



## Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 11:43 pm GMT

PDB ID : 7B5K  
EMDB ID : EMD-12035  
Title : E. coli 70S containing suppressor tRNA in the A-site stabilized by a Negamycin analogue and P-site tRNA-nascent chain.  
Authors : Albers, S.; Beckert, B.; Matthies, M.; Schuster, R.; Riedner, M.; Seuring, C.; Sanyal, S.; Torda, A.; Wilson, N.D.; Ignatova, Z.  
Deposited on : 2020-12-03  
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation 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.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

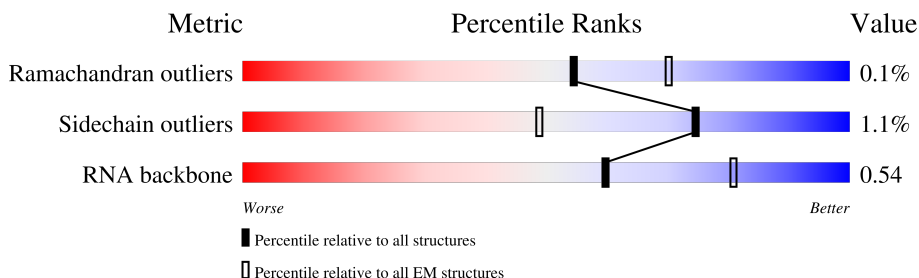
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	2897	
2	B	120	
3	C	271	
4	D	209	
5	E	201	
6	F	177	
7	G	176	
8	H	149	

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Mol	Chain	Length	Quality of chain
9	J	142	16% 100%
10	K	123	21% 98%
11	L	144	29% 98%
12	M	136	12% 99%
13	N	118	8% 97%
14	O	117	61% 100%
15	P	114	21% 100%
16	Q	117	21% 100%
17	R	103	48% 99%
18	S	110	18% 100%
19	T	93	40% 100%
20	U	102	70% 100%
21	V	94	64% 99%
22	W	76	9% 99%
23	X	77	18% 99%
24	Y	62	73% 100%
25	Z	58	19% 100%
26	0	56	27% 100%
27	1	51	31% 100%
28	2	46	• 96%
29	3	64	• 95%
30	4	38	24% 97%
31	5	66	97% 97%
32	a	1533	31% 83% 15%
33	b	224	90% 98%

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Mol	Chain	Length	Quality of chain
34	c	206	53% 100%
35	d	205	96% 99%
36	e	155	32% 98%
37	f	106	78% 100%
38	g	151	81% 99%
39	h	129	47% 99%
40	i	127	72% 98%
41	j	99	78% 96%
42	k	117	49% 99%
43	l	123	37% 98%
44	m	114	73% 96%
45	n	101	59% 98%
46	o	88	55% 100%
47	p	82	85% 98%
48	q	80	66% 100%
49	r	55	40% 100%
50	s	82	78% 96%
51	t	86	86% 100%
52	u	56	77% 98%
53	v	8	12% 100%
54	x	77	16% 83% 17%
55	z	76	68% 72% 26%
56	9	76	93% 61% 37%
57	6	11	27% 73% 27%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	ERY	A	3237	X	-	-	-

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 148612 atoms, of which 36 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	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	C	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	D	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	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	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.



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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	1	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1533	Total	C	N	O	P	0	0
			32908	14684	6037	10654	1533		

- Molecule 33 is a protein called 30S ribosomal protein S2.

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

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

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

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called 30S ribosomal protein S14.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

- Molecule 48 is a protein called 30S ribosomal protein S17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

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

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	82	Total	C	N	O	S	0	0
			656	419	125	110	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

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

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 53 is a protein called ermC Nacent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	8	Total	C	N	O		0	0
			63	46	8	9			

- Molecule 54 is a RNA chain called P-site Isoleucine tRNA (77-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	77	Total	C	N	O	P	0	0
			1646	734	296	539	77		

- Molecule 55 is a RNA chain called atRNA synthetic Stop tRNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	76	Total	C	N	O	P	0	0
			1633	726	301	530	76		

- Molecule 56 is a RNA chain called E-site val tRNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	9	76	Total	C	N	O	P	0	0
			1616	722	289	530	75		

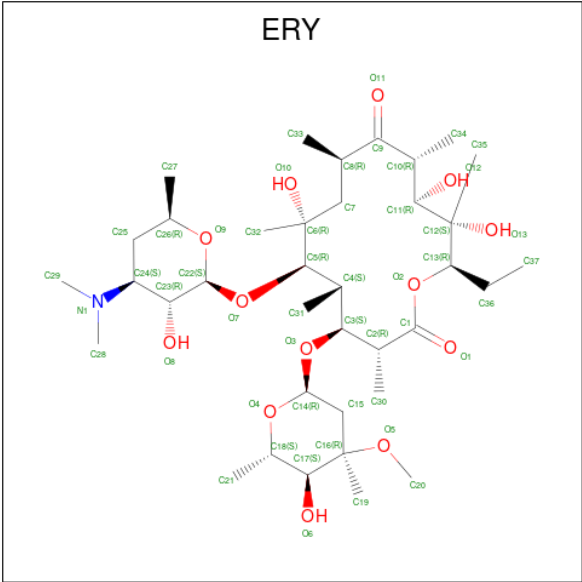
- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	11	Total	C	N	O	P	0	0
			234	105	42	76	11		

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

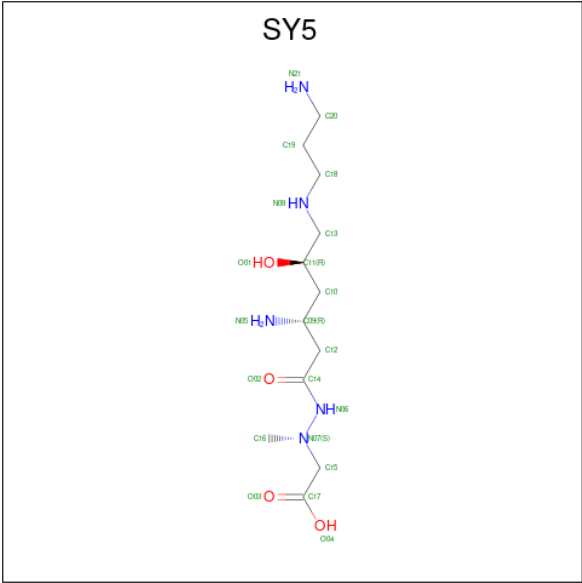
Mol	Chain	Residues	Atoms		AltConf
58	A	236	Total	Mg	0
			236	236	
58	B	1	Total	Mg	0
			1	1	
58	C	2	Total	Mg	0
			2	2	
58	D	1	Total	Mg	0
			1	1	
58	E	1	Total	Mg	0
			1	1	
58	Q	1	Total	Mg	0
			1	1	
58	0	1	Total	Mg	0
			1	1	
58	a	115	Total	Mg	0
			115	115	
58	m	1	Total	Mg	0
			1	1	

- Molecule 59 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>).



Mol	Chain	Residues	Atoms				AltConf
59	A	1	Total	C	N	O	0
			51	37	1	13	

- Molecule 60 is 2-[[[(3 {R},5 {R})-3-azanyl-6-(3-azanylpropylamino)-5-oxidanyl-hexanoyl]amino]-methyl-amino]ethanoic acid (three-letter code: SY5) (formula: C<sub>12</sub>H<sub>27</sub>N<sub>5</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					AltConf
60	a	1	Total	C	H	N	O	0
			78	24	36	10	8	
60	a	1	Total	C	H	N	O	0
			78	24	36	10	8	

- Molecule 61 is water.

