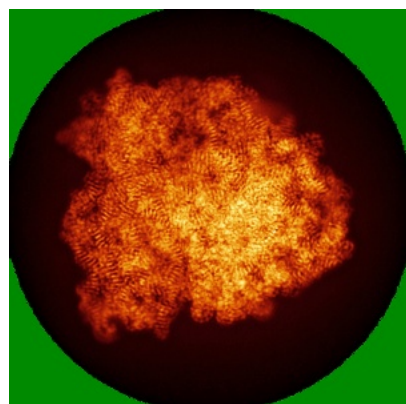


Z Index: 136

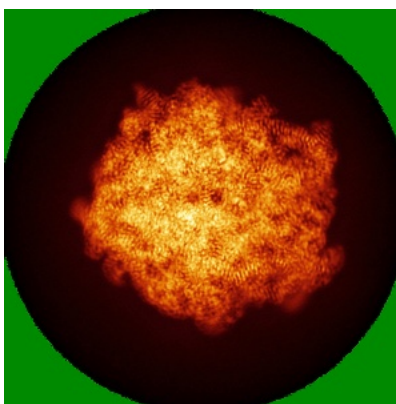
The images above show the largest variance slices of the map in three orthogonal directions.

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

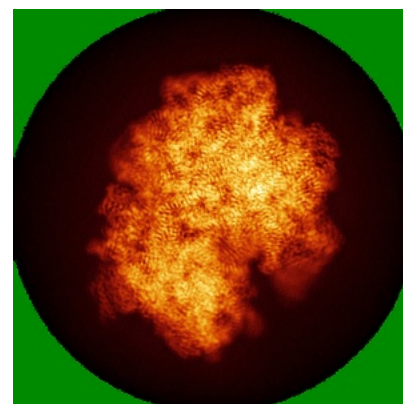
### 6.4.1 Primary map



X

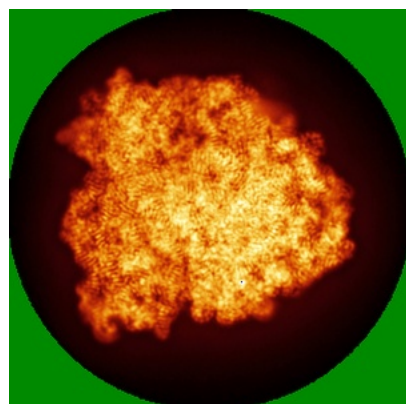


Y

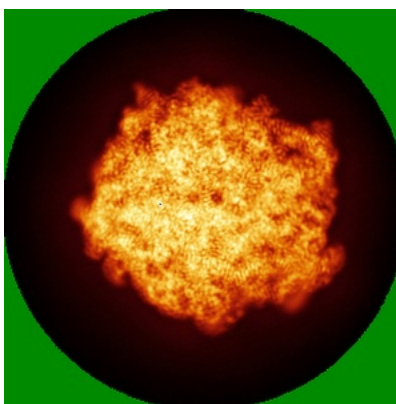


Z

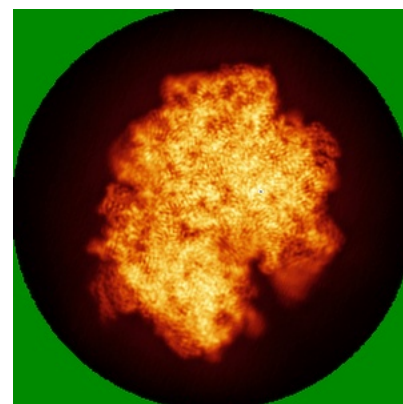
### 6.4.2 Raw map



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](#)

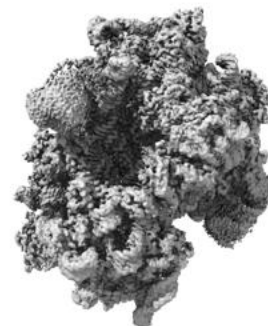
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

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.

