



## wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 02:17 PM EDT

PDB ID : 5KCR  
EMDB ID : EMD-8237  
Title : Cryo-EM structure of the Escherichia coli 70S ribosome in complex with antibiotic Avilamycin C, mRNA and P-site tRNA at 3.6Å resolution  
Authors : Arenz, S.; Juette, M.F.; Graf, M.; Nguyen, F.; Huter, P.; Polikanov, Y.S.; Blanchard, S.C.; Wilson, D.N.  
Deposited on : 2016-06-06  
Resolution : 3.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

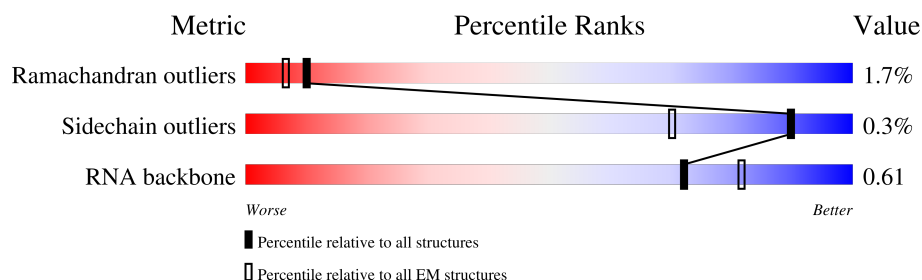
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1A	2904	
2	1B	120	
3	1D	273	
4	1E	209	
5	1F	201	
6	1G	179	
7	1H	177	
8	1I	149	

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Mol	Chain	Length	Quality of chain
9	1J	165	 82% 78% 18%
10	1K	142	 91% 92% 6%
11	1N	142	 98%
12	1O	123	 13% 99%
13	1P	144	 12% 100%
14	1Q	136	 8% 95% 5%
15	1R	127	 9% 97%
16	1S	117	 14% 100%
17	1T	115	 14% 98%
18	1U	118	 98%
19	1V	103	 13% 99%
20	1W	110	 10% 100%
21	1X	100	 17% 92% 7%
22	1Y	104	 17% 97%
23	1Z	94	 11% 100%
24	10	85	 6% 89% 11%
25	11	78	 17% 99%
26	12	63	 14% 98%
27	13	59	 12% 95%
28	15	57	 16% 98%
29	16	55	 91% 93% 7%
30	17	46	 7% 100%
31	18	65	 6% 98%
32	19	38	 11% 100%
33	1a	1539	 85% 15%

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Mol	Chain	Length	Quality of chain
34	1b	241	
35	1c	233	
36	1d	206	
37	1e	167	
38	1f	135	
39	1g	179	
40	1h	130	
41	1i	130	
42	1j	103	
43	1k	129	
44	1l	124	
45	1m	118	
46	1n	101	
47	1o	89	
48	1p	82	
49	1q	84	
50	1r	75	
51	1s	92	
52	1t	87	
53	1u	71	
54	1v	9	
55	1x	87	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145689 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	2897	Total	C	N	O	P	8	0
			62361	27826	11476	20155	2904		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1847	G	A	conflict	GB 802133627

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1D	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1E	209	Total	C	N	O	S	1	0
			1576	986	290	296	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1F	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1G	177	Total	C	N	O	S	0	0
			1404	896	246	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1I	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1J	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1K	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1N	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1O	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1P	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1Q	136	Total	C	N	O	S	2	0
			1090	696	211	177	6		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1R	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1S	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1T	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	1U	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1V	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1W	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1X	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1Y	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1Z	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	10	76	Total	C	N	O	S	1	0
			591	365	121	104	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	11	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	12	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	13	58	Total	C	N	O	S	2	0
			463	290	90	81	2		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	15	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	16	51	Total	C	N	O	S	0	0
			414	266	76	72			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	17	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	18	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	19	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 33 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1a	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1e	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1n	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1o	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	1r	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1u	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

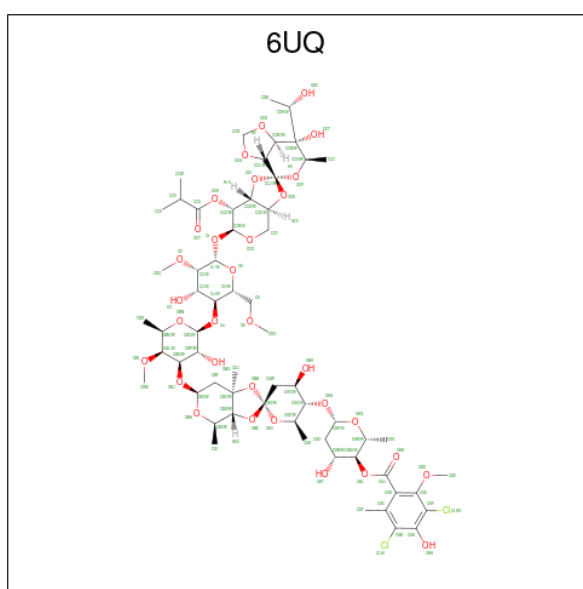
- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1v	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1x	87	Total	C	N	O	P	0	0
			1861	829	333	612	87		

- Molecule 56 is (2R,3S,4R,6S)-4-hydroxy-6-{{[(2R,3aR,4R,4'R,5'S,6S,6'R,7aR)-4'-hydroxy-6-{{[(2S,3R,4R,5S,6R)-3-hydroxy-2-{{[(2R,3S,4S,5S,6S)-4-hydroxy-6-{{(2R,3aS,3a'R,6S,6'R,7R,7'R,7aR,7a'R)-7'-hydroxy-7'-[(1S)-1-hydroxyethyl]-6'-methyl-7-[(2-methylpropanoyl)oxy]octahydro-4H-2,4'-spirobi[[1,3]dioxolo[4,5-c]pyran]-6-yl}oxy)-5-methoxy-2-(methoxymethyl)tetrahydro-2H-pyran-3-yl}oxy}-5-methoxy-6-methyltetrahydro-2H-pyran-4-yl}oxy}-4,6',7a-trimethyloctahydro-4H-spiro[1,3-dioxolo[4,5-c]pyran-2,2'-pyran]-5'-yl}oxy}-2-methyltetrahydro-2H-pyran-3-yl 3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoate (non-preferred name) (three-letter code: 6UQ) (formula: C<sub>61</sub>H<sub>90</sub>Cl<sub>2</sub>O<sub>32</sub>).



Mol	Chain	Residues	Atoms				AltConf
56	1A	1	Total	C	Cl	O	0
			95	61	2	32	

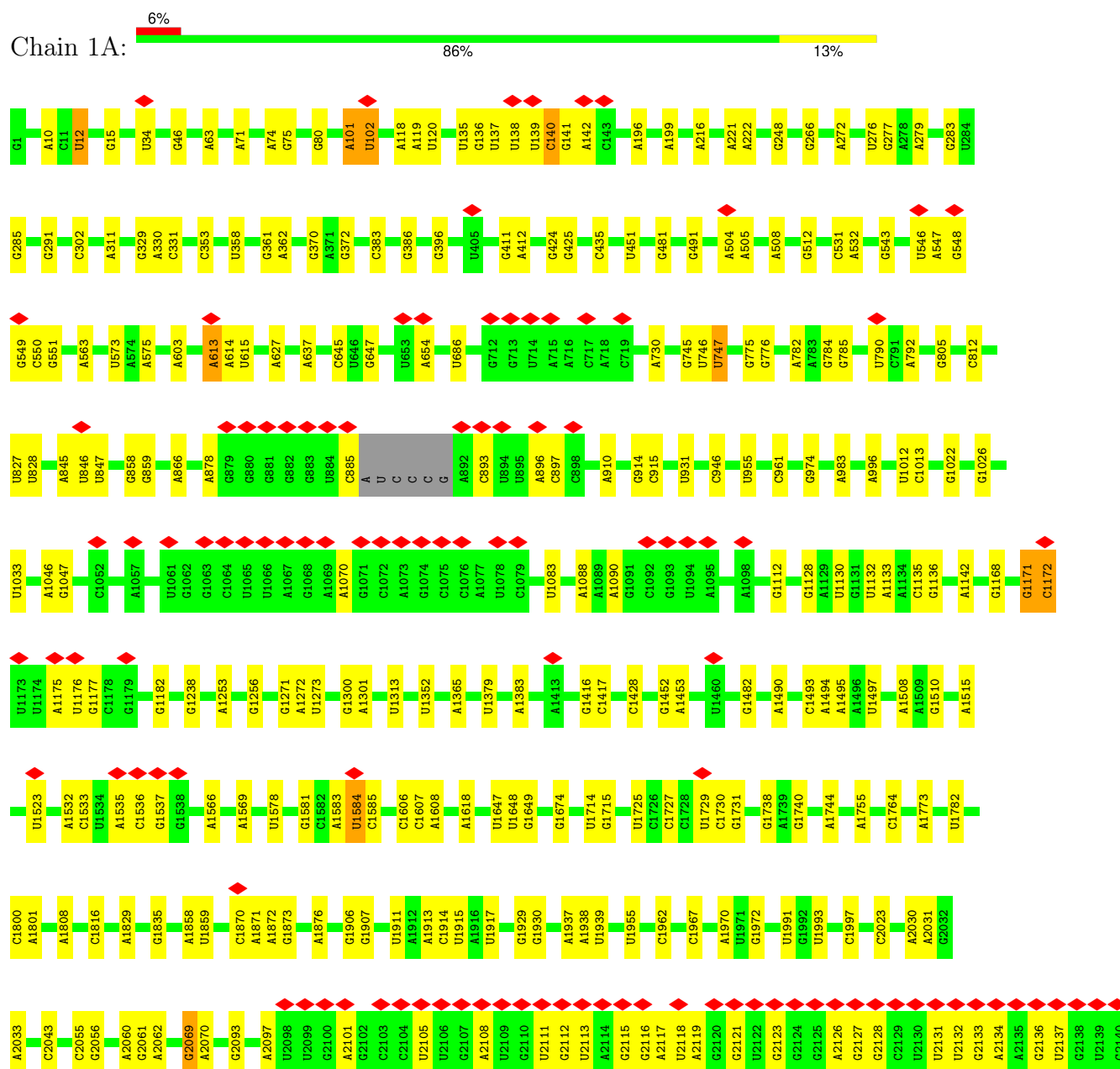
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

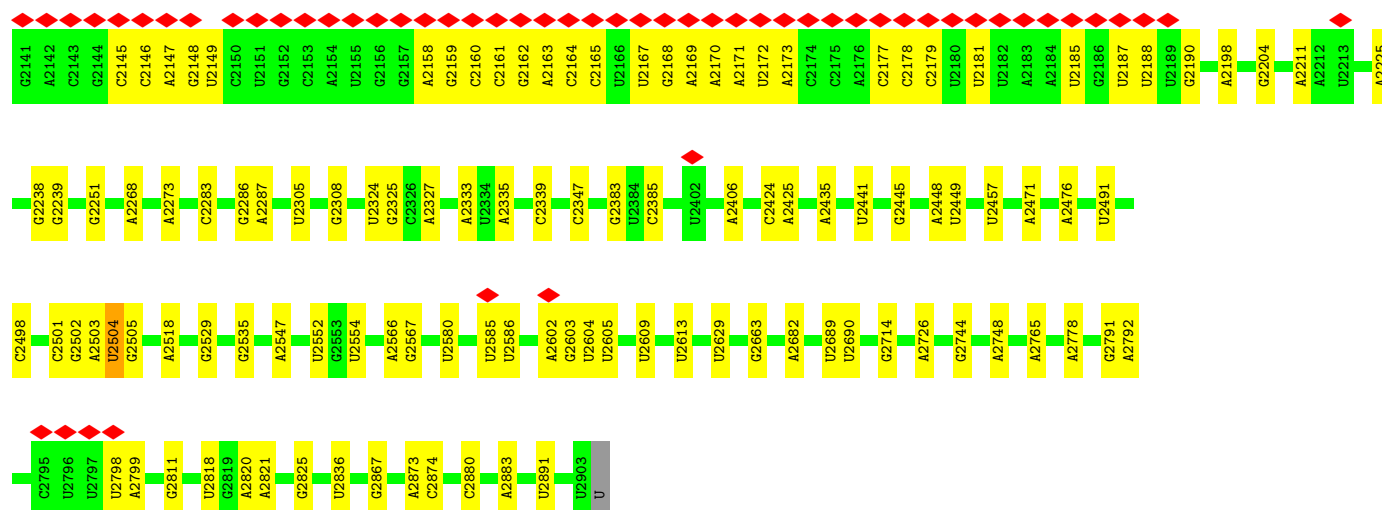
Mol	Chain	Residues	Atoms		AltConf
57	19	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

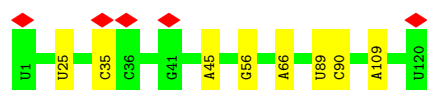
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 23S Ribosomal RNA