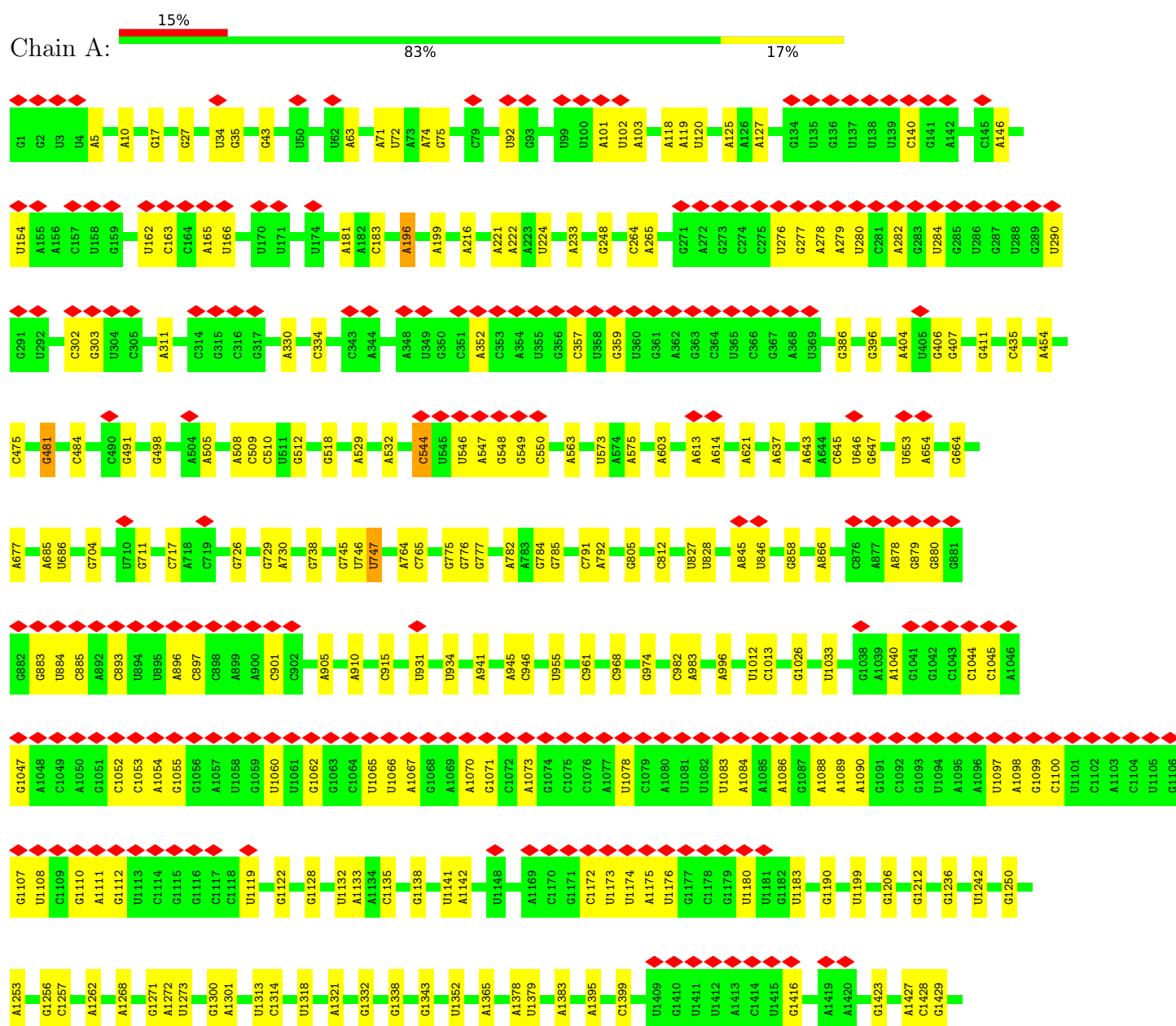
Mol	Chain	Residues	Atoms		AltConf
61	A	611	Total 611	O 611	0
61	C	3	Total 3	O 3	0
61	D	1	Total 1	O 1	0
61	L	1	Total 1	O 1	0
61	N	1	Total 1	O 1	0
61	a	221	Total 221	O 221	0
61	d	3	Total 3	O 3	0
61	e	1	Total 1	O 1	0
61	l	1	Total 1	O 1	0
61	n	4	Total 4	O 4	0
61	o	1	Total 1	O 1	0
61	p	1	Total 1	O 1	0
61	t	2	Total 2	O 2	0
61	z	3	Total 3	O 3	0

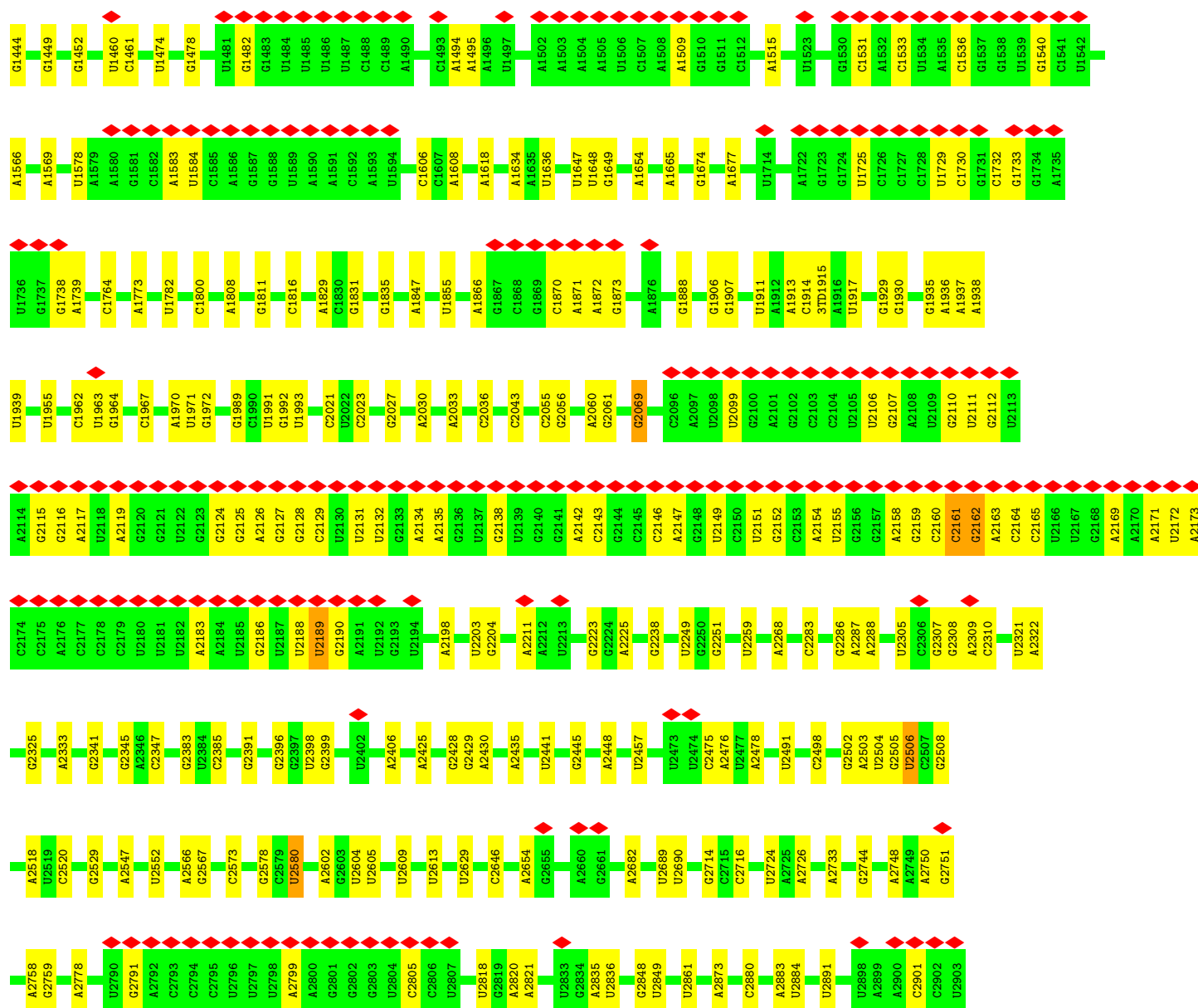


### 3 Residue-property plots

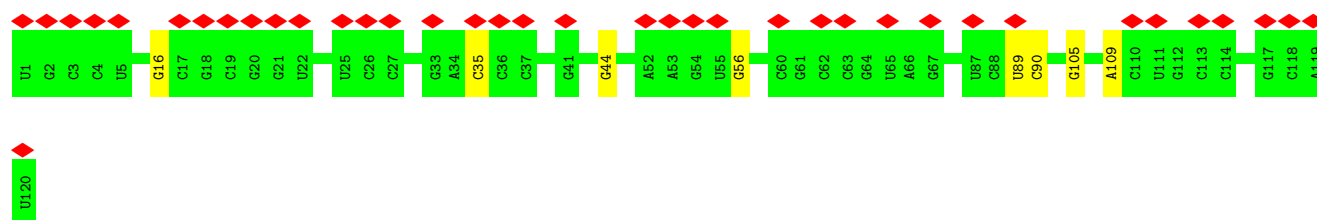
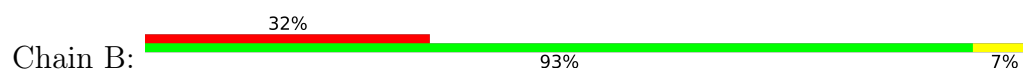
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 rRNA



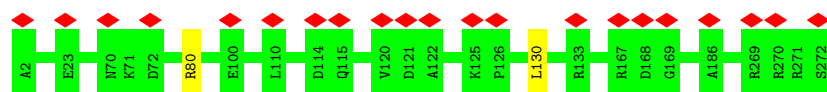


### • Molecule 2: 5S rRNA

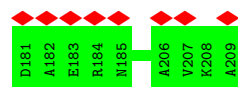
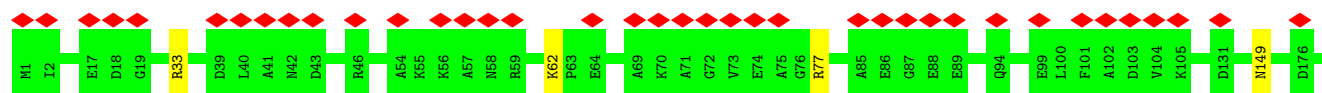


### • Molecule 3: 50S ribosomal protein L2

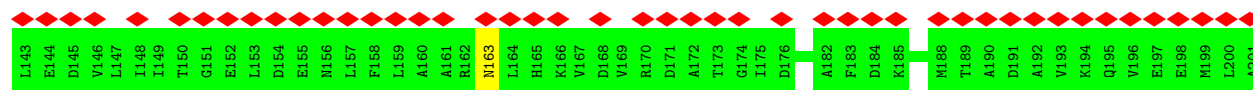
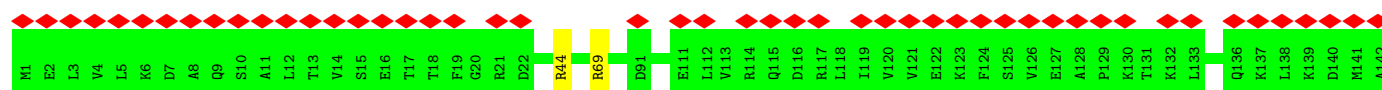