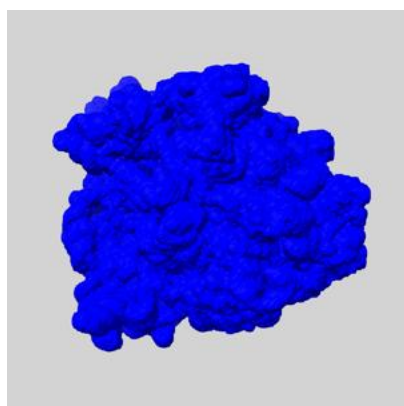
## 6.6 Mask visualisation [i](#)

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

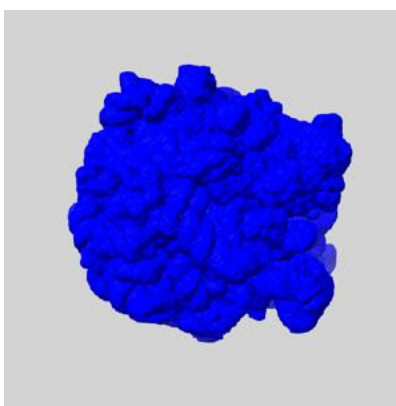
A mask typically either:

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

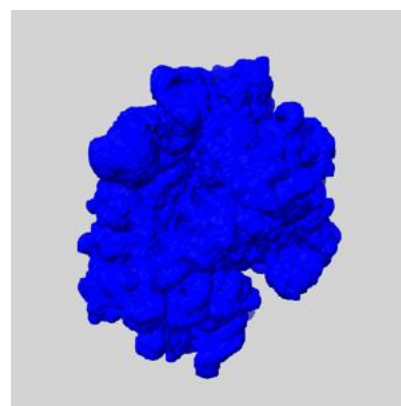
### 6.6.1 emd\_13458\_msk\_1.map [i](#)