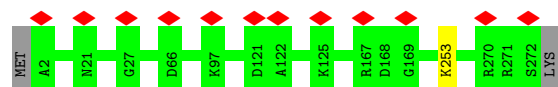




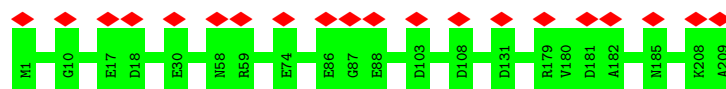
- Molecule 2: 5S Ribosomal RNA



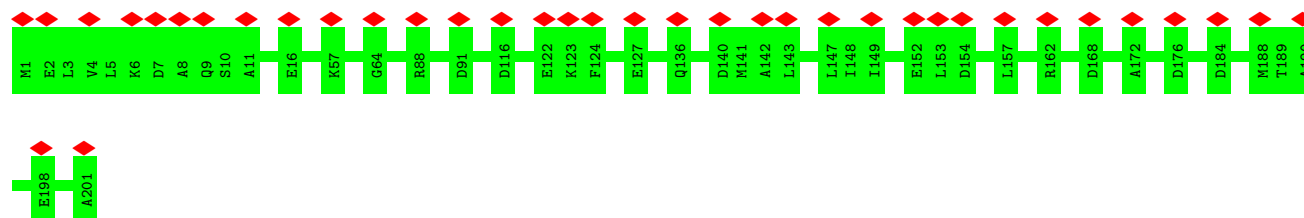
- Molecule 3: 50S ribosomal protein L2



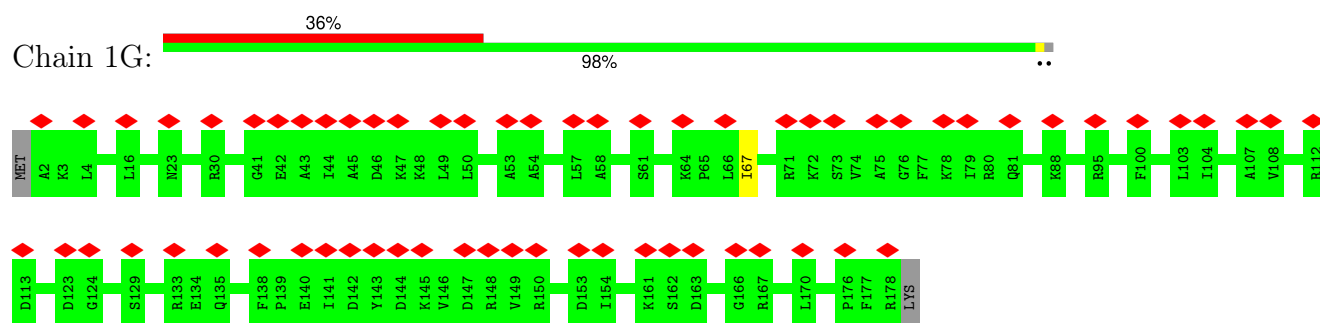
- Molecule 4: 50S ribosomal protein L3



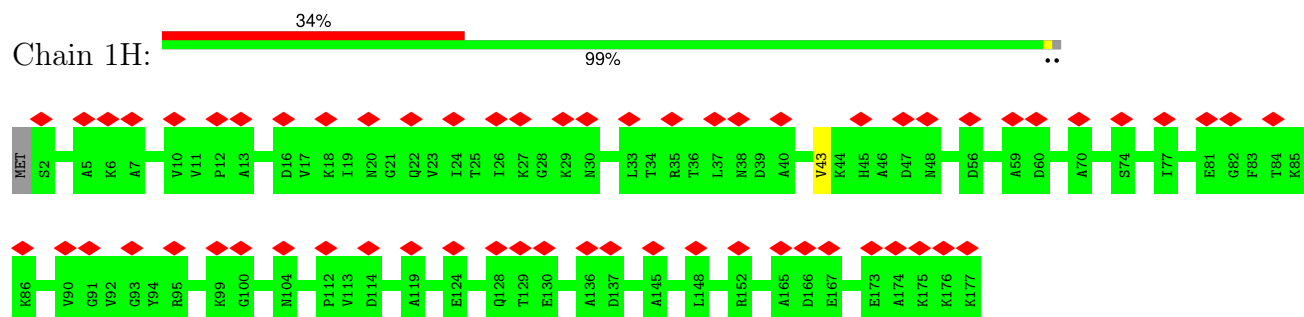
- Molecule 5: 50S ribosomal protein L4



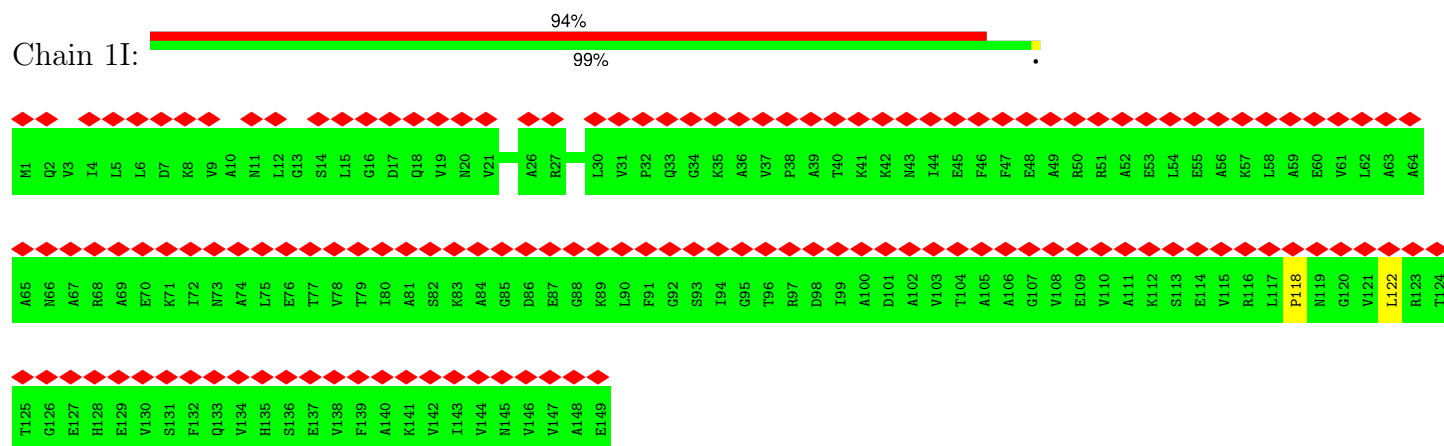
- Molecule 6: 50S ribosomal protein L5



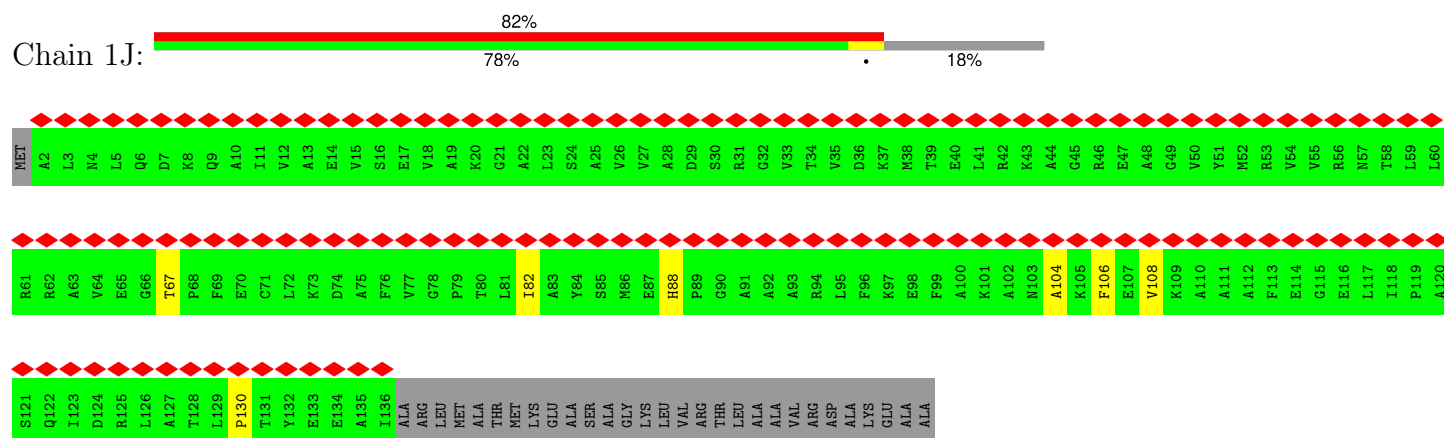
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L9

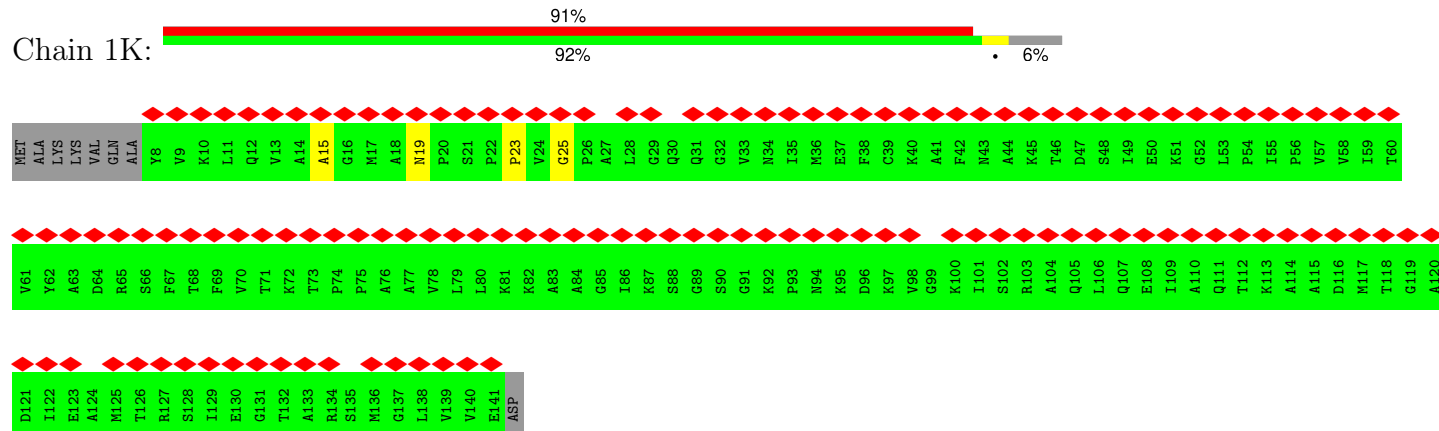


• Molecule 9: 50S ribosomal protein L10

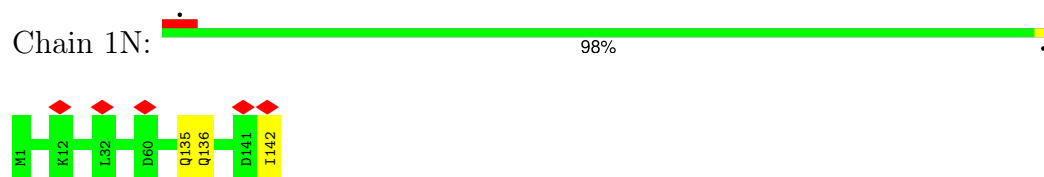




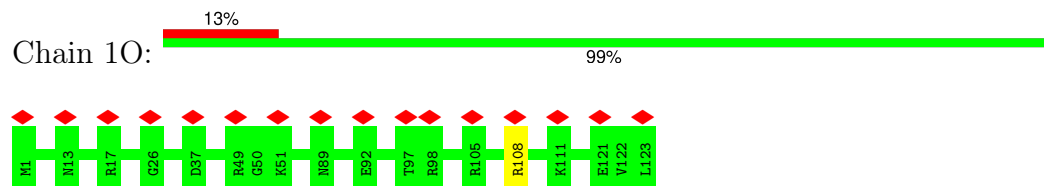
- Molecule 10: 50S ribosomal protein L11



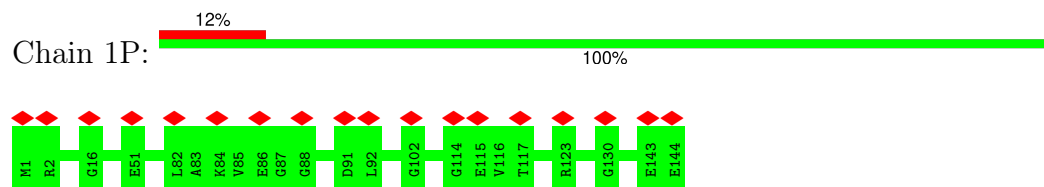
- Molecule 11: 50S ribosomal protein L13



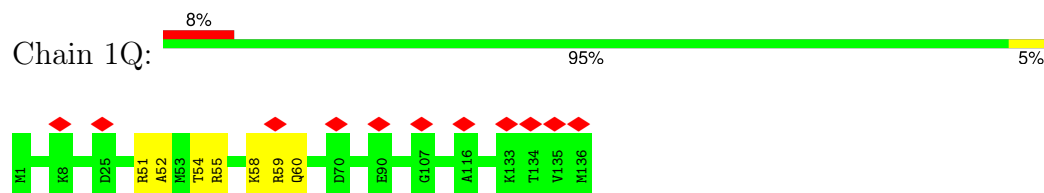
- Molecule 12: 50S ribosomal protein L14