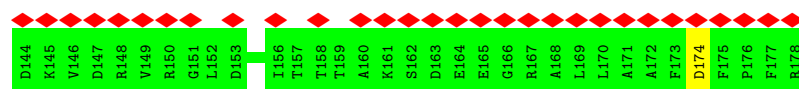
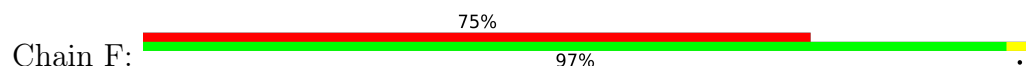
• Molecule 4: 50S ribosomal protein L3



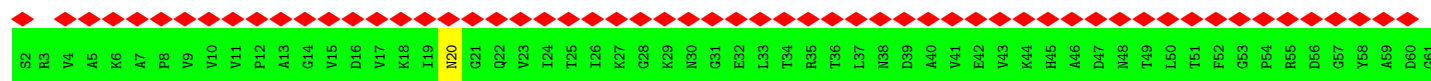
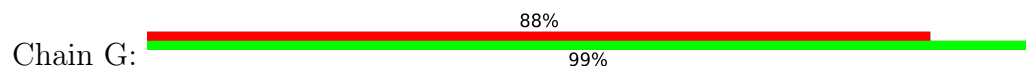
• Molecule 5: 50S ribosomal protein L4

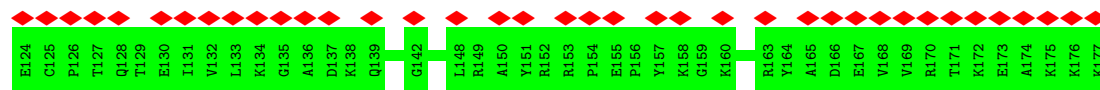
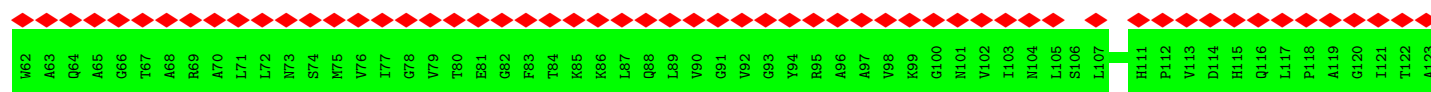


• Molecule 6: 50S ribosomal protein L5

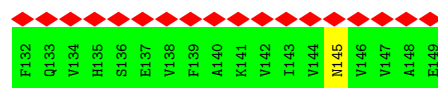
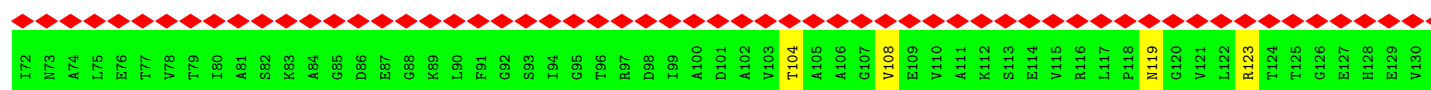
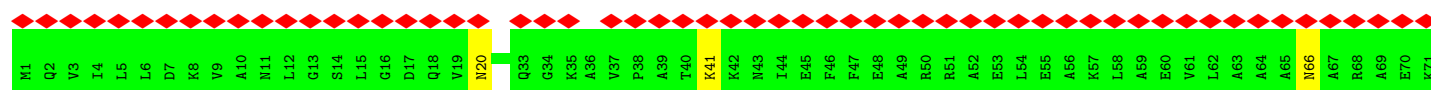


• Molecule 7: 50S ribosomal protein L6

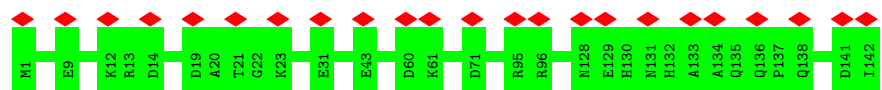




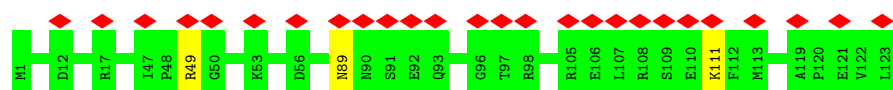
• Molecule 8: 50S ribosomal protein L9



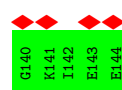
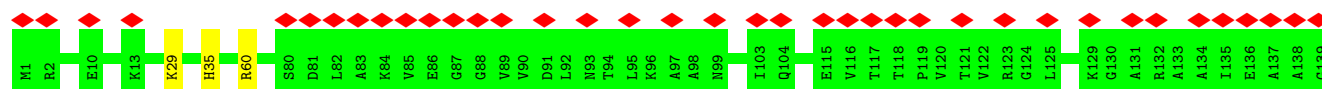
• Molecule 9: 50S ribosomal protein L13



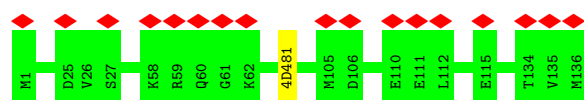
• Molecule 10: 50S ribosomal protein L14



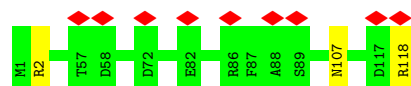
• Molecule 11: 50S ribosomal protein L15



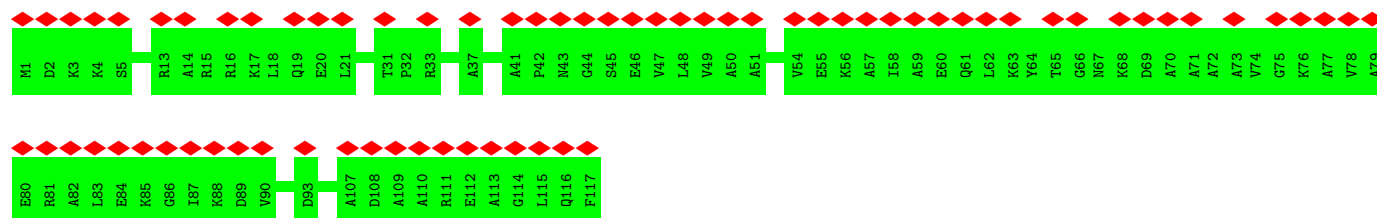
• Molecule 12: 50S ribosomal protein L16



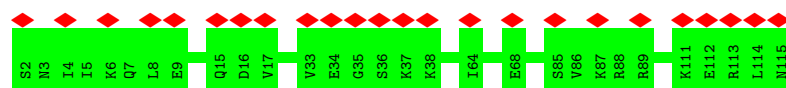
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18



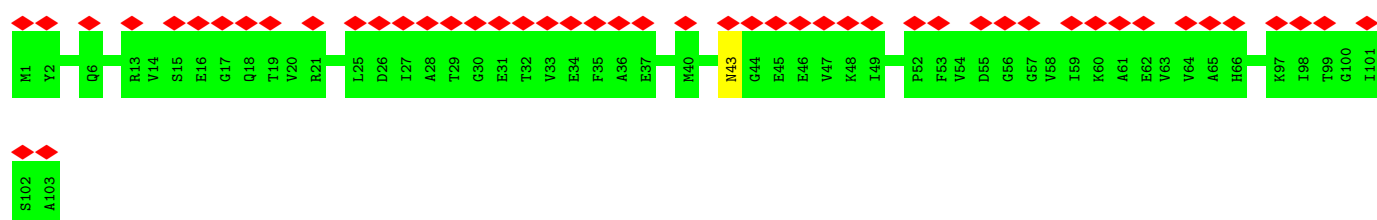
- Molecule 15: 50S ribosomal protein L19



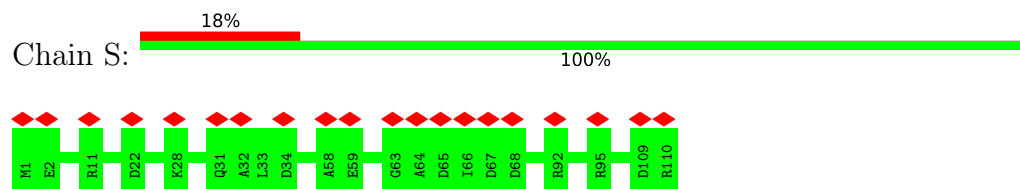
- Molecule 16: 50S ribosomal protein L20



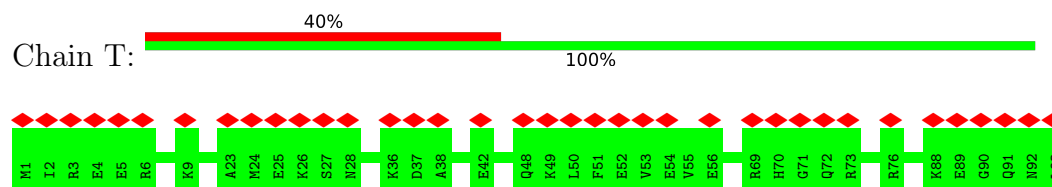
- Molecule 17: 50S ribosomal protein L21