X



Y

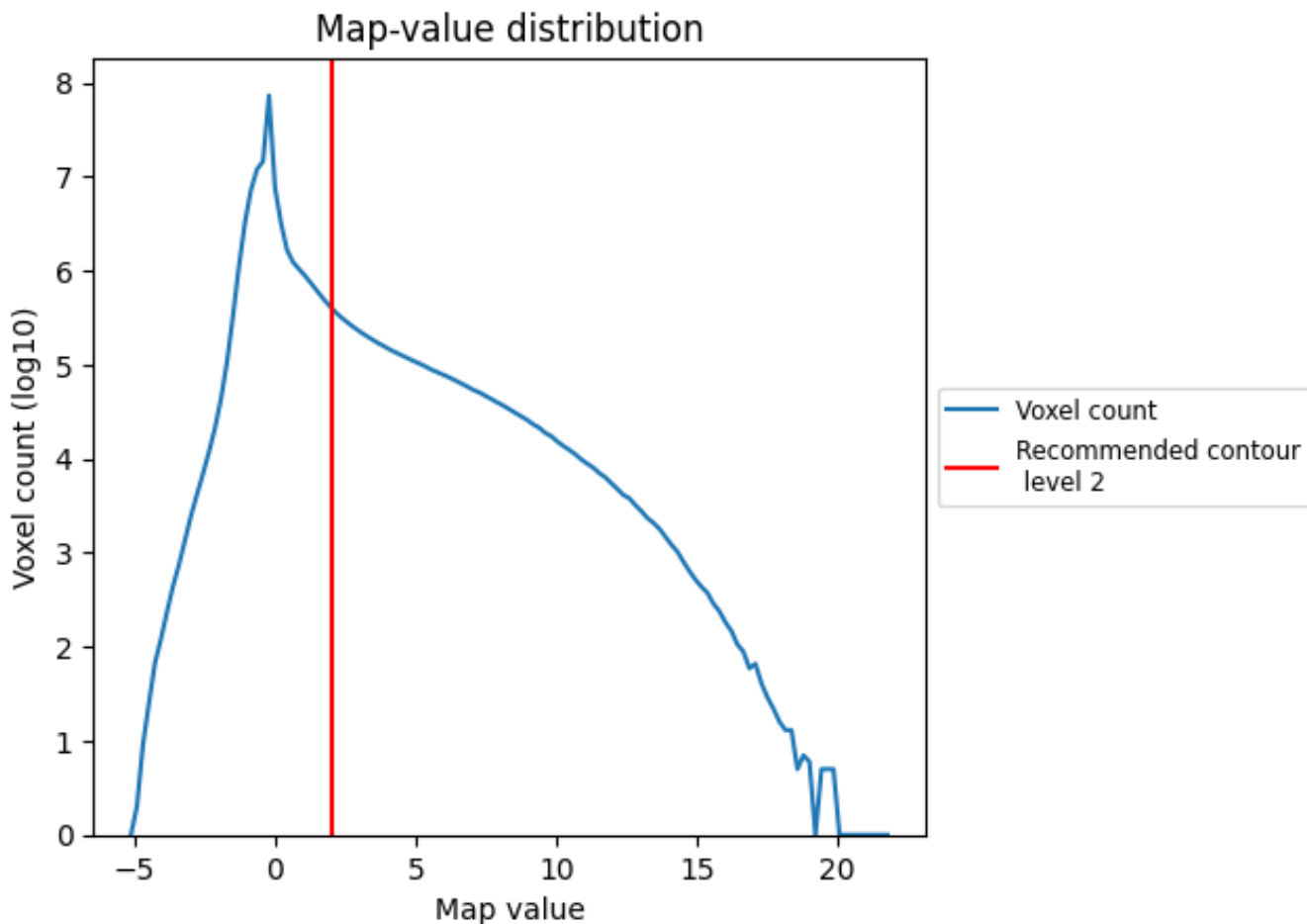


Z

## 7 Map analysis [i](#)

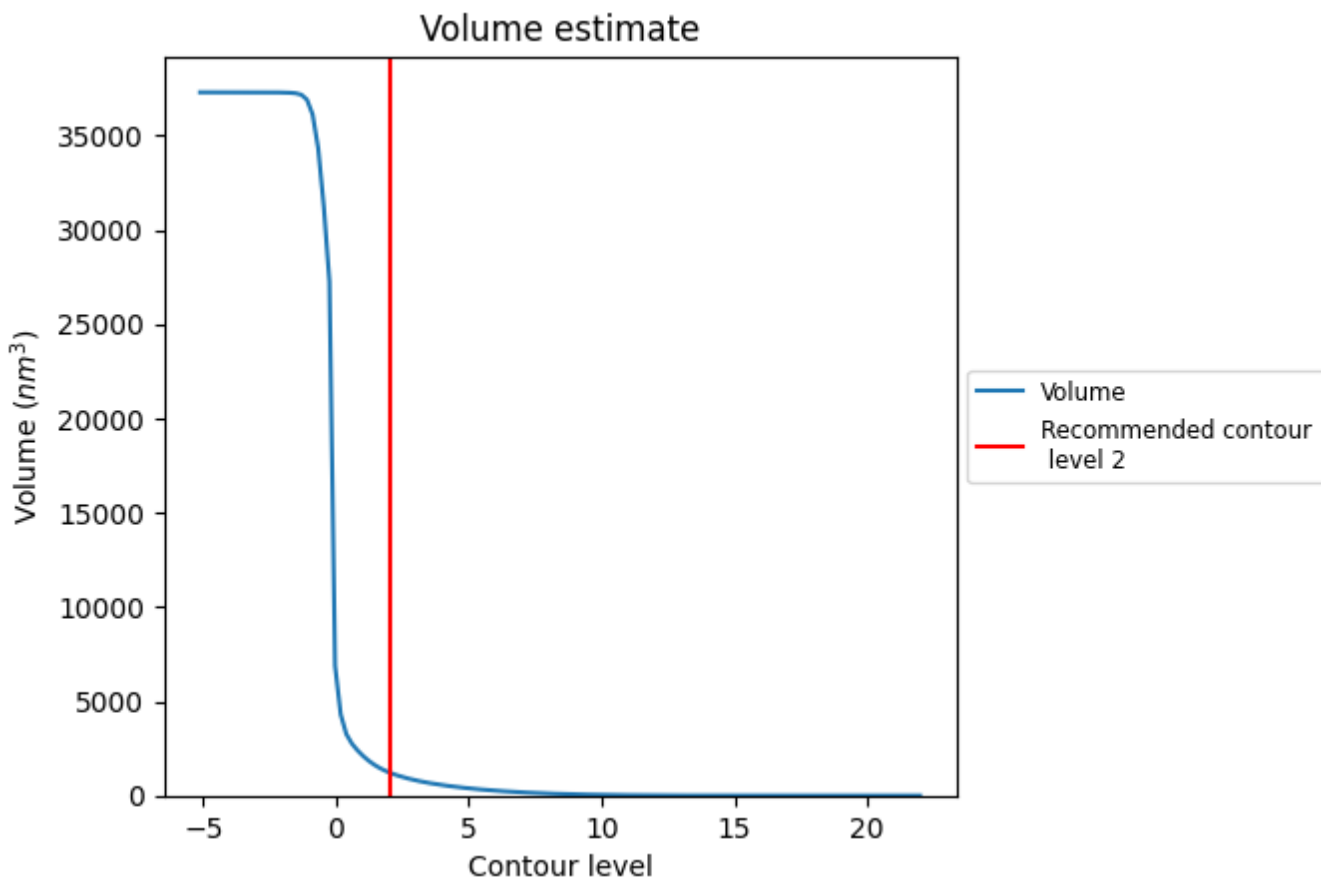
This section contains the results of statistical analysis of the map.