- Molecule 13: 50S ribosomal protein L15

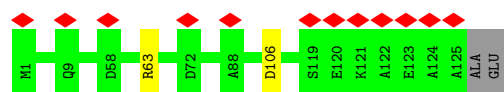


- Molecule 14: 50S ribosomal protein L16

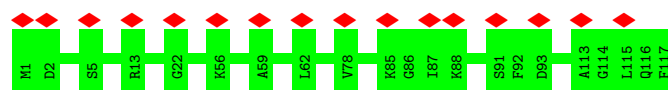


- Molecule 15: 50S ribosomal protein L17

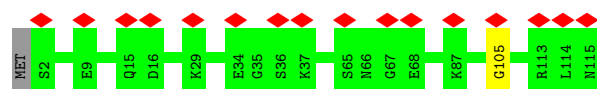




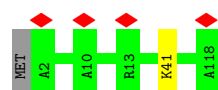
- Molecule 16: 50S ribosomal protein L18



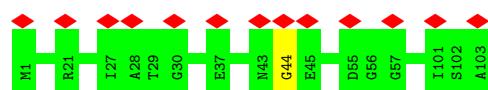
- Molecule 17: 50S ribosomal protein L19



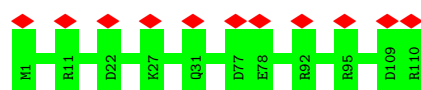
- Molecule 18: 50S ribosomal protein L20



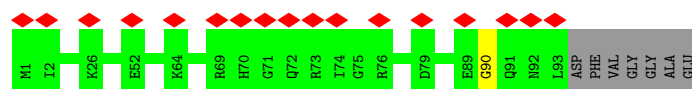
- Molecule 19: 50S ribosomal protein L21



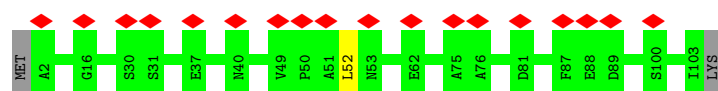
- Molecule 20: 50S ribosomal protein L22



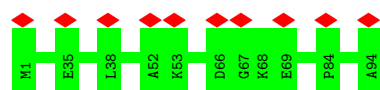
- Molecule 21: 50S ribosomal protein L23



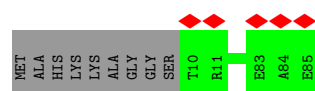
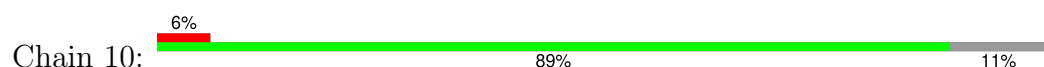
- Molecule 22: 50S ribosomal protein L24



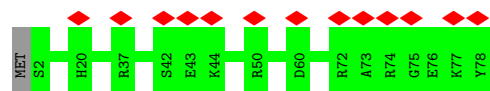
- Molecule 23: 50S ribosomal protein L25



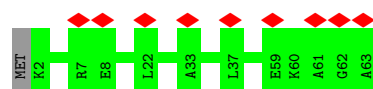
- Molecule 24: 50S ribosomal protein L27



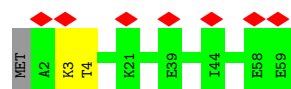
- Molecule 25: 50S ribosomal protein L28



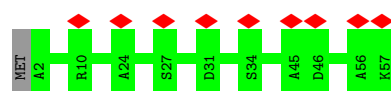
- Molecule 26: 50S ribosomal protein L29



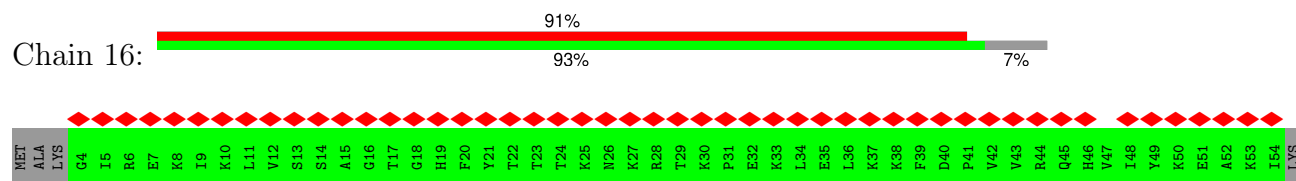
- Molecule 27: 50S ribosomal protein L30



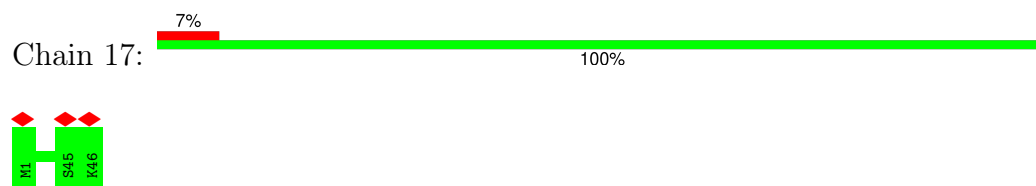
- Molecule 28: 50S ribosomal protein L32



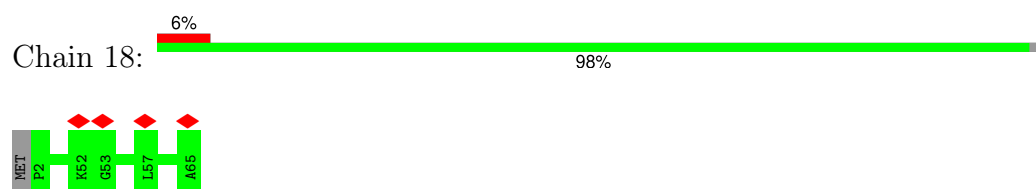
- Molecule 29: 50S ribosomal protein L33



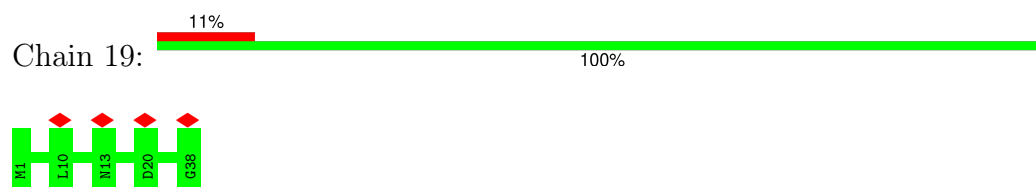
- Molecule 30: 50S ribosomal protein L34



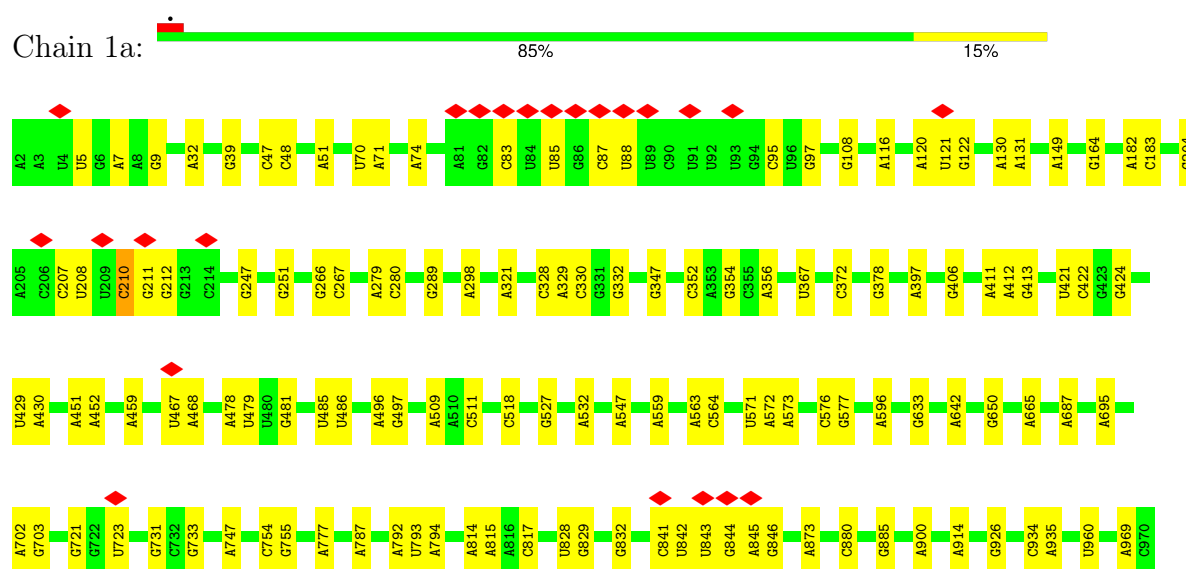
- Molecule 31: 50S ribosomal protein L35

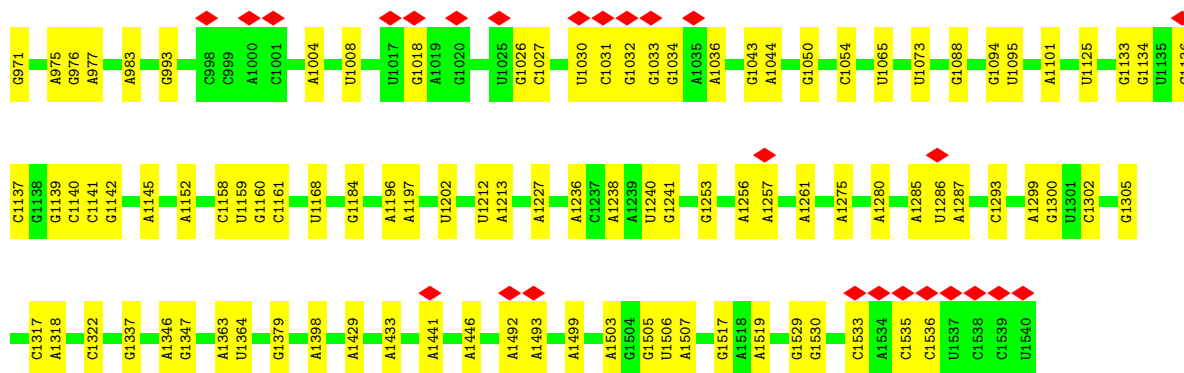


- Molecule 32: 50S ribosomal protein L36

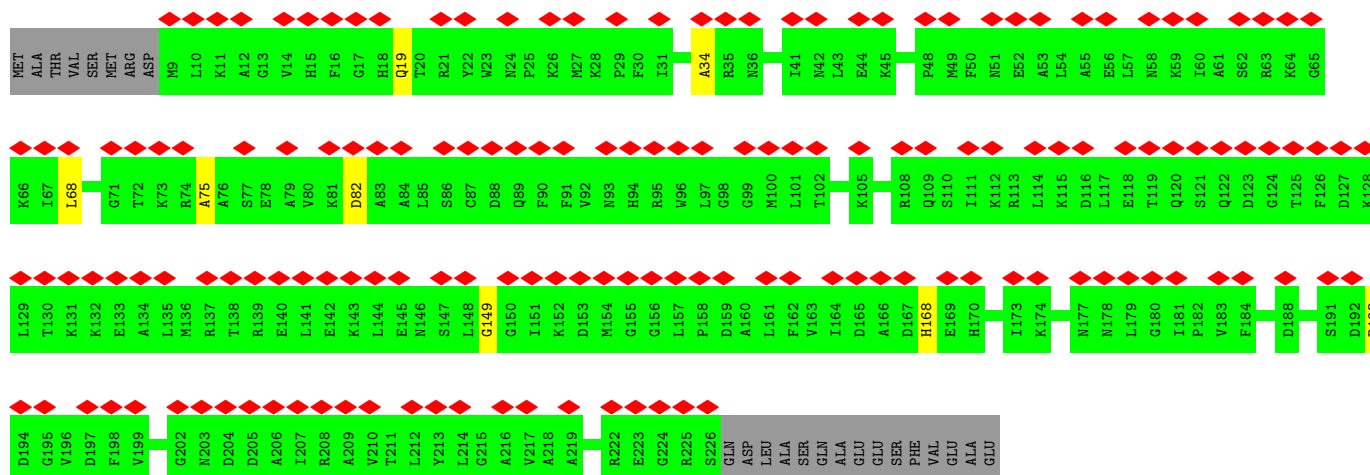
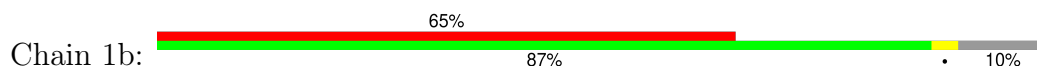