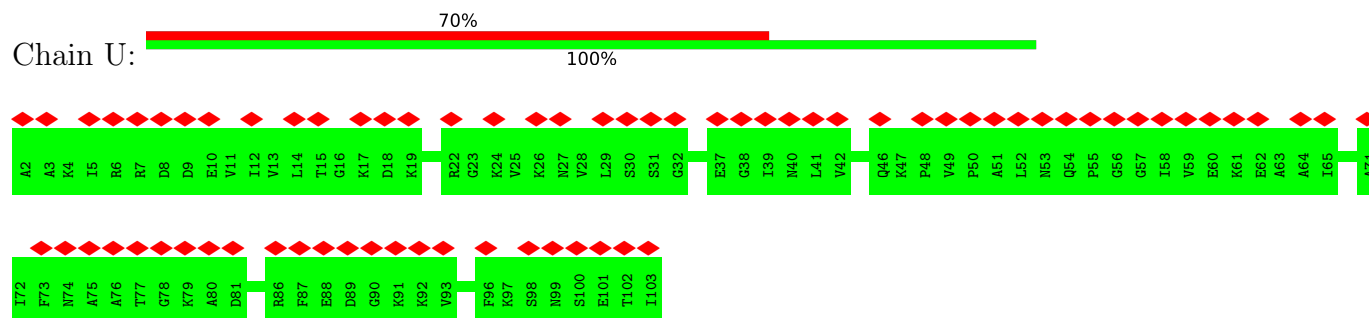
- Molecule 18: 50S ribosomal protein L22



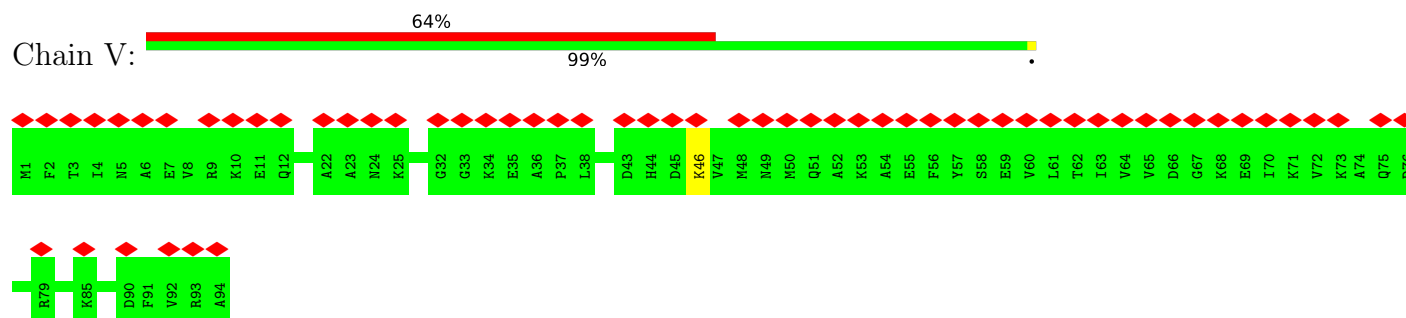
- Molecule 19: 50S ribosomal protein L23



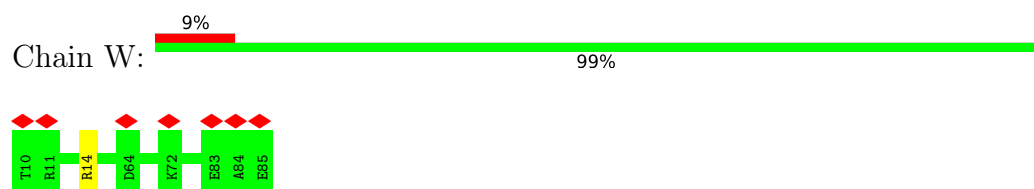
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25

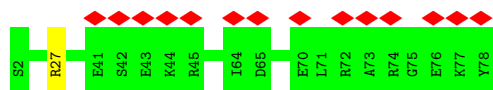


- Molecule 22: 50S ribosomal protein L27

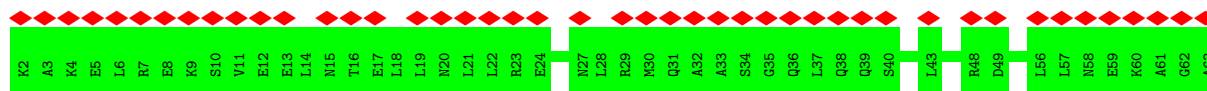
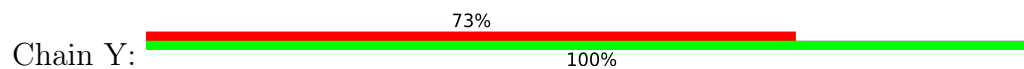


- Molecule 23: 50S ribosomal protein L28

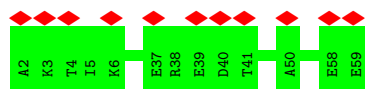




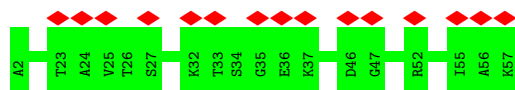
- Molecule 24: 50S ribosomal protein L29



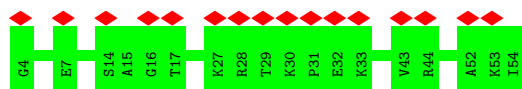
- Molecule 25: 50S ribosomal protein L30



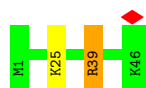
- Molecule 26: 50S ribosomal protein L32



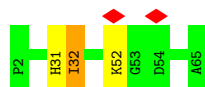
- Molecule 27: 50S ribosomal protein L33



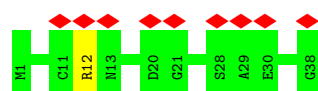
- Molecule 28: 50S ribosomal protein L34



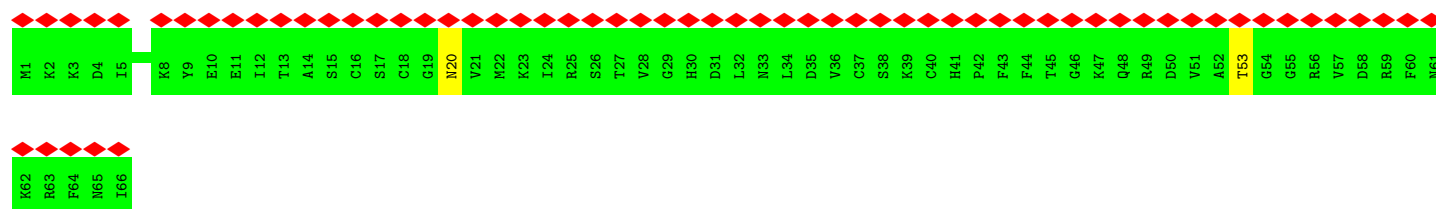
- Molecule 29: 50S ribosomal protein L35



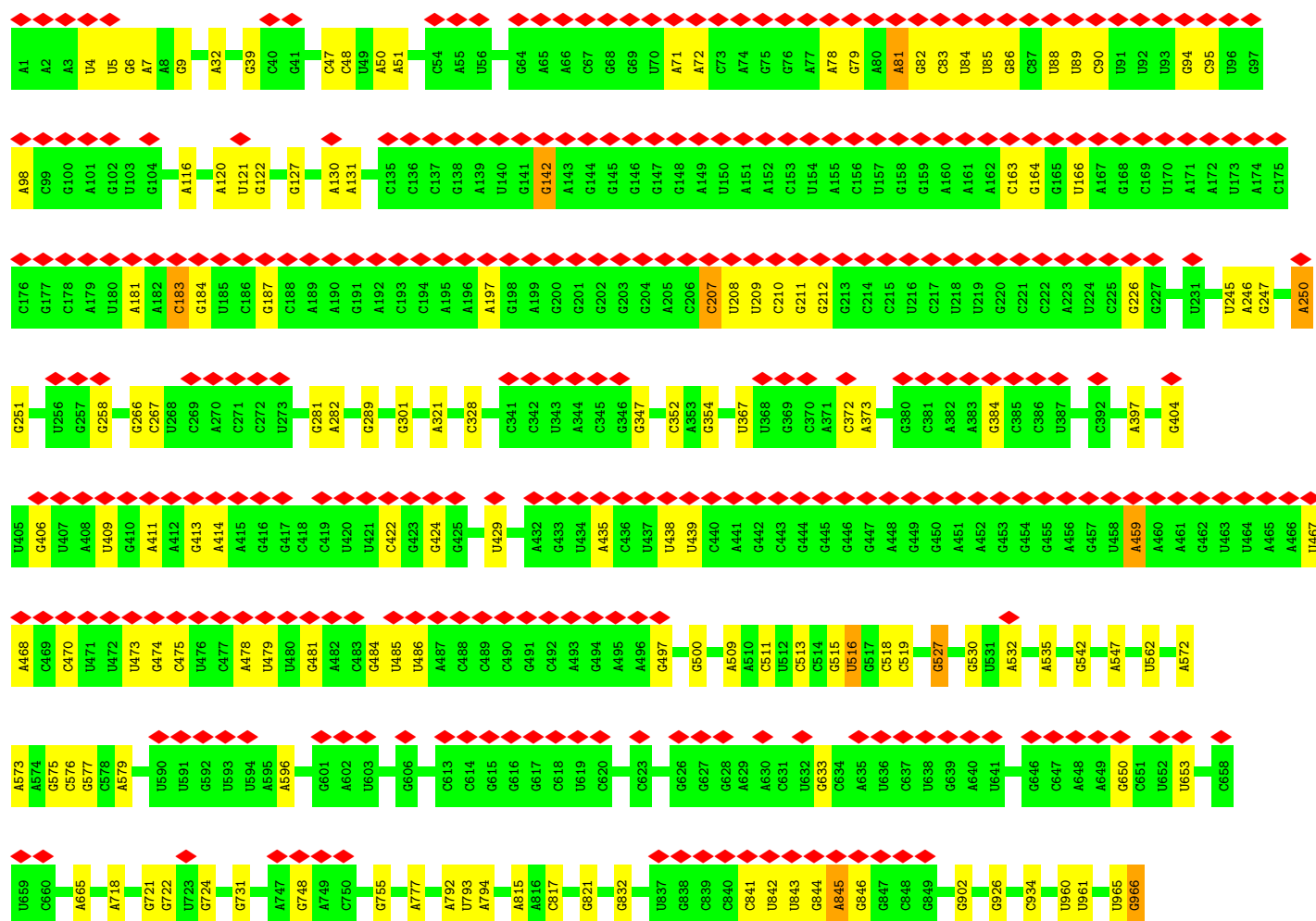
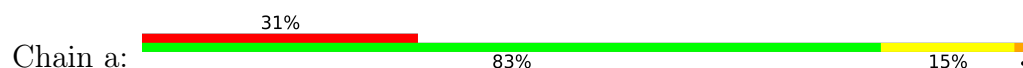
- Molecule 30: 50S ribosomal protein L36