### 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.

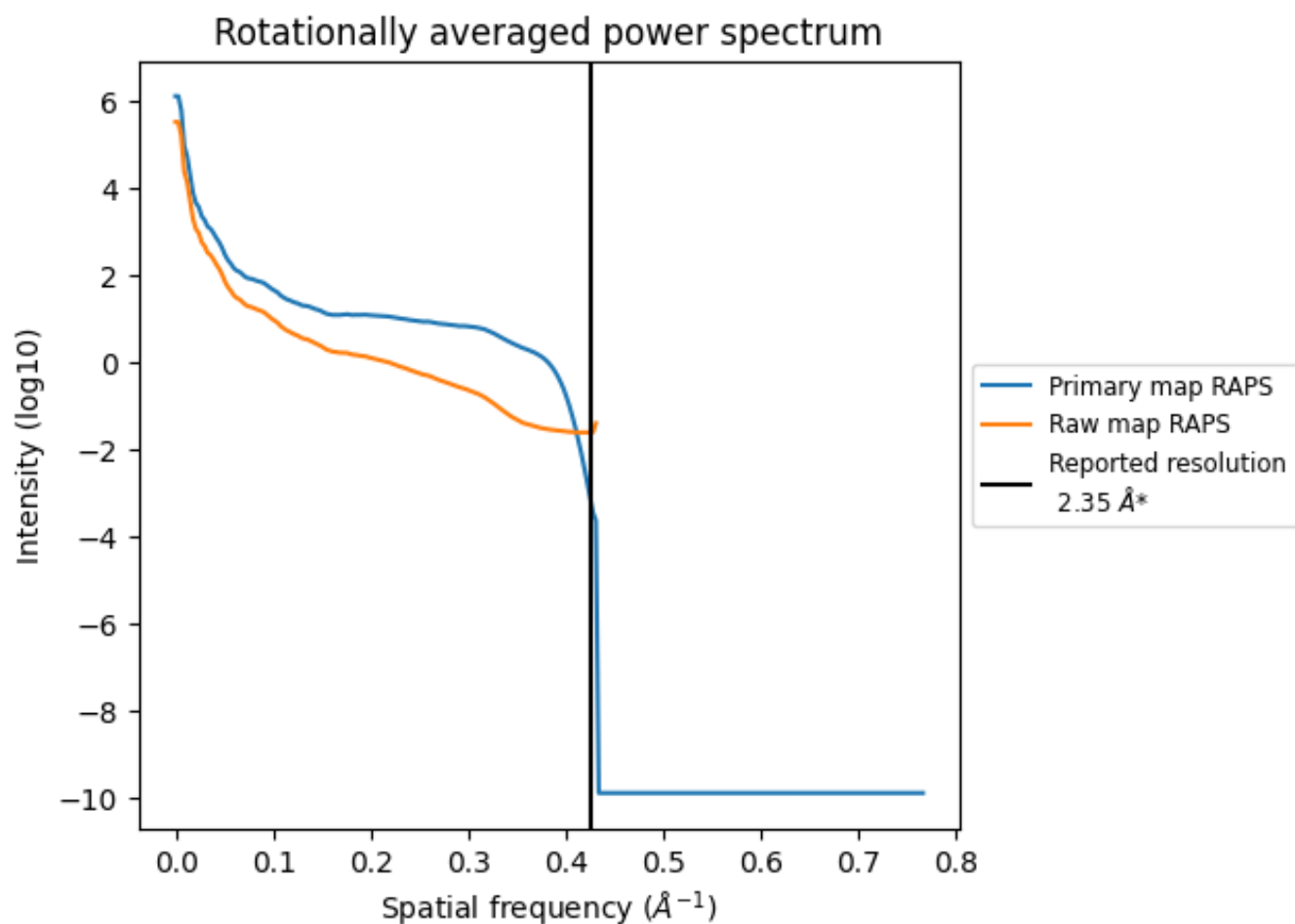
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1226 nm<sup>3</sup>; this corresponds to an approximate mass of 1108 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