- Molecule 33: 16S Ribosomal RNA

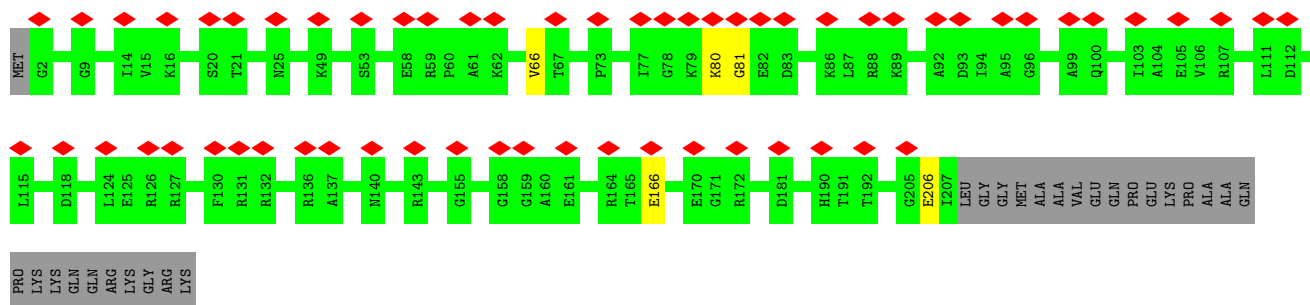
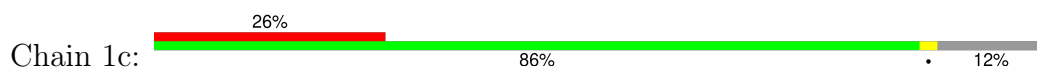




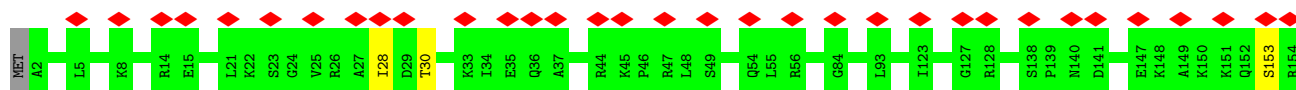
• Molecule 34: 30S ribosomal protein S2

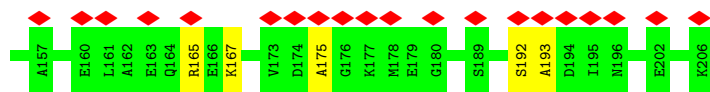


• Molecule 35: 30S ribosomal protein S3

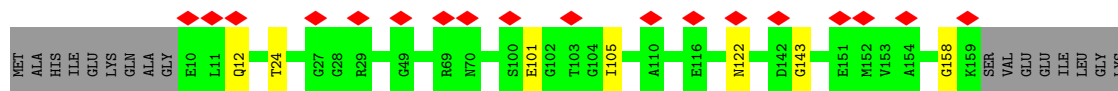
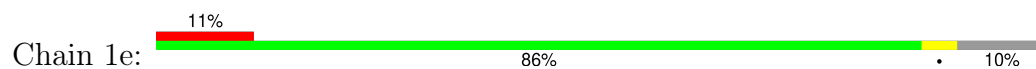


• Molecule 36: 30S ribosomal protein S4

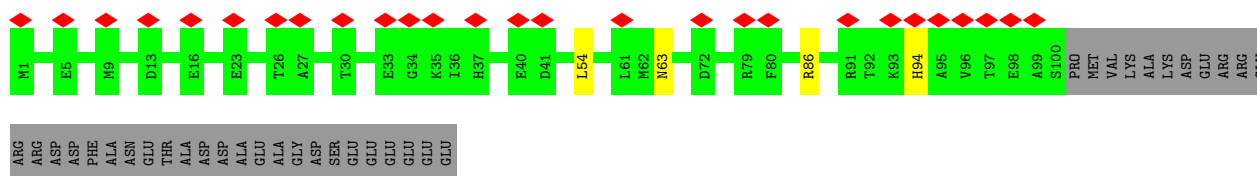




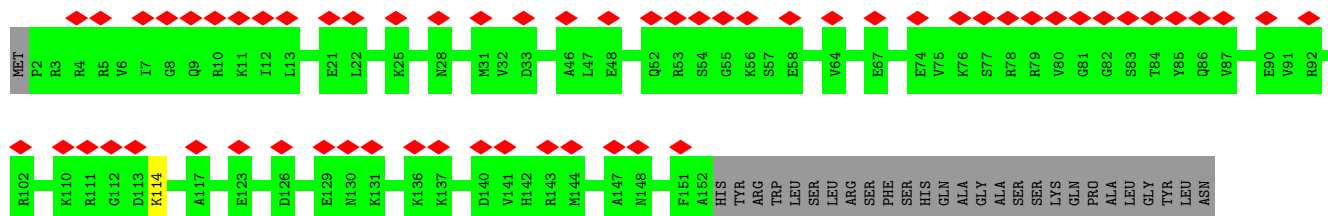
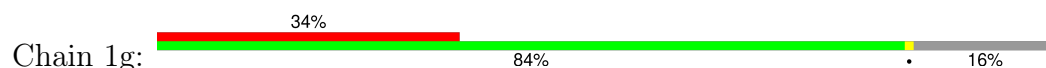
- Molecule 37: 30S ribosomal protein S5



- Molecule 38: 30S ribosomal protein S6



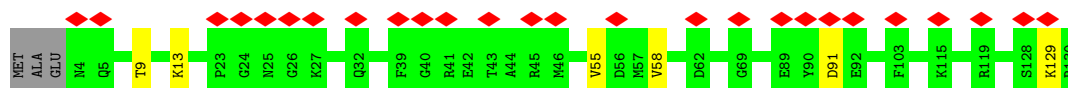
- Molecule 39: 30S ribosomal protein S7



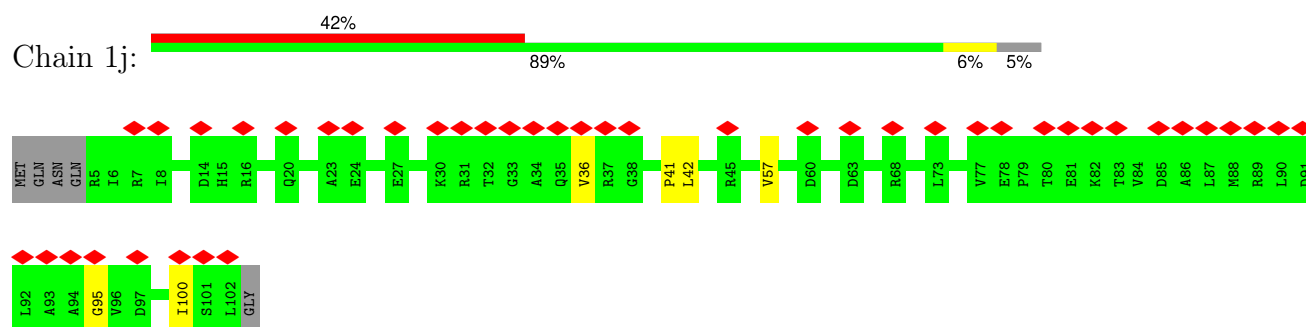
- Molecule 40: 30S ribosomal protein S8



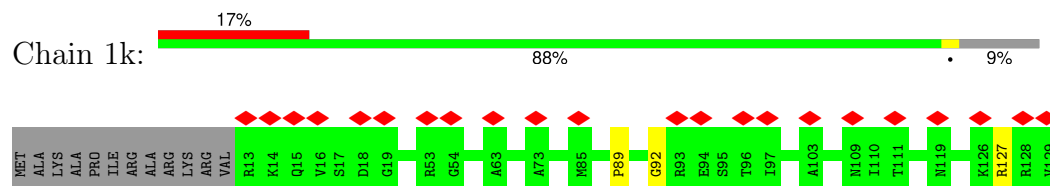
- Molecule 41: 30S ribosomal protein S9



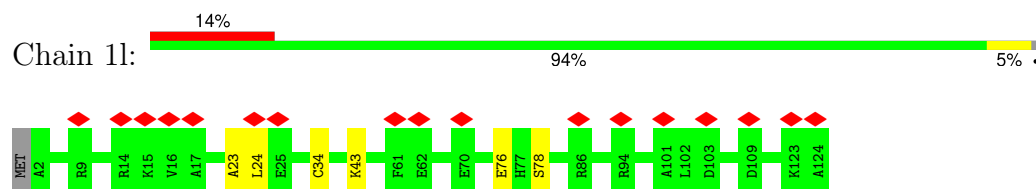
- Molecule 42: 30S ribosomal protein S10



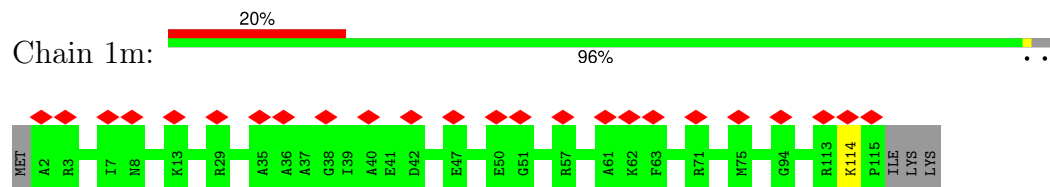
- Molecule 43: 30S ribosomal protein S11



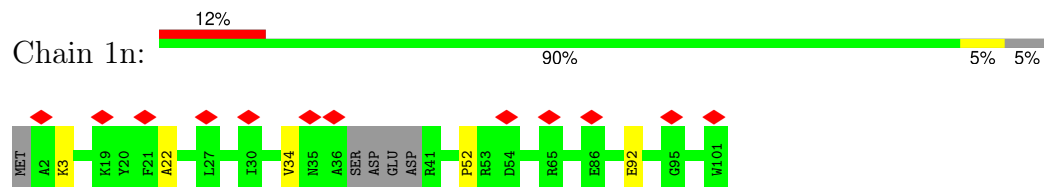
- Molecule 44: 30S ribosomal protein S12



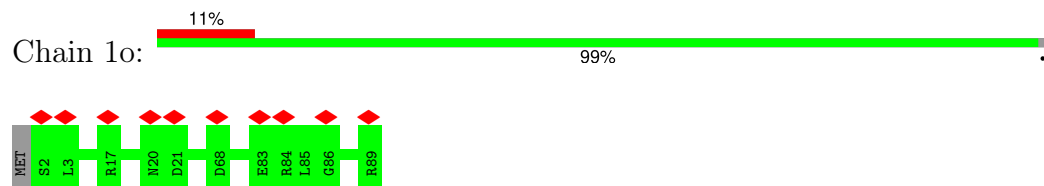
- Molecule 45: 30S ribosomal protein S13



- Molecule 46: 30S ribosomal protein S14

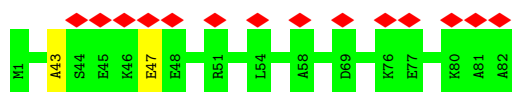


- Molecule 47: 30S ribosomal protein S15

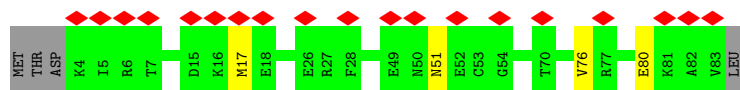
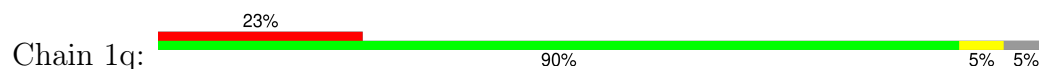


- Molecule 48: 30S ribosomal protein S16

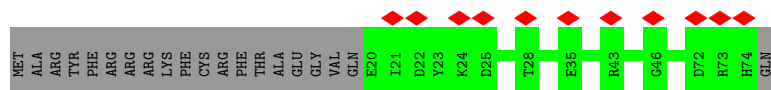
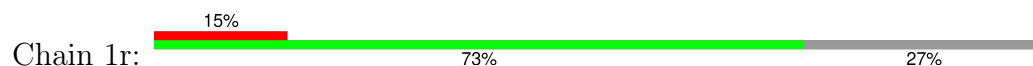




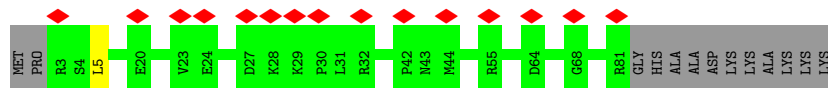
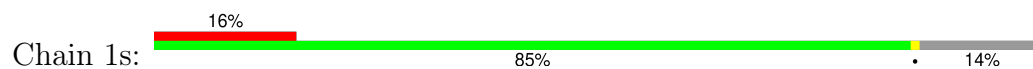
- Molecule 49: 30S ribosomal protein S17



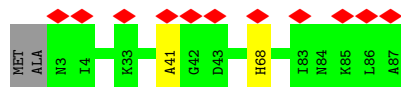
- Molecule 50: 30S ribosomal protein S18



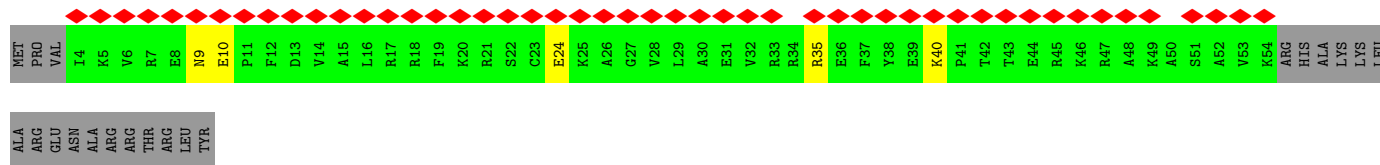
- Molecule 51: 30S ribosomal protein S19