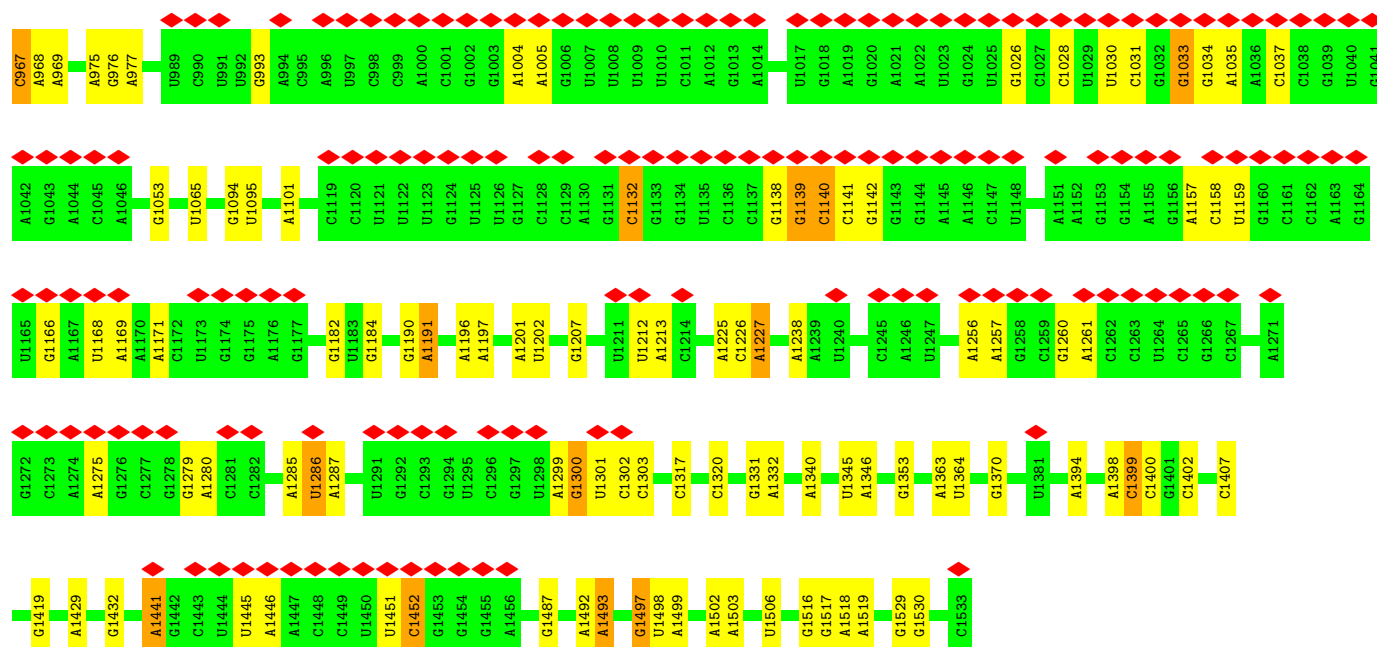
- Molecule 31: 50S ribosomal protein L31



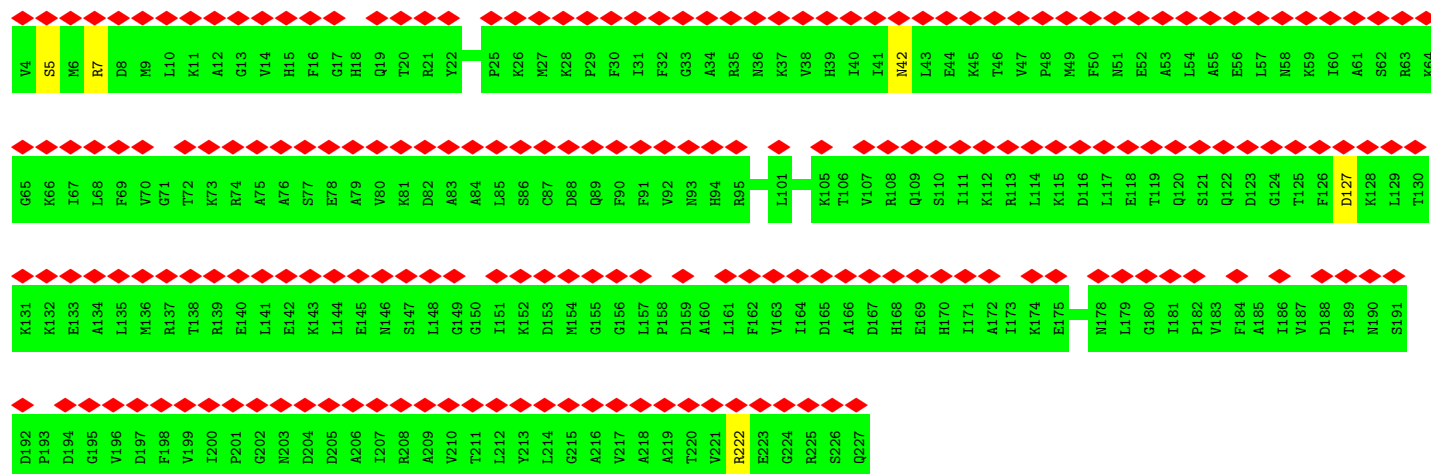
- Molecule 32: 16S rRNA



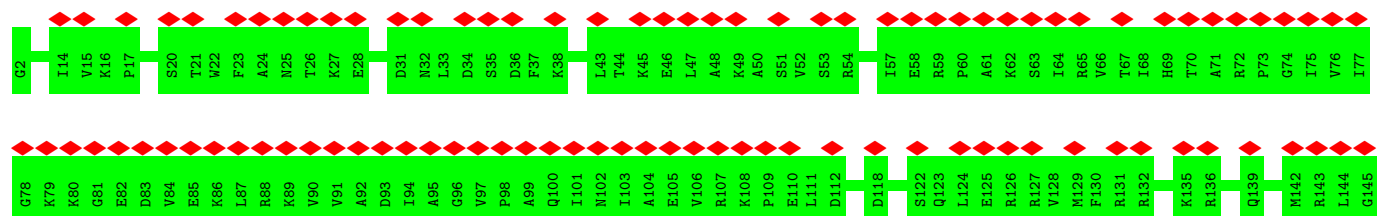


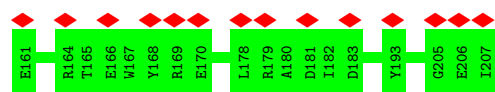


• Molecule 33: 30S ribosomal protein S2

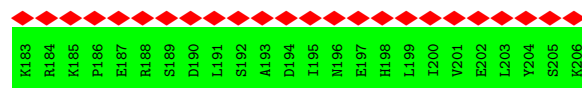
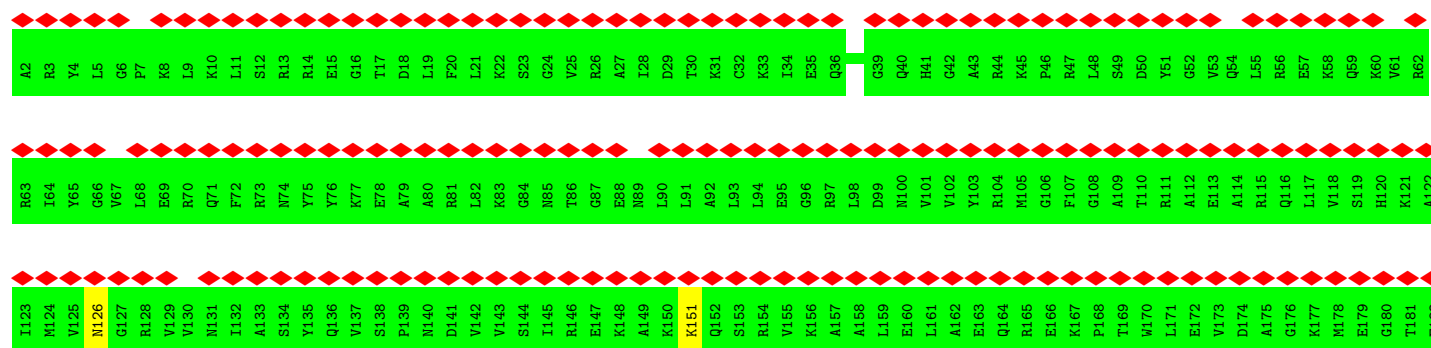