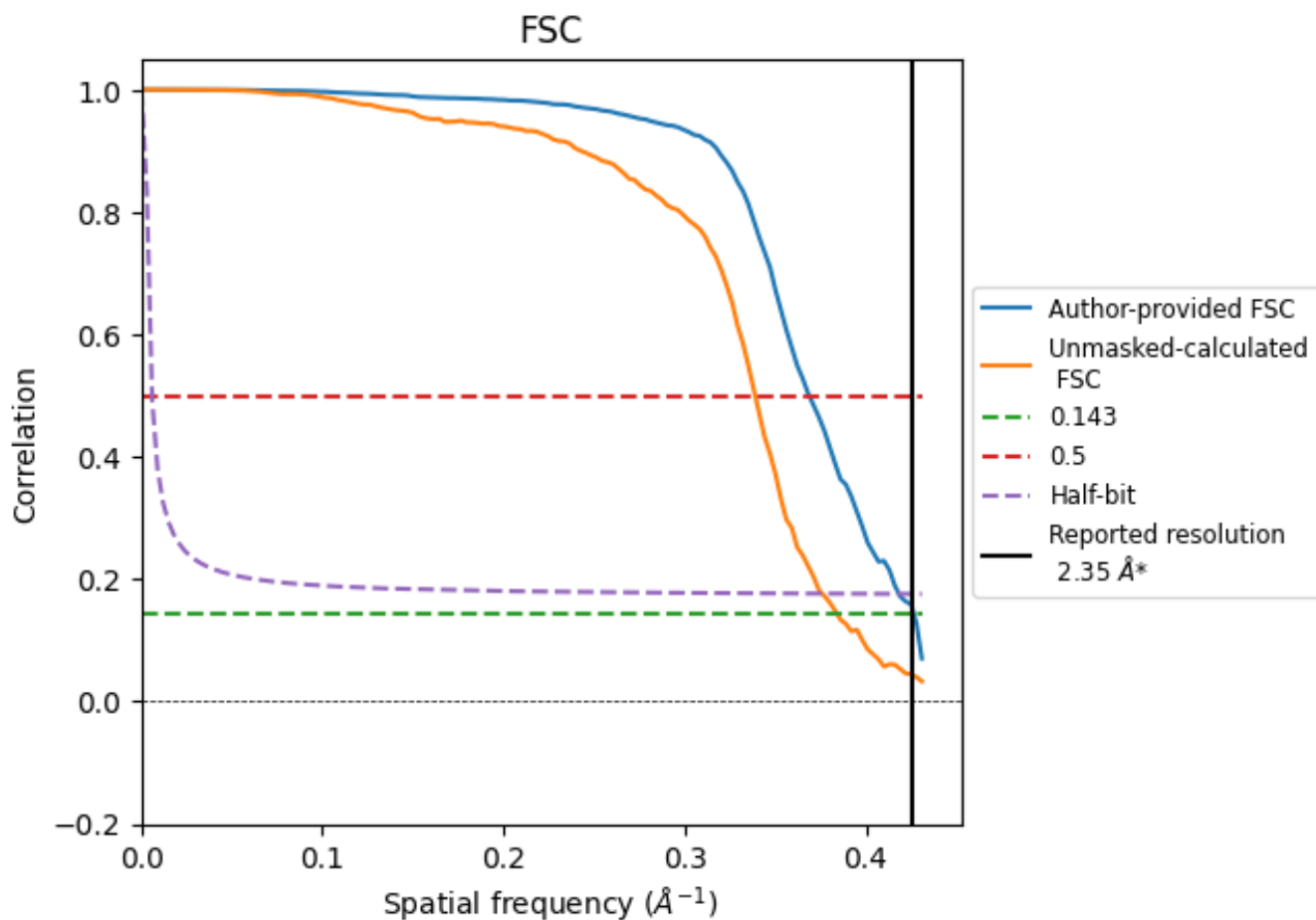


\*Reported resolution corresponds to spatial frequency of 0.426 Å<sup>-1</sup>

## 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 0.426 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

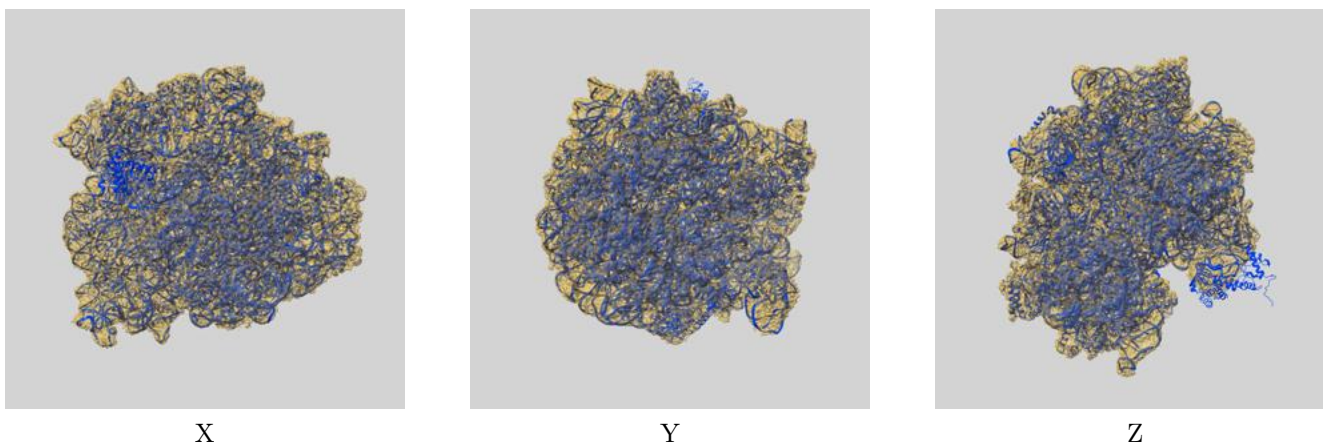
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.34	2.71	2.39
Unmasked-calculated*	2.60	2.95	2.66