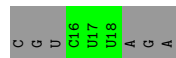
- Molecule 52: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S21

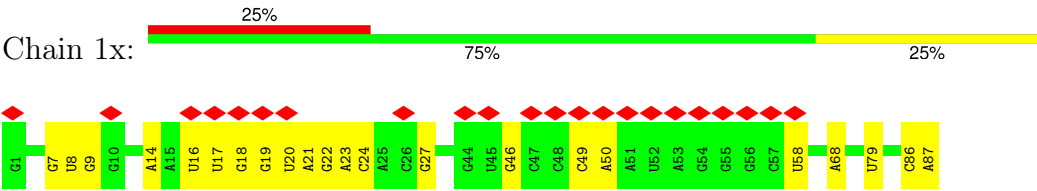


- Molecule 54: mRNA





● Molecule 55: P-site tRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61651	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 ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.004	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.000801	Depositor
Map size (Å)	407.74402, 407.74402, 407.74402	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1A	0.27	0/69297	0.81	26/108106 (0.0%)
2	1B	0.23	0/2872	0.77	0/4478
3	1D	0.29	0/2121	0.54	0/2852
4	1E	0.28	0/1576	0.50	0/2119
5	1F	0.27	0/1571	0.47	0/2113
6	1G	0.30	0/1428	0.51	0/1919
7	1H	0.28	0/1343	0.49	0/1816
8	1I	0.29	0/1121	0.51	0/1515
9	1J	0.31	0/1037	0.59	0/1400
10	1K	0.29	0/993	0.53	0/1341
11	1N	0.38	0/1152	0.54	0/1551
12	1O	0.30	0/955	0.51	0/1279
13	1P	0.28	0/1062	0.52	0/1413
14	1Q	0.29	0/1115	0.50	0/1488
15	1R	0.27	0/1006	0.49	0/1345
16	1S	0.28	0/910	0.48	0/1219
17	1T	0.29	0/929	0.53	0/1242
18	1U	0.29	0/960	0.43	0/1278
19	1V	0.27	0/829	0.51	0/1107
20	1W	0.25	0/864	0.47	0/1156
21	1X	0.27	0/744	0.50	0/994
22	1Y	0.30	0/787	0.52	0/1051
23	1Z	0.28	0/766	0.48	0/1025
24	10	0.29	0/598	0.49	0/790
25	11	0.26	0/635	0.47	0/848
26	12	0.24	0/502	0.41	0/667
27	13	0.27	0/467	0.42	0/623
28	15	0.30	0/450	0.51	0/599
29	16	0.38	0/421	0.55	0/561
30	17	0.32	0/380	0.59	0/498
31	18	0.27	0/513	0.49	0/676
32	19	0.26	0/303	0.48	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	1a	0.25	0/36966	0.73	12/57666 (0.0%)
34	1b	0.25	0/1735	0.42	0/2338
35	1c	0.24	0/1651	0.40	0/2225
36	1d	0.25	0/1665	0.43	0/2227
37	1e	0.26	0/1118	0.46	0/1504
38	1f	0.25	0/835	0.43	0/1128
39	1g	0.24	0/1195	0.39	0/1602
40	1h	0.26	0/989	0.45	0/1326
41	1i	0.25	0/1034	0.47	0/1375
42	1j	0.25	0/796	0.49	0/1077
43	1k	0.25	0/893	0.43	0/1205
44	1l	0.27	0/969	0.48	0/1300
45	1m	0.23	0/892	0.43	0/1193
46	1n	0.23	0/785	0.41	0/1043
47	1o	0.24	0/718	0.41	0/959
48	1p	0.24	0/659	0.43	0/884
49	1q	0.26	0/657	0.47	0/881
50	1r	0.24	0/462	0.40	0/621
51	1s	0.25	0/652	0.41	0/877
52	1t	0.23	0/671	0.38	0/888
53	1u	0.26	0/430	0.48	0/570
54	1v	0.33	0/65	0.91	0/98
55	1x	0.25	0/2080	0.76	0/3242
All	All	0.27	0/157624	0.72	38/235695 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1N	0	1
27	13	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1a	1158	C	N1-C2-O2	8.80	124.18	118.90
1	1A	1584	U	C2-N1-C1'	8.32	127.68	117.70
1	1A	1584	U	N1-C2-O2	8.29	128.61	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1a	1158	C	C2-N1-C1'	8.29	127.91	118.80
33	1a	210	C	N1-C2-O2	8.01	123.70	118.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	13	3[B]	LYS	Peptide
11	1N	135	GLN	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	
3	1D	269/273 (98%)	251 (93%)	17 (6%)	1 (0%)	30	63
4	1E	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
5	1F	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
6	1G	175/179 (98%)	164 (94%)	11 (6%)	0	100	100
7	1H	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
8	1I	147/149 (99%)	132 (90%)	13 (9%)	2 (1%)	9	40
9	1J	133/165 (81%)	114 (86%)	13 (10%)	6 (4%)	2	18
10	1K	132/142 (93%)	122 (92%)	6 (4%)	4 (3%)	3	26
11	1N	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
12	1O	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	16	51
13	1P	142/144 (99%)	137 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1Q	136/136 (100%)	126 (93%)	8 (6%)	2 (2%)	8	39
15	1R	123/127 (97%)	117 (95%)	5 (4%)	1 (1%)	16	51
16	1S	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
17	1T	112/115 (97%)	108 (96%)	3 (3%)	1 (1%)	14	48
18	1U	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
19	1V	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	13	46
20	1W	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
21	1X	91/100 (91%)	87 (96%)	3 (3%)	1 (1%)	12	45
22	1Y	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	13	46
23	1Z	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	10	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
25	11	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
26	12	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
27	13	57/59 (97%)	55 (96%)	1 (2%)	1 (2%)	7	35
28	15	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	16	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
30	17	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
31	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	19	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
34	1b	216/241 (90%)	189 (88%)	19 (9%)	8 (4%)	2	22
35	1c	204/233 (88%)	180 (88%)	19 (9%)	5 (2%)	4	29
36	1d	203/206 (98%)	187 (92%)	8 (4%)	8 (4%)	2	21
37	1e	148/167 (89%)	124 (84%)	17 (12%)	7 (5%)	2	18
38	1f	98/135 (73%)	84 (86%)	10 (10%)	4 (4%)	2	20
39	1g	149/179 (83%)	141 (95%)	7 (5%)	1 (1%)	19	53
40	1h	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
41	1i	125/130 (96%)	113 (90%)	6 (5%)	6 (5%)	2	17
42	1j	96/103 (93%)	83 (86%)	7 (7%)	6 (6%)	1	13
43	1k	115/129 (89%)	99 (86%)	13 (11%)	3 (3%)	4	28
44	1l	121/124 (98%)	106 (88%)	9 (7%)	6 (5%)	1	17
45	1m	112/118 (95%)	102 (91%)	9 (8%)	1 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	1n	92/101 (91%)	79 (86%)	8 (9%)	5 (5%)	1	15
47	1o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
48	1p	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	4	29
49	1q	78/84 (93%)	62 (80%)	12 (15%)	4 (5%)	1	16
50	1r	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
51	1s	77/92 (84%)	72 (94%)	4 (5%)	1 (1%)	10	41
52	1t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	5	30
53	1u	49/71 (69%)	36 (74%)	8 (16%)	5 (10%)	0	6
All	All	5755/6150 (94%)	5333 (93%)	326 (6%)	96 (2%)	10	37

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	1K	15	ALA
10	1K	19	ASN
14	1Q	51	ARG
22	1Y	52	LEU
36	1d	30	THR

### 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	
3	1D	216/218 (99%)	216 (100%)	0	100	100
4	1E	163/163 (100%)	163 (100%)	0	100	100
5	1F	165/165 (100%)	165 (100%)	0	100	100
6	1G	147/150 (98%)	146 (99%)	1 (1%)	81	90
7	1H	137/138 (99%)	136 (99%)	1 (1%)	81	90
8	1I	114/114 (100%)	114 (100%)	0	100	100
9	1J	103/123 (84%)	102 (99%)	1 (1%)	73	85
10	1K	104/110 (94%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	1N	116/116 (100%)	114 (98%)	2 (2%)	56	75
12	1O	104/104 (100%)	104 (100%)	0	100	100
13	1P	103/103 (100%)	103 (100%)	0	100	100
14	1Q	111/109 (102%)	106 (96%)	5 (4%)	23	53
15	1R	102/103 (99%)	101 (99%)	1 (1%)	73	85
16	1S	87/87 (100%)	87 (100%)	0	100	100
17	1T	99/100 (99%)	99 (100%)	0	100	100
18	1U	89/90 (99%)	88 (99%)	1 (1%)	70	83
19	1V	84/84 (100%)	84 (100%)	0	100	100
20	1W	93/93 (100%)	93 (100%)	0	100	100
21	1X	80/84 (95%)	80 (100%)	0	100	100
22	1Y	83/85 (98%)	83 (100%)	0	100	100
23	1Z	78/78 (100%)	78 (100%)	0	100	100
24	10	58/63 (92%)	58 (100%)	0	100	100
25	11	67/68 (98%)	67 (100%)	0	100	100
26	12	54/55 (98%)	54 (100%)	0	100	100
27	13	49/49 (100%)	49 (100%)	0	100	100
28	15	47/48 (98%)	47 (100%)	0	100	100
29	16	45/49 (92%)	45 (100%)	0	100	100
30	17	38/38 (100%)	38 (100%)	0	100	100
31	18	51/52 (98%)	51 (100%)	0	100	100
32	19	34/34 (100%)	34 (100%)	0	100	100
34	1b	180/199 (90%)	180 (100%)	0	100	100
35	1c	170/190 (90%)	170 (100%)	0	100	100
36	1d	172/173 (99%)	172 (100%)	0	100	100
37	1e	113/126 (90%)	113 (100%)	0	100	100
38	1f	87/116 (75%)	87 (100%)	0	100	100
39	1g	124/147 (84%)	124 (100%)	0	100	100
40	1h	104/105 (99%)	104 (100%)	0	100	100
41	1i	105/107 (98%)	105 (100%)	0	100	100
42	1j	86/90 (96%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	1k	90/99 (91%)	90 (100%)	0	100	100
44	1l	103/104 (99%)	103 (100%)	0	100	100
45	1m	92/96 (96%)	92 (100%)	0	100	100
46	1n	79/84 (94%)	79 (100%)	0	100	100
47	1o	75/77 (97%)	75 (100%)	0	100	100
48	1p	65/65 (100%)	65 (100%)	0	100	100
49	1q	74/78 (95%)	74 (100%)	0	100	100
50	1r	48/65 (74%)	48 (100%)	0	100	100
51	1s	70/79 (89%)	70 (100%)	0	100	100
52	1t	65/66 (98%)	65 (100%)	0	100	100
53	1u	44/61 (72%)	44 (100%)	0	100	100
All	All	4767/5000 (95%)	4755 (100%)	12 (0%)	90	96

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	1Q	58	LYS
14	1Q	59	ARG
18	1U	41	LYS
14	1Q	60	GLN
11	1N	136	GLN

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

Mol	Chain	Res	Type
26	12	58	ASN
36	1d	116	GLN
50	1r	52	GLN
27	13	20	HIS
31	18	26	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2884/2904 (99%)	360 (12%)	10 (0%)
2	1B	119/120 (99%)	8 (6%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	1a	1538/1539 (99%)	226 (14%)	0
54	1v	2/9 (22%)	0	0
55	1x	86/87 (98%)	22 (25%)	0
All	All	4629/4659 (99%)	616 (13%)	10 (0%)

5 of 616 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	A
1	1A	12	U
1	1A	15	G
1	1A	34	U
1	1A	46	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2406	A
1	1A	2585	U
1	1A	2873	A
1	1A	2118	U
1	1A	2127	G