• Molecule 34: 30S ribosomal protein S3

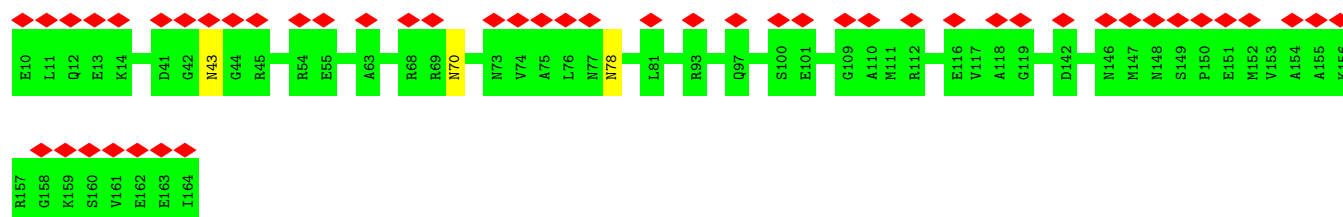




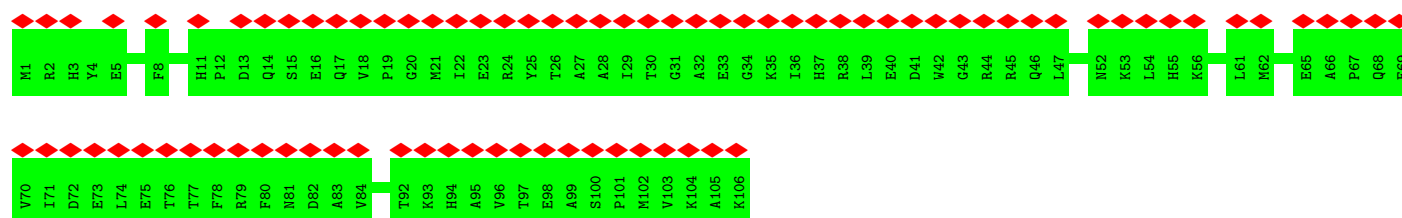
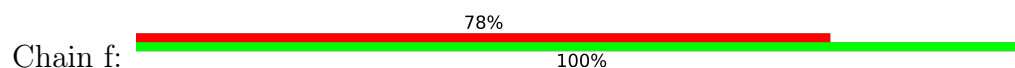
- Molecule 35: 30S ribosomal protein S4



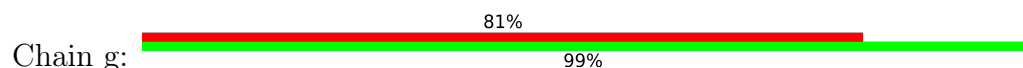
- Molecule 36: 30S ribosomal protein S5

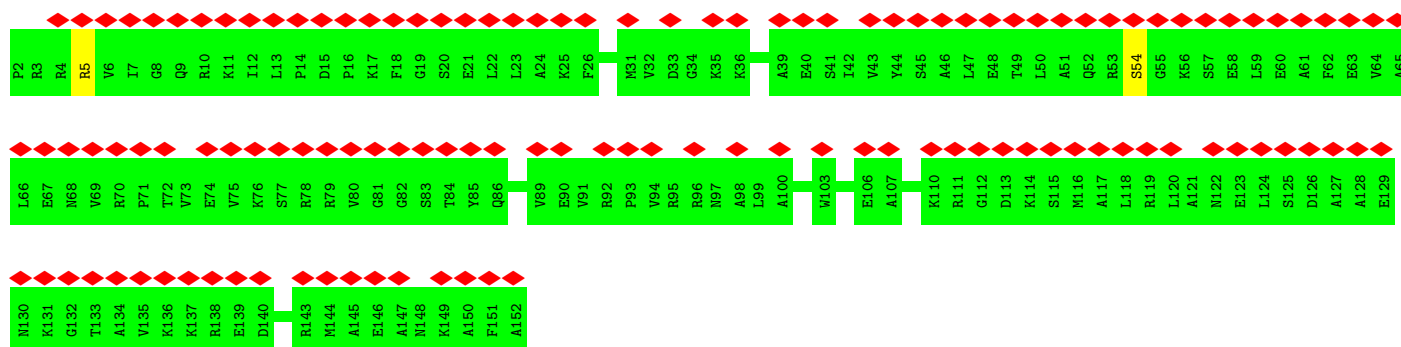


- Molecule 37: 30S ribosomal protein S6

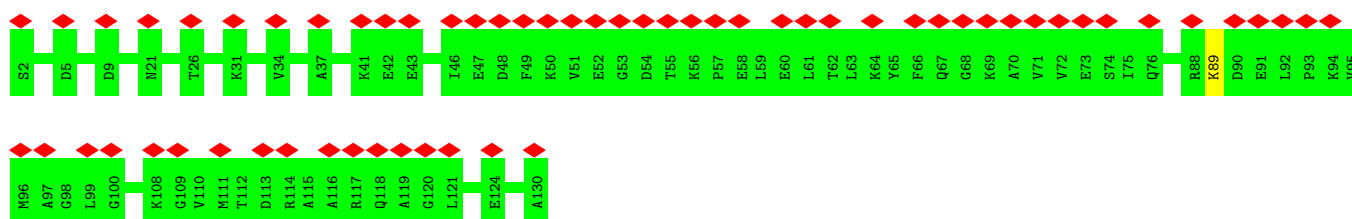


- Molecule 38: 30S ribosomal protein S7





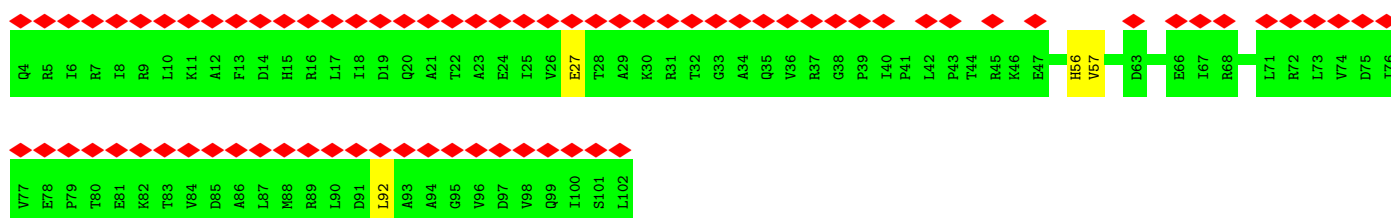
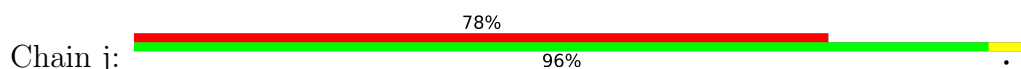
• Molecule 39: 30S ribosomal protein S8



• Molecule 40: 30S ribosomal protein S9

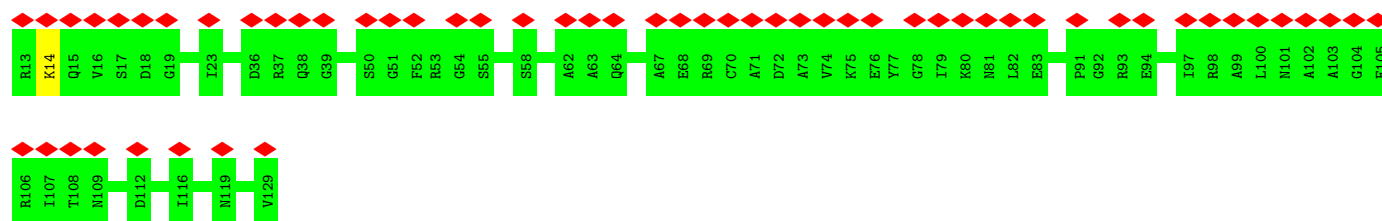


• Molecule 41: 30S ribosomal protein S10



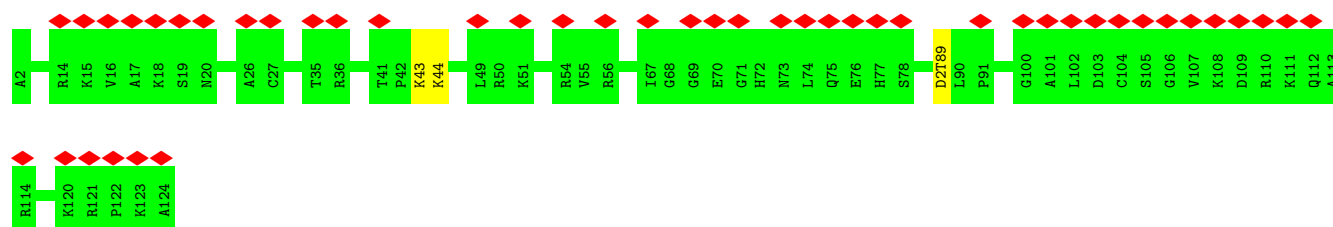
• Molecule 42: 30S ribosomal protein S11





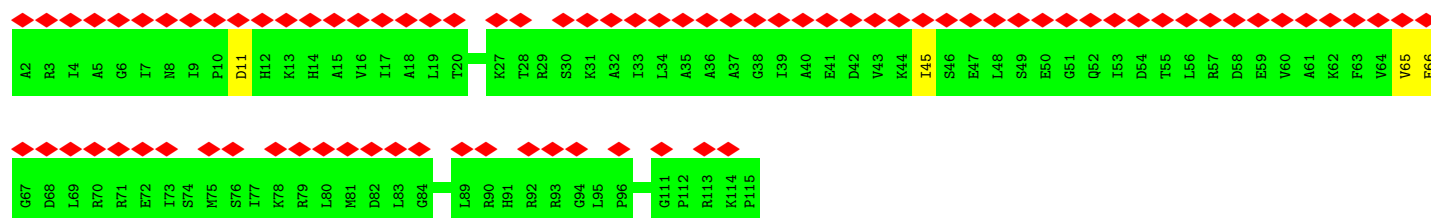
- Molecule 43: 30S ribosomal protein S12