\*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 2.60 differs from the reported value 2.35 by more than 10 %

## 9 Map-model fit [i](#)

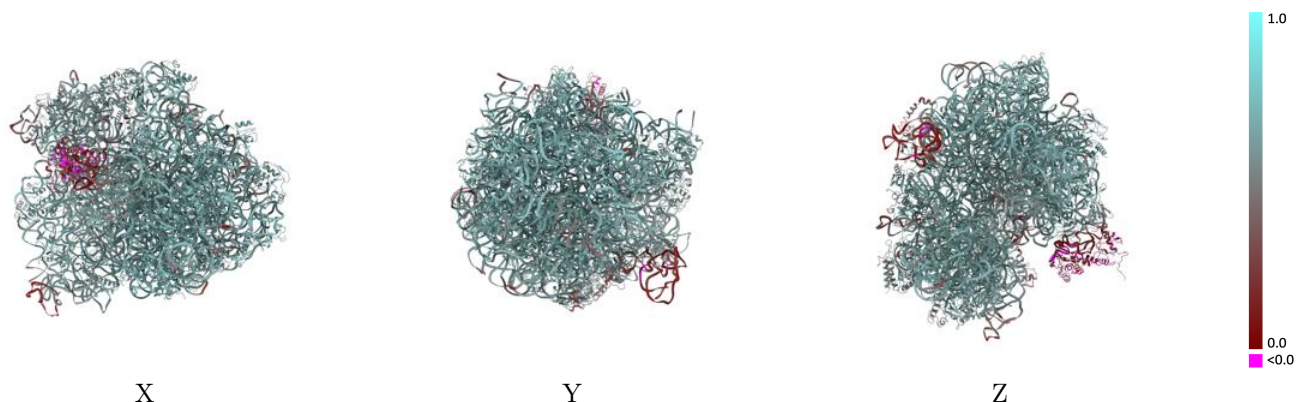
This section contains information regarding the fit between EMDB map EMD-13458 and PDB model 7PJS. Per-residue inclusion information can be found in section 3 on page 17.