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

26 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	$\# Z  > 2$
1	OMG	1A	2251	1,55	19,26,27	0.89	1 (5%)	21,38,41	1.04	2 (9%)
1	PSU	1A	1917	1	18,21,22	1.42	2 (11%)	21,30,33	2.20	4 (19%)
1	PSU	1A	2504	1	18,21,22	1.40	2 (11%)	21,30,33	2.06	4 (19%)
1	OMU	1A	2552	1	19,22,23	1.22	2 (10%)	25,31,34	1.82	5 (20%)
1	PSU	1A	2580	1	18,21,22	1.39	3 (16%)	21,30,33	2.12	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	6MZ	1A	1618	1	17,25,26	0.96	1 (5%)	15,36,39	2.31	4 (26%)
1	G7M	1A	2069	1	20,26,27	1.13	1 (5%)	16,39,42	1.60	4 (25%)
1	H2U	1A	2449	1	18,21,22	1.01	2 (11%)	19,30,33	1.11	3 (15%)
1	PSU	1A	955	1	18,21,22	1.38	2 (11%)	21,30,33	2.24	4 (19%)
1	PSU	1A	746	1	18,21,22	1.42	2 (11%)	21,30,33	2.06	4 (19%)
1	2MA	1A	2503	1	17,25,26	1.03	0	16,37,40	1.36	2 (12%)
1	2MG	1A	2445	1	18,26,27	0.87	1 (5%)	16,38,41	1.46	5 (31%)
1	PSU	1A	2605	1	18,21,22	1.39	3 (16%)	21,30,33	2.18	4 (19%)
1	1MG	1A	745	1	19,26,27	0.96	1 (5%)	18,39,42	1.25	2 (11%)
1	5MU	1A	747	1	19,22,23	1.37	5 (26%)	27,32,35	2.12	6 (22%)
1	PSU	1A	2457	1	18,21,22	1.42	2 (11%)	21,30,33	2.16	5 (23%)
1	PSU	1A	2604	1	18,21,22	1.37	2 (11%)	21,30,33	2.00	4 (19%)
4	MEQ	1E	150[A]	4	8,9,10	0.60	0	5,10,12	0.72	0
1	OMC	1A	2498	1	19,22,23	0.79	0	25,31,34	1.04	1 (4%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.09	4 (19%)
1	2MG	1A	1835	1	18,26,27	0.91	1 (5%)	16,38,41	1.23	1 (6%)
1	6MZ	1A	2030	1	17,25,26	0.96	1 (5%)	15,36,39	2.58	5 (33%)
1	5MU	1A	1939	1	19,22,23	1.43	6 (31%)	27,32,35	2.14	6 (22%)
1	PSU	1A	1915	1	18,21,22	1.37	2 (11%)	21,30,33	2.12	4 (19%)
1	5MC	1A	1962	1	19,22,23	1.66	3 (15%)	26,32,35	1.06	2 (7%)
4	MEQ	1E	150[B]	4	8,9,10	0.65	0	5,10,12	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1A	2251	1,55	-	0/5/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2504	1	-	1/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	1A	2580	1	-	0/7/25/26	0/2/2/2
1	6MZ	1A	1618	1	-	0/5/27/28	0/3/3/3
1	G7M	1A	2069	1	-	1/3/25/26	0/3/3/3
1	H2U	1A	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	1A	955	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	746	1	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	1A	2503	1	-	2/3/25/26	0/3/3/3
1	2MG	1A	2445	1	-	1/5/27/28	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	1A	745	1	-	0/3/25/26	0/3/3/3
1	5MU	1A	747	1	-	1/7/25/26	0/2/2/2
1	PSU	1A	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2604	1	-	0/7/25/26	0/2/2/2
4	MEQ	1E	150[A]	4	-	2/8/9/11	-
1	OMC	1A	2498	1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MG	1A	1835	1	-	2/5/27/28	0/3/3/3
1	6MZ	1A	2030	1	-	2/5/27/28	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/7/25/26	0/2/2/2
4	MEQ	1E	150[B]	4	-	4/8/9/11	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1962	5MC	C5-C4	6.04	1.48	1.44
1	1A	2457	PSU	C6-C5	3.67	1.39	1.35
1	1A	1917	PSU	C6-C5	3.67	1.39	1.35
1	1A	2504	PSU	C6-C5	3.58	1.39	1.35
1	1A	2604	PSU	C6-C5	3.53	1.39	1.35

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1917	PSU	N1-C2-N3	6.94	122.49	115.17
1	1A	955	PSU	N1-C2-N3	6.85	122.40	115.17
1	1A	2457	PSU	N1-C2-N3	6.79	122.33	115.17
1	1A	2605	PSU	N1-C2-N3	6.68	122.21	115.17
1	1A	2030	6MZ	C2-N1-C6	6.61	121.73	116.60

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	746	PSU	C2'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
1	1A	746	PSU	C2'-C1'-C5-C6
1	1A	746	PSU	O4'-C1'-C5-C6
4	1E	150[B]	MEQ	C-CA-CB-CG
4	1E	150[B]	MEQ	CG-CD-NE2-CE

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
56	6UQ	1A	3001	1	101,105,105	1.61	14 (13%)	130,164,164	2.02	39 (30%)

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	6UQ	1A	3001	1	-	15/47/211/211	0/11/11/11

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1A	3001	6UQ	OCP-CCJ	6.29	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1A	3001	6UQ	CDF-CAC	-5.53	1.40	1.51
56	1A	3001	6UQ	OBQ-CBP	5.12	1.55	1.43
56	1A	3001	6UQ	CAD-CAJ	-4.28	1.40	1.50
56	1A	3001	6UQ	OCS-CCR	3.74	1.47	1.41

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	3001	6UQ	CCC-OCH-CCU	-7.60	105.14	117.76
56	1A	3001	6UQ	CBC-CBF-CBG	-6.43	104.14	114.99
56	1A	3001	6UQ	OCI-CCD-CCE	-4.64	97.02	103.48
56	1A	3001	6UQ	CCZ-CCO-CCN	-4.30	104.75	115.31
56	1A	3001	6UQ	O1-CCB-OCG	4.18	117.57	108.92

There are no chirality outliers.

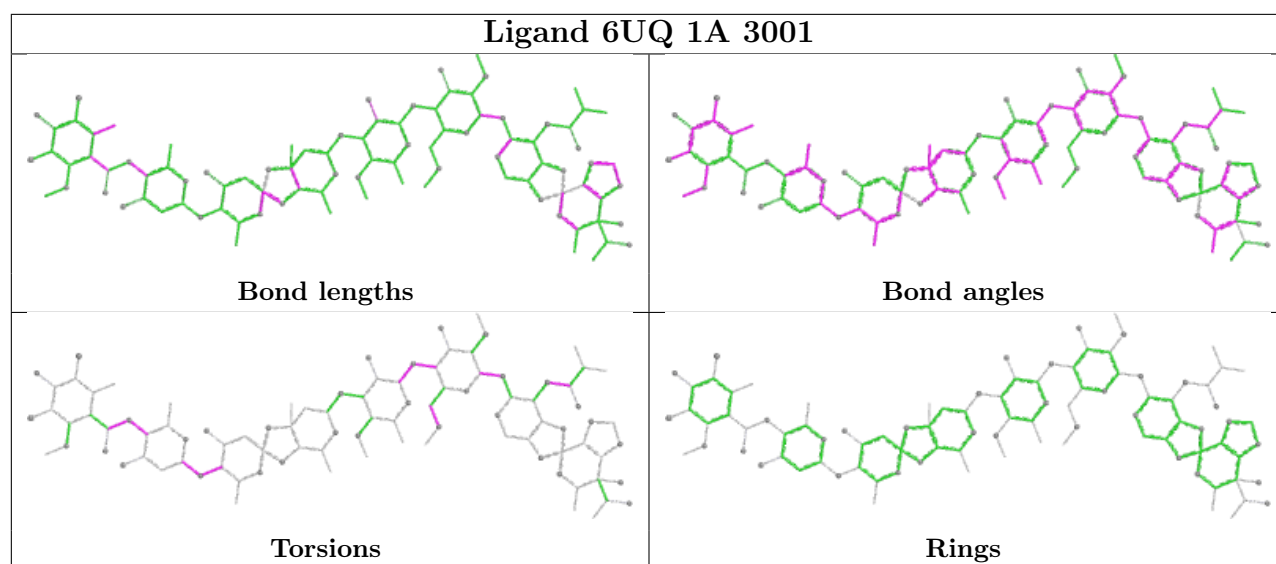
5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	1A	3001	6UQ	C2-C1-O1-CCB
56	1A	3001	6UQ	C3-C4-O4-CBO
56	1A	3001	6UQ	CAD-CAJ-OAL-CAM
56	1A	3001	6UQ	CCV-CCU-OCH-CCC
56	1A	3001	6UQ	OCY-CCU-OCH-CCC

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



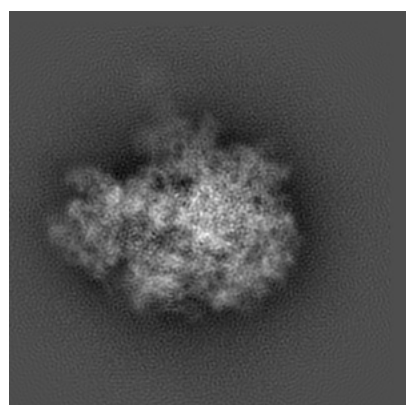
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8237. These allow visual inspection of the internal detail of the map and identification of artifacts.

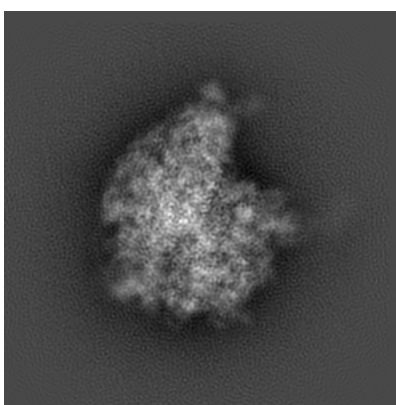
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

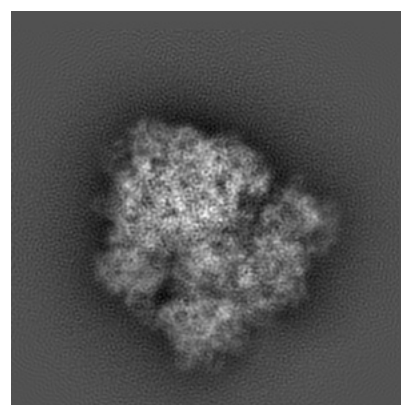
#### 6.1.1 Primary map



X



Y

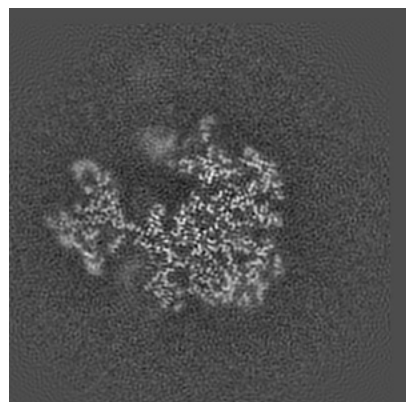


Z

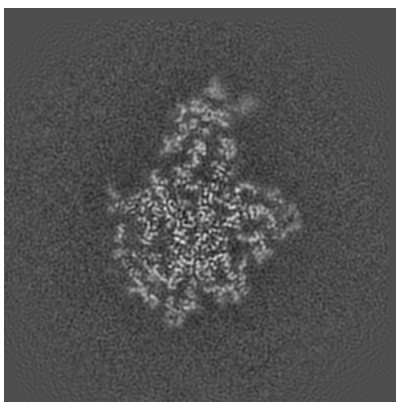
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

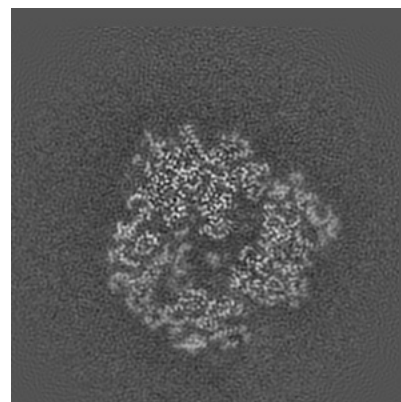
#### 6.2.1 Primary map



X Index: 184



Y Index: 184



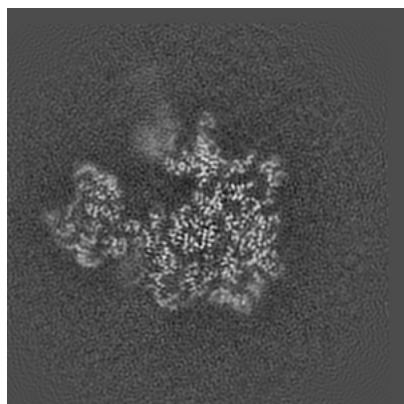
Z Index: 184



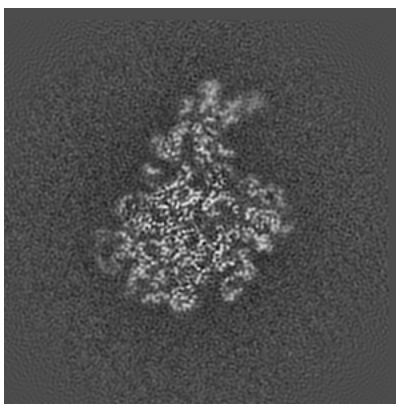
The images above show central slices of the map in three orthogonal directions.