Chain l: 37% 98%



- Molecule 44: 30S ribosomal protein S13

Chain m: 73% 96%



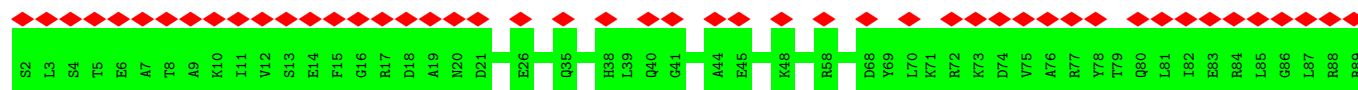
- Molecule 45: 30S ribosomal protein S14

Chain n: 59% 98%

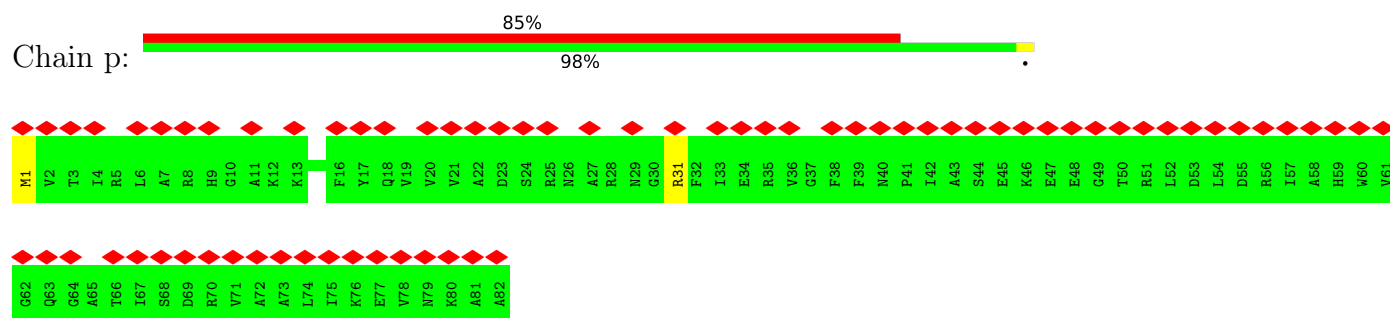


- Molecule 46: 30S ribosomal protein S15

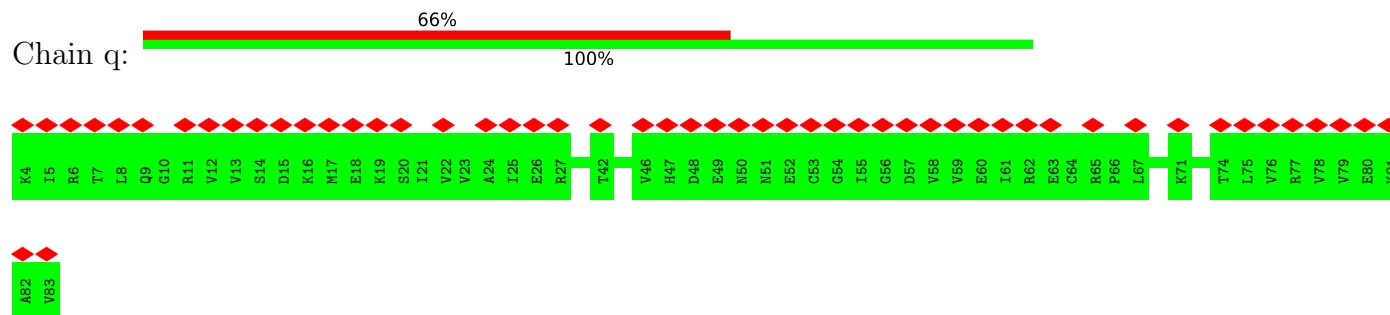
Chain o: 55% 100%



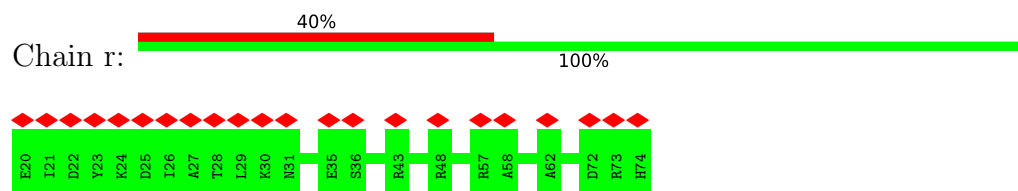
- Molecule 47: 30S ribosomal protein S16



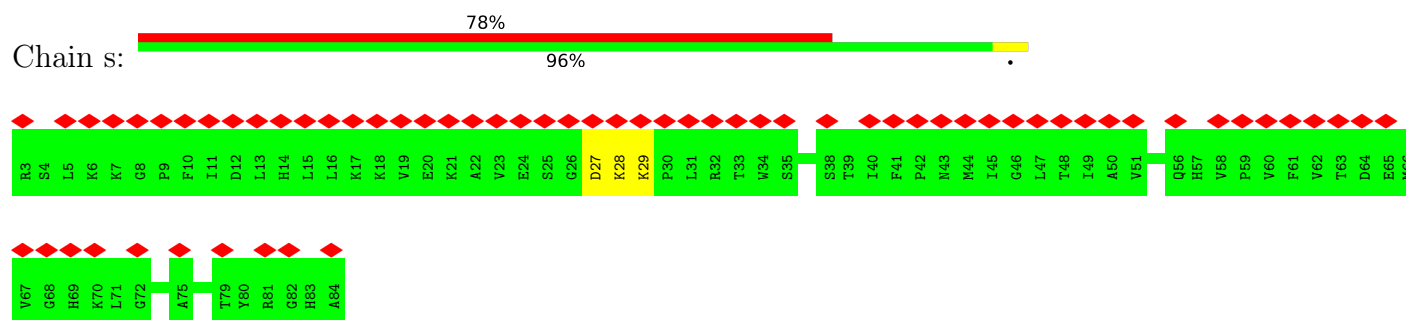
- Molecule 48: 30S ribosomal protein S17



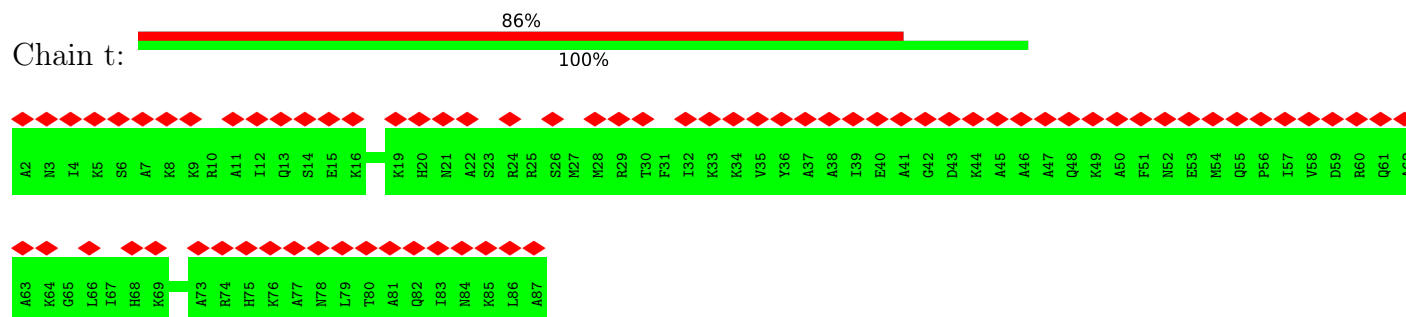
- Molecule 49: 30S ribosomal protein S18



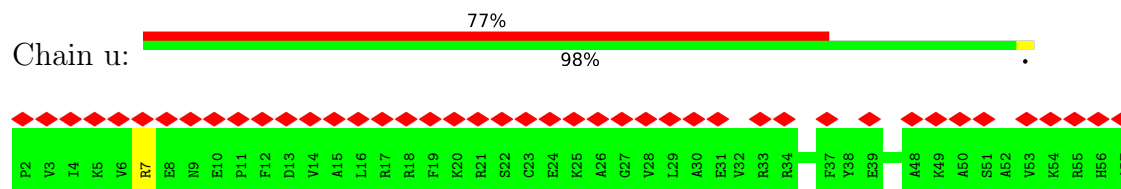
- Molecule 50: 30S ribosomal protein S19



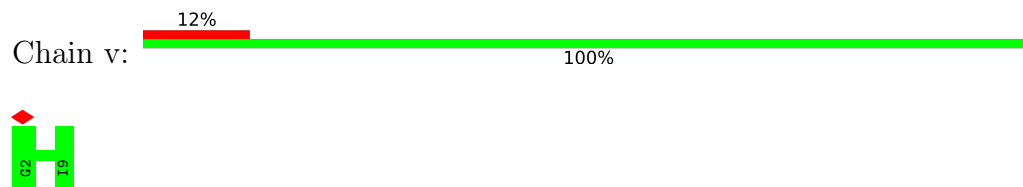
- Molecule 51: 30S ribosomal protein S20