### 9.1 Map-model overlay [i](#)



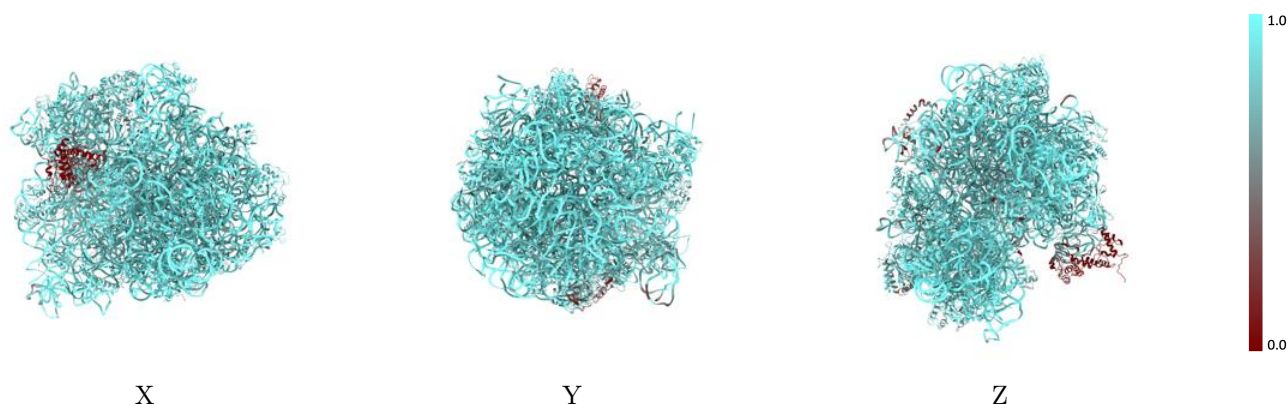
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