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

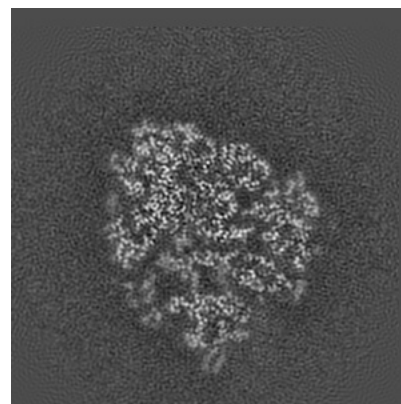
### 6.3.1 Primary map



X Index: 179



Y Index: 175

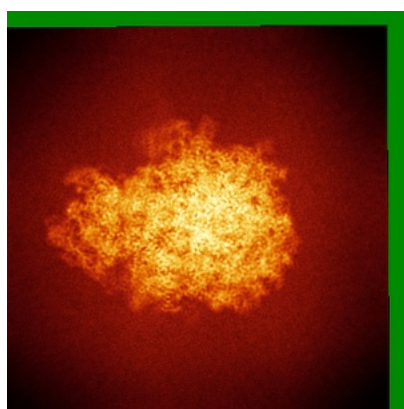


Z Index: 177

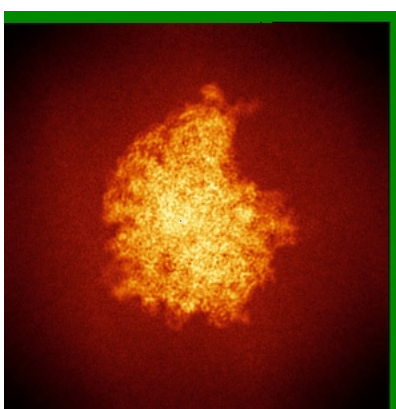
The images above show the largest variance slices of the map in three orthogonal directions.

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

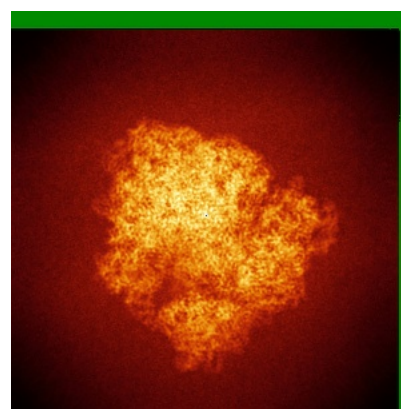
### 6.4.1 Primary map



X



Y

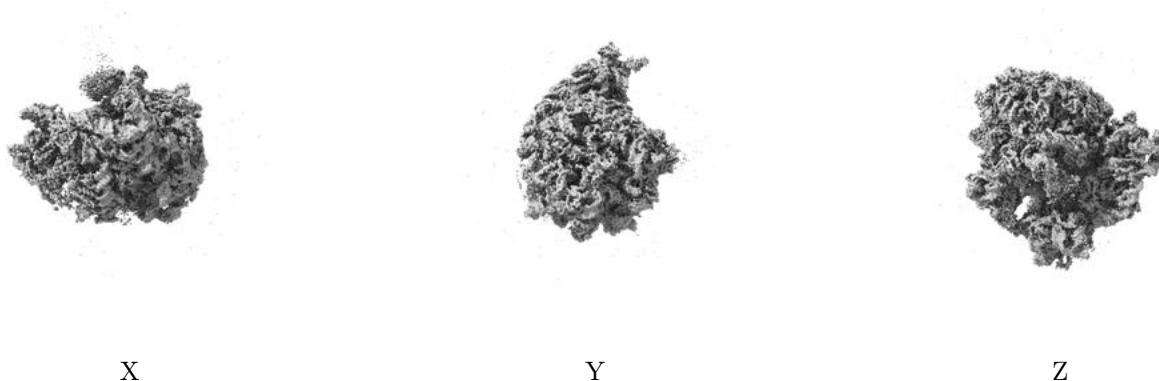


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.000801. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

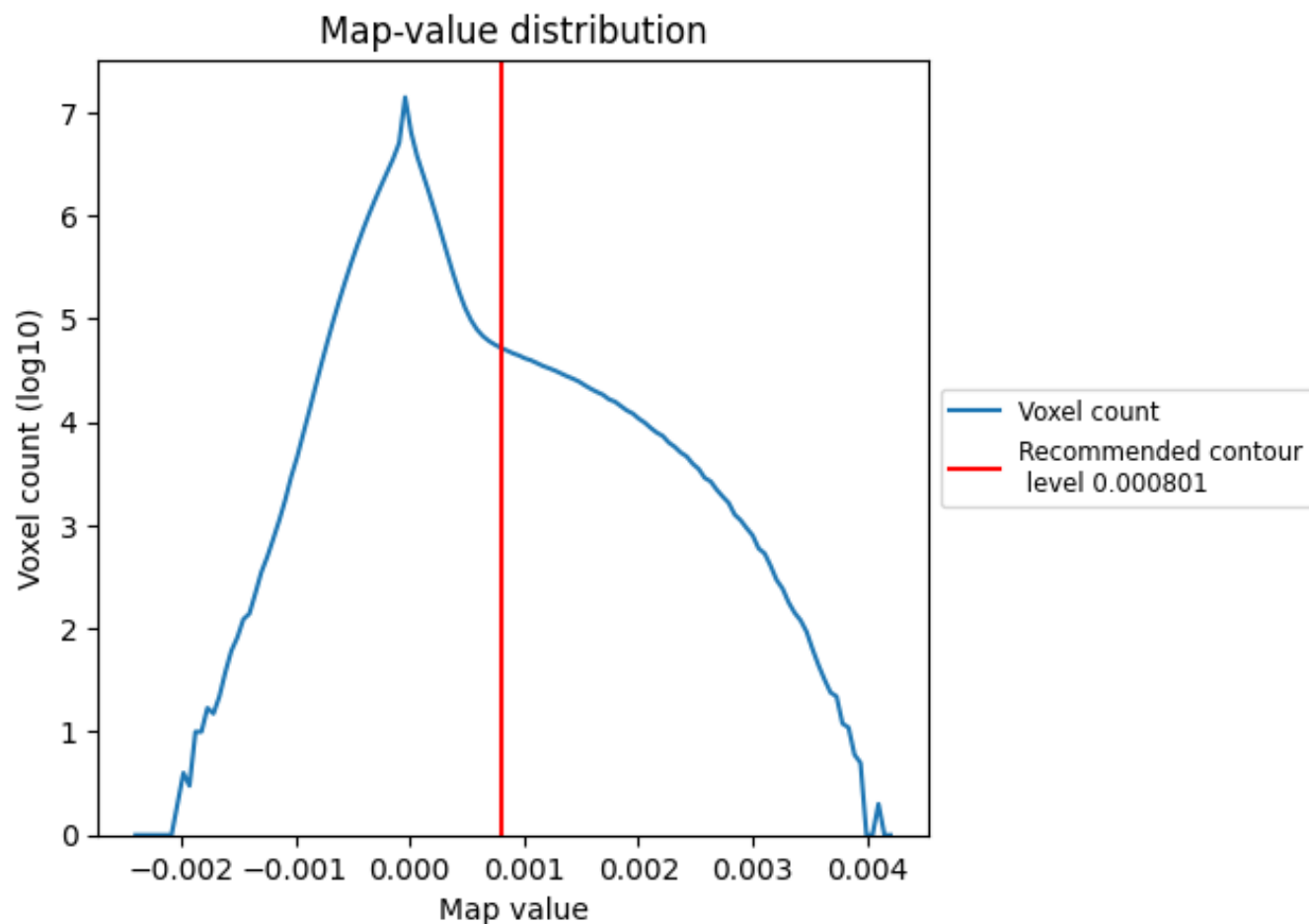
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

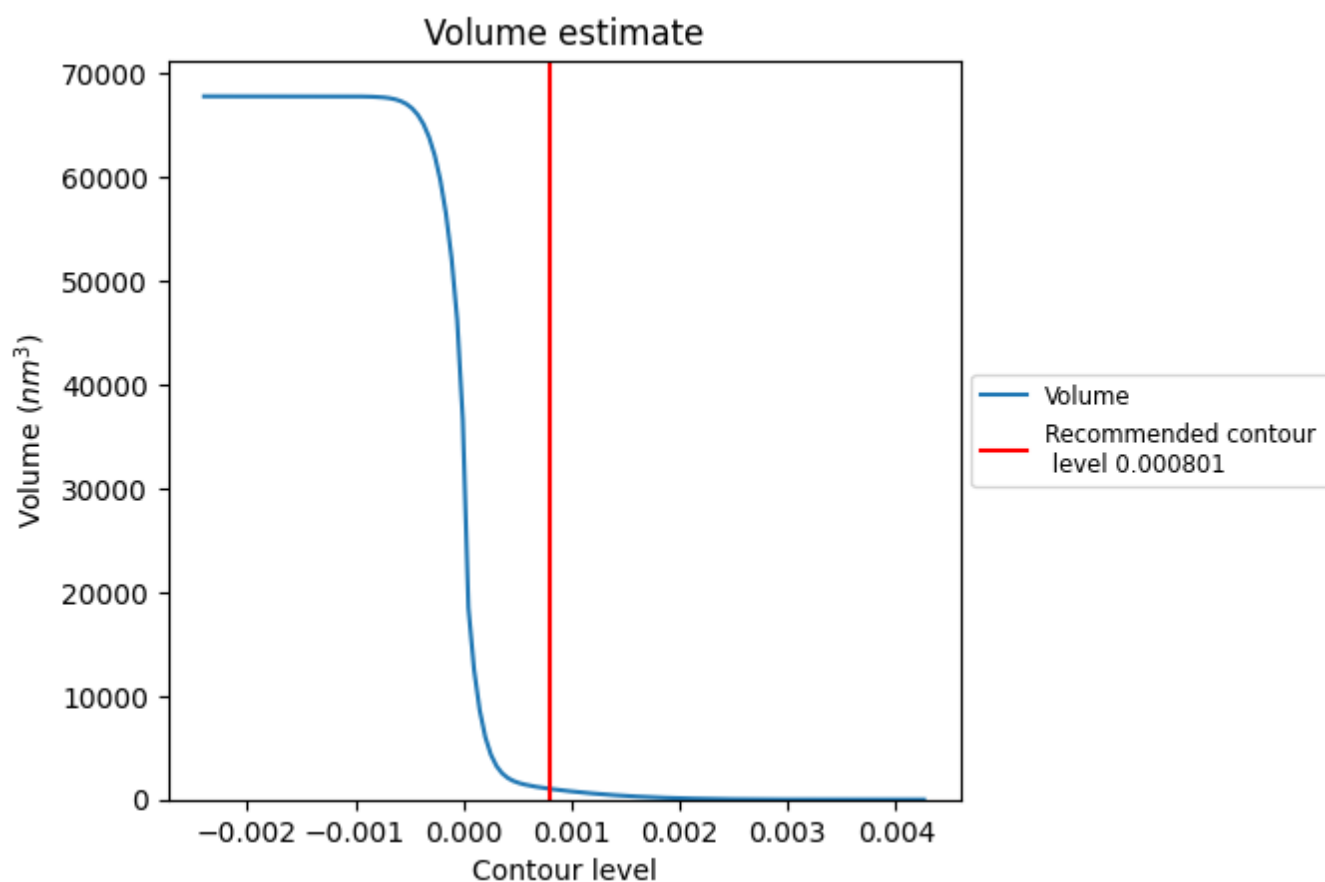
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

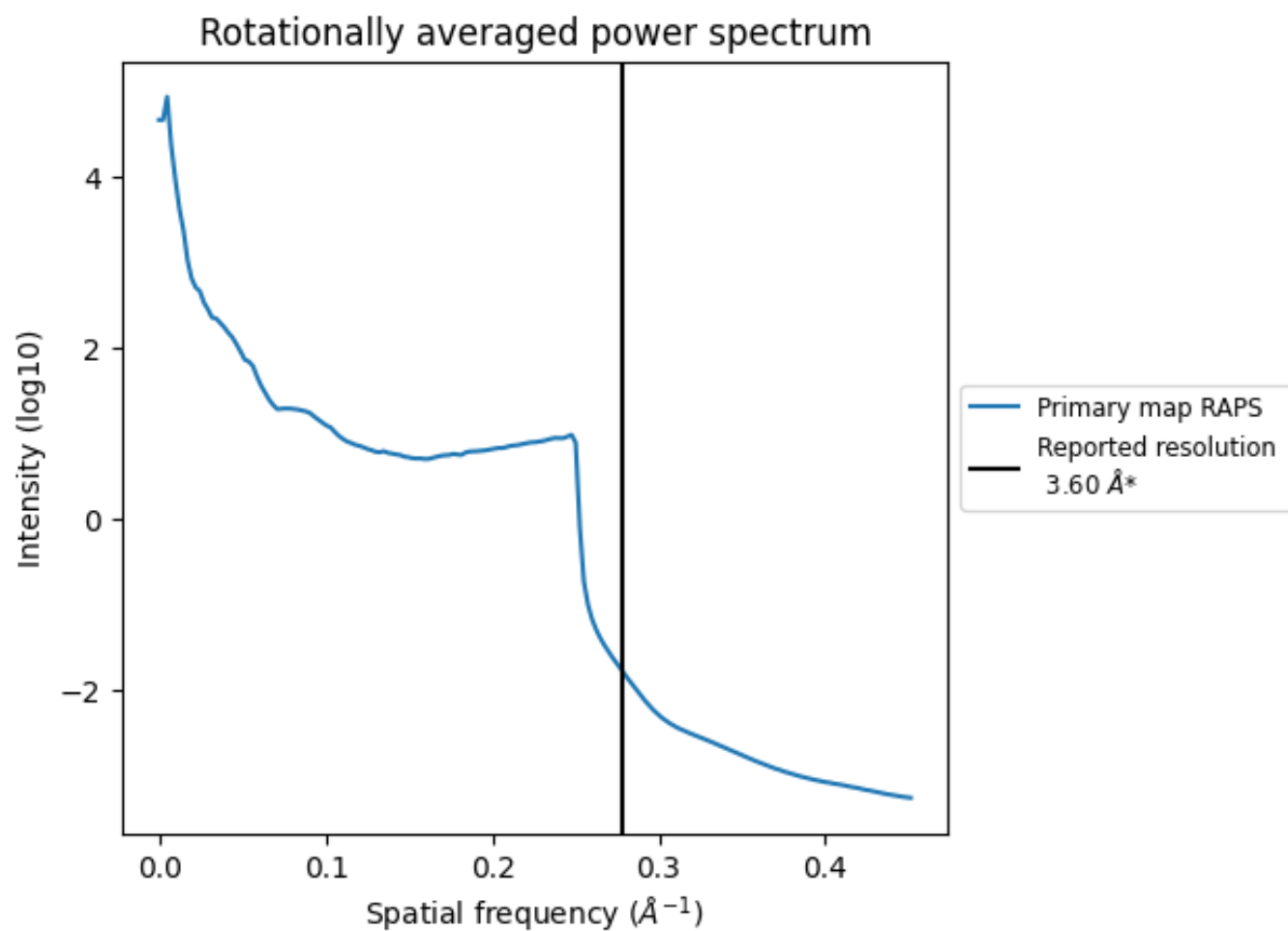
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1035 nm<sup>3</sup>; this corresponds to an approximate mass of 935 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

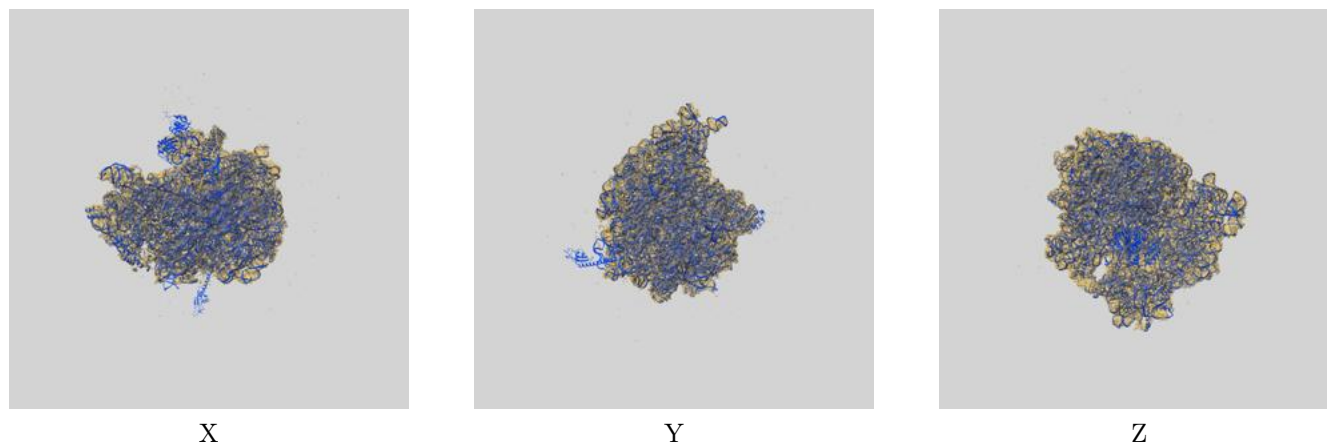
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

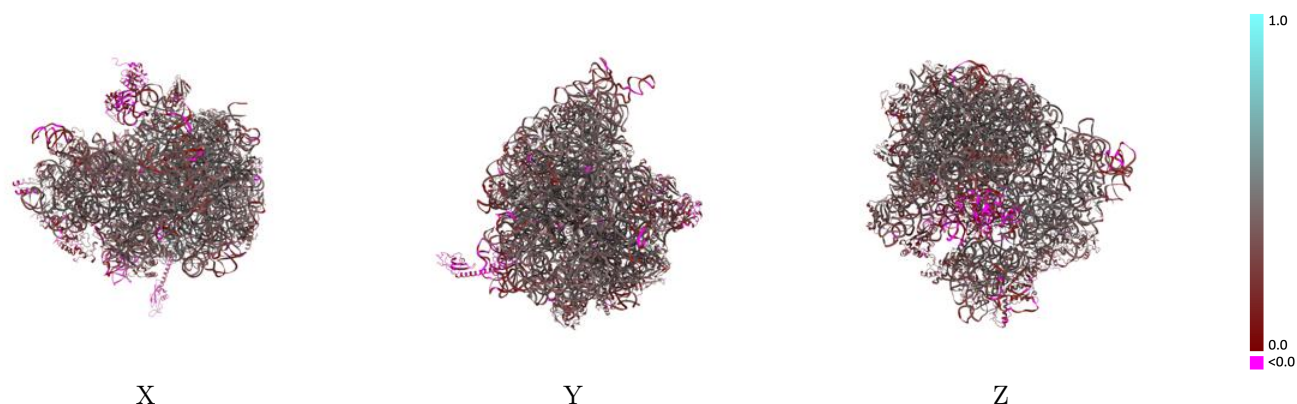
This section contains information regarding the fit between EMDB map EMD-8237 and PDB model 5KCR. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



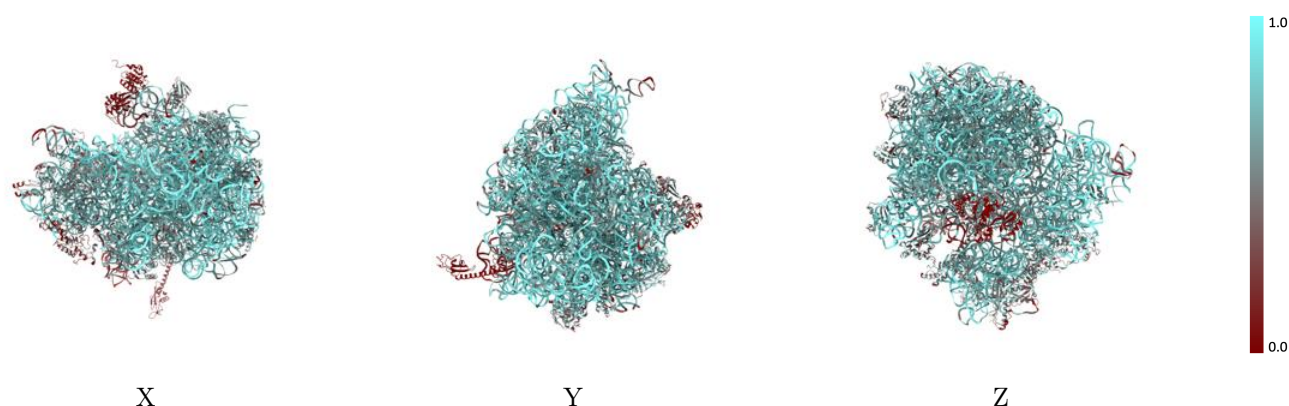
The images above show the 3D surface view of the map at the recommended contour level 0.000801 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

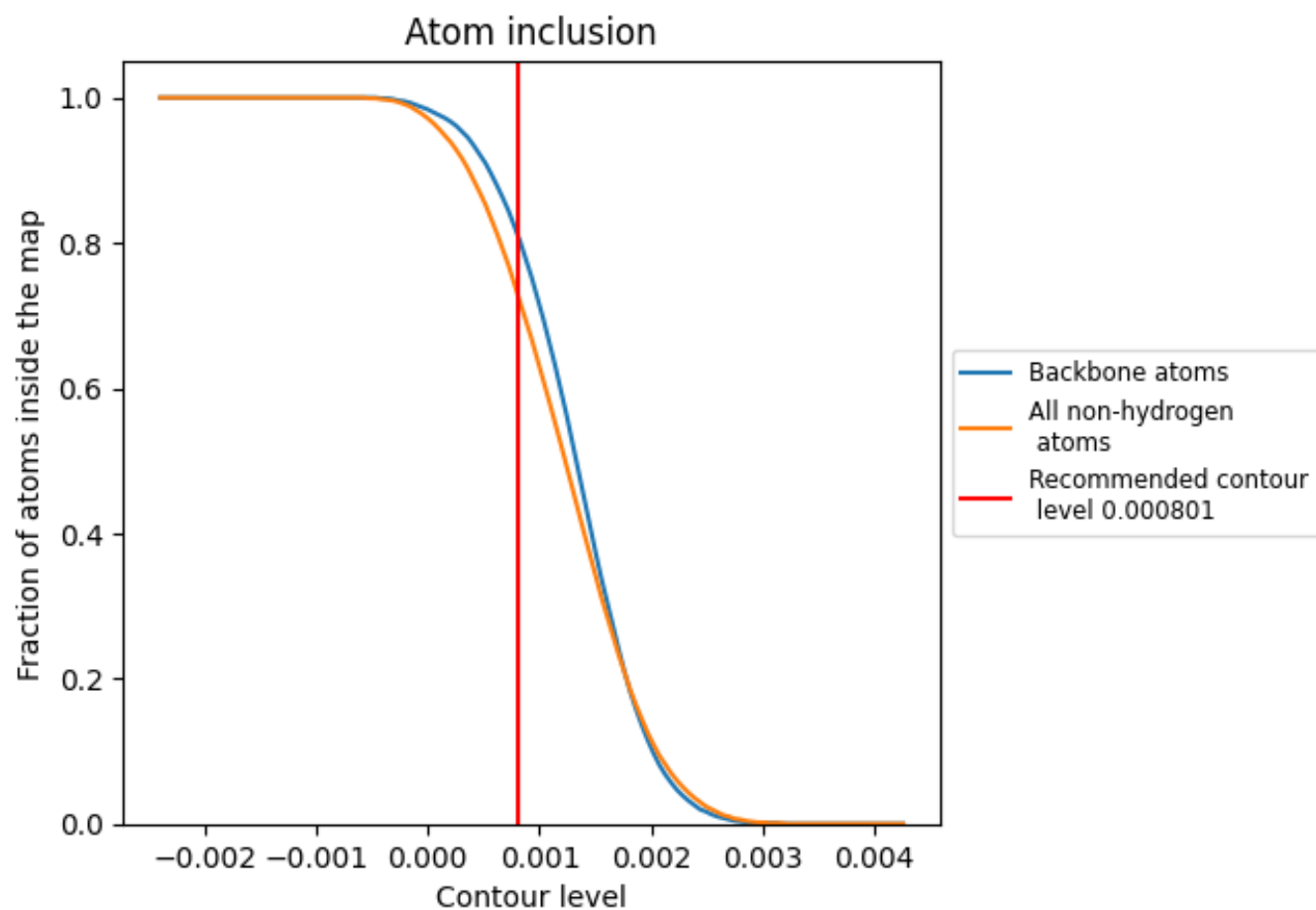
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.000801).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ











































The table lists the average atom inclusion at the recommended contour level (0.000801) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7310	 0.3460
10	 0.6440	 0.3860
11	 0.6220	 0.3870
12	 0.5810	 0.3060
13	 0.6480	 0.3530
15	 0.6380	 0.3700
16	 0.0890	 0.2680
17	 0.6620	 0.3850
18	 0.6600	 0.4210
19	 0.6350	 0.3780
1A	 0.8190	 0.3620
1B	 0.8400	 0.3410
1D	 0.6640	 0.4220
1E	 0.6320	 0.3860
1F	 0.5760	 0.3480
1G	 0.4850	 0.1980
1H	 0.5200	 0.2800
1I	 0.0570	 0.0530
1J	 0.0210	 0.0330
1K	 0.0650	 0.0660
1N	 0.6450	 0.3820
1O	 0.5890	 0.3850
1P	 0.6190	 0.3820
1Q	 0.6450	 0.4050
1R	 0.6510	 0.3740
1S	 0.6290	 0.3100
1T	 0.6060	 0.3660
1U	 0.6960	 0.3960
1V	 0.6300	 0.3580
1W	 0.6080	 0.3870
1X	 0.5480	 0.3320
1Y	 0.5820	 0.3280
1Z	 0.6130	 0.3150
1a	 0.8330	 0.3660
1b	 0.2620	 0.1940



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Chain	Atom inclusion	Q-score
1c	 0.5330	 0.3340
1d	 0.5430	 0.3100
1e	 0.6000	 0.3560
1f	 0.5350	 0.2650
1g	 0.4540	 0.2570
1h	 0.5980	 0.3520
1i	 0.5560	 0.2820
1j	 0.4320	 0.2610
1k	 0.5470	 0.3110
1l	 0.6180	 0.3710
1m	 0.5550	 0.3080
1n	 0.6180	 0.3260
1o	 0.6140	 0.3360
1p	 0.6110	 0.3480
1q	 0.5630	 0.3220
1r	 0.6190	 0.3260
1s	 0.5570	 0.3070
1t	 0.6230	 0.3160
1u	 0.1650	 0.1750
1v	 0.9330	 0.4890
1x	 0.5880	 0.2480