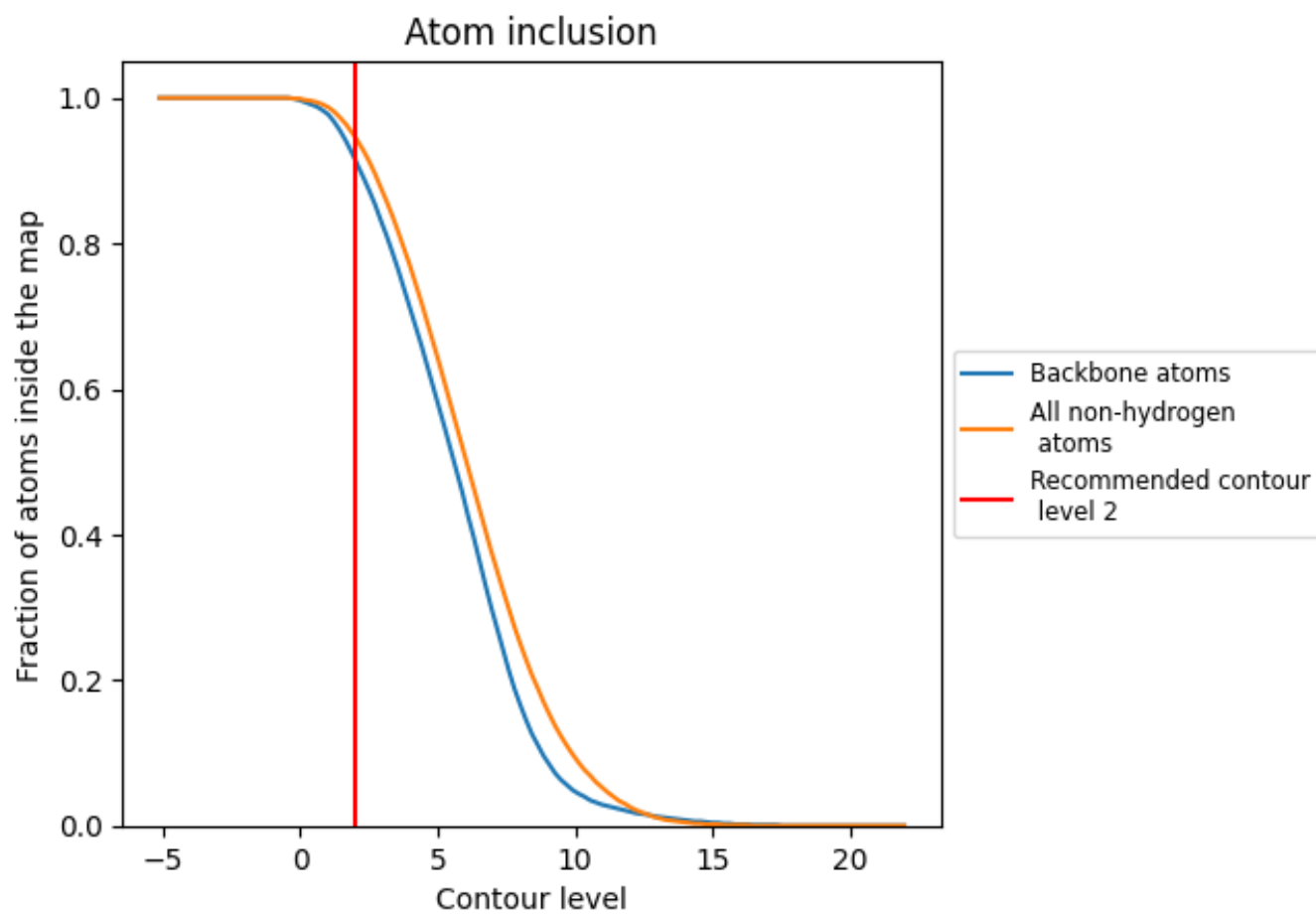
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

















































The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.6120
0	 0.9420	 0.6510
1	 0.8880	 0.6290
2	 0.9690	 0.6800
3	 0.9700	 0.6790
4	 0.9450	 0.6330
5	 0.0110	 0.1310
6	 0.7910	 0.4950
A	 0.9770	 0.6210
B	 0.9860	 0.6220
C	 0.9530	 0.6650
D	 0.9430	 0.6540
E	 0.9280	 0.6360
F	 0.8580	 0.5430
G	 0.8690	 0.5500
H	 0.4660	 0.4410
I	 0.0660	 0.1220
J	 0.9510	 0.6580
K	 0.9170	 0.6450
L	 0.9490	 0.6460
M	 0.9430	 0.6570
N	 0.9630	 0.6610
O	 0.9490	 0.6180
P	 0.9230	 0.6460
Q	 0.9780	 0.6770
R	 0.9220	 0.6350
S	 0.9230	 0.6500
T	 0.9210	 0.6280
U	 0.9180	 0.6050
V	 0.9050	 0.6210
W	 0.9520	 0.6680
X	 0.9350	 0.6560
Y	 0.9130	 0.5980
Z	 0.9290	 0.6480
a	 0.9860	 0.6170



*Continued on next page...*

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Chain	Atom inclusion	Q-score
b	 0.7670	 0.5510
c	 0.9110	 0.6110
d	 0.9090	 0.5930
e	 0.9430	 0.6420
f	 0.8910	 0.5810
g	 0.8710	 0.5700
h	 0.9390	 0.6410
i	 0.9370	 0.6050
j	 0.8540	 0.5490
k	 0.9210	 0.6120
l	 0.9210	 0.6400
m	 0.9340	 0.5990
n	 0.9580	 0.6230
o	 0.9170	 0.6100
p	 0.9270	 0.6120
q	 0.9070	 0.6170
r	 0.9300	 0.6120
s	 0.9170	 0.5940
t	 0.9290	 0.6080
u	 0.8120	 0.5500
v	 0.9140	 0.5720
w	 0.8880	 0.5260
y	 0.5240	 0.5310
z	 0.9390	 0.5990