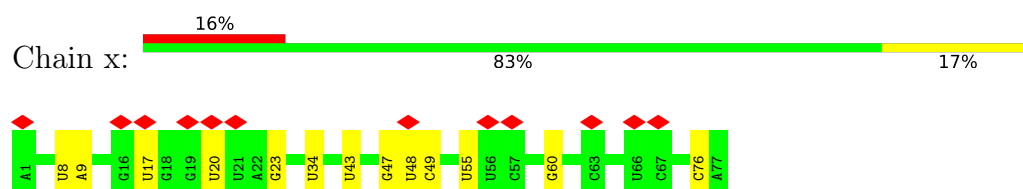
- Molecule 52: 30S ribosomal protein S21



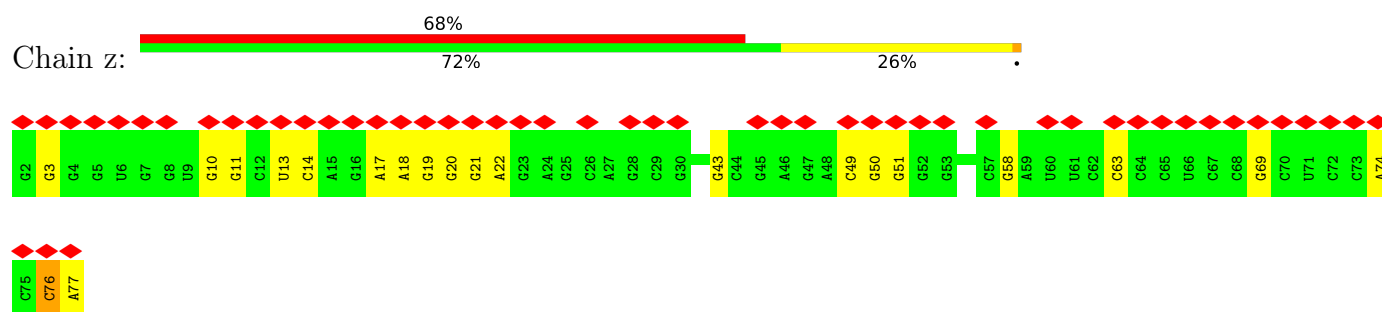
- Molecule 53: ermC Nacent chain



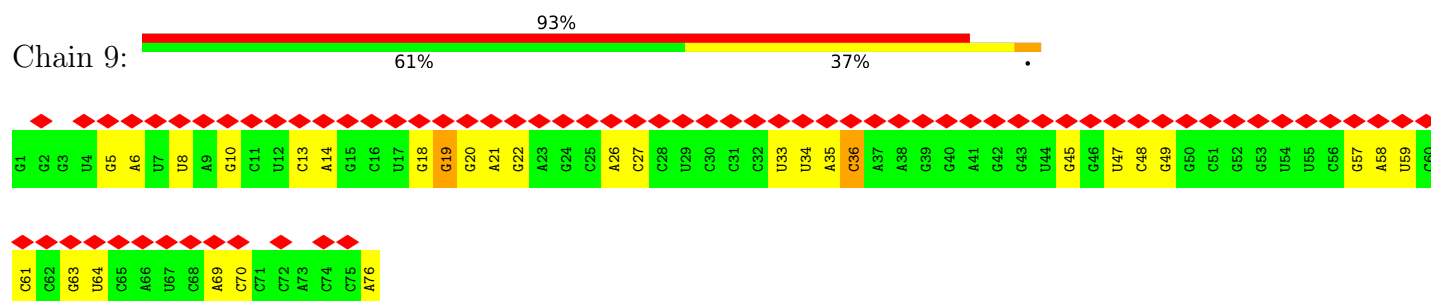
- Molecule 54: P-site Isoleucine tRNA (77-MER)



- Molecule 55: atRNA synthetic Stop tRNA (76-MER)

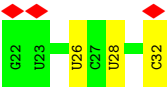


- Molecule 56: E-site val tRNA (76-MER)



- Molecule 57: mRNA





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.448	Depositor
Minimum map value	-0.189	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.083	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96000004, 0.96000004, 0.96000004	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, OMG, MA6, SY5, PSU, G7M, OMC, D2T, MG, 2MG, 4D4, UR3, ERY, MEQ, 2MA, OMU, 6MZ, 5MC, 4OC, 1MG, 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	A	0.71	0/69120	0.90	23/107824 (0.0%)
2	B	0.57	0/2872	0.86	0/4478
3	C	0.42	0/2121	0.59	0/2852
4	D	0.38	0/1576	0.56	0/2119
5	E	0.35	0/1571	0.58	0/2113
6	F	0.36	0/1434	0.65	1/1926 (0.1%)
7	G	0.33	0/1343	0.60	0/1816
8	H	0.32	0/1121	0.71	0/1515
9	J	0.38	0/1152	0.54	0/1551
10	K	0.36	0/955	0.58	0/1279
11	L	0.37	0/1062	0.62	0/1413
12	M	0.37	0/1081	0.59	0/1443
13	N	0.39	0/958	0.57	0/1281
14	O	0.33	0/910	0.60	0/1219
15	P	0.37	0/929	0.59	0/1242
16	Q	0.43	0/960	0.57	0/1278
17	R	0.39	0/829	0.58	0/1107
18	S	0.33	0/864	0.57	0/1156
19	T	0.34	0/744	0.57	0/994
20	U	0.33	0/787	0.55	0/1051
21	V	0.36	0/766	0.57	0/1025
22	W	0.40	0/587	0.56	0/776
23	X	0.34	0/635	0.57	0/848
24	Y	0.32	0/502	0.61	0/667
25	Z	0.33	0/453	0.58	0/605
26	0	0.39	0/450	0.65	0/599
27	1	0.42	0/421	0.56	0/561
28	2	0.43	0/380	0.77	1/498 (0.2%)
29	3	0.37	0/513	0.67	0/676
30	4	0.39	0/303	0.55	0/397
31	5	0.33	0/531	0.76	0/709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	a	0.60	0/36568	0.96	62/57042 (0.1%)
33	b	0.32	0/1784	0.62	0/2403
34	c	0.35	0/1651	0.58	0/2225
35	d	0.33	0/1665	0.61	0/2227
36	e	0.38	0/1157	0.60	0/1557
37	f	0.35	0/881	0.58	0/1189
38	g	0.35	0/1195	0.63	1/1602 (0.1%)
39	h	0.36	0/989	0.57	0/1326
40	i	0.33	0/1034	0.61	0/1375
41	j	0.35	0/805	0.65	0/1089
42	k	0.33	0/893	0.57	0/1205
43	l	0.38	0/960	0.67	1/1286 (0.1%)
44	m	0.33	0/892	0.65	0/1193
45	n	0.35	0/811	0.66	1/1081 (0.1%)
46	o	0.31	0/722	0.54	0/964
47	p	0.33	0/659	0.59	0/884
48	q	0.36	0/657	0.62	0/881
49	r	0.35	0/462	0.56	0/621
50	s	0.31	0/672	0.58	0/904
51	t	0.27	0/676	0.50	0/895
52	u	0.35	0/472	0.58	0/627
53	v	0.43	0/64	0.46	0/85
54	x	0.56	0/1840	0.90	1/2867 (0.0%)
55	z	0.46	0/1826	0.91	1/2848 (0.0%)
56	9	0.36	0/1804	0.93	5/2808 (0.2%)
57	6	0.64	0/261	0.83	0/404
All	All	0.60	0/159330	0.85	97/238606 (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
6	F	0	1
8	H	0	5
11	L	0	1
29	3	0	1
31	5	0	1
33	b	0	1
41	j	0	3
44	m	0	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
50	s	0	2
All	All	0	18

There are no bond length outliers.

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2188	U	OP2-P-O3'	-11.20	80.55	105.20
1	A	2188	U	OP1-P-O3'	-10.12	82.93	105.20
28	2	39	ARG	NE-CZ-NH2	-9.37	115.61	120.30
32	a	1497	G	C2-N3-C4	9.15	116.47	111.90
32	a	1493	A	C8-N9-C4	-8.95	102.22	105.80
32	a	1497	G	N1-C2-N3	-8.50	118.80	123.90
1	A	512	G	O4'-C1'-N9	8.23	114.79	108.20
32	a	542	G	C8-N9-C1'	-8.21	116.32	127.00
32	a	542	G	C4-N9-C1'	7.90	136.77	126.50
32	a	530	G	O4'-C1'-N9	7.71	114.37	108.20
32	a	1497	G	C5-C6-O6	-7.47	124.11	128.60
1	A	2506	U	N3-C2-O2	-7.19	117.17	122.20
6	F	174	ASP	CB-CG-OD1	7.11	124.70	118.30
32	a	1227	A	O4'-C1'-N9	7.11	113.89	108.20
32	a	542	G	O4'-C1'-N9	-6.77	102.78	108.20
32	a	81	A	O4'-C1'-N9	-6.59	102.93	108.20
1	A	1047	G	O4'-C1'-N9	6.57	113.45	108.20
32	a	1493	A	P-O3'-C3'	-6.56	111.83	119.70
1	A	2848	G	O4'-C1'-N9	6.55	113.44	108.20
56	9	36	C	C2-N1-C1'	6.52	125.97	118.80
1	A	2189	U	OP1-P-OP2	6.51	129.37	119.60
32	a	1452	C	P-O3'-C3'	6.46	127.45	119.70
32	a	1399	C	P-O3'-C3'	6.41	127.39	119.70
32	a	1261	A	O4'-C1'-N9	6.38	113.31	108.20
32	a	1493	A	N7-C8-N9	6.34	116.97	113.80
32	a	1452	C	O4'-C1'-N1	6.34	113.27	108.20
1	A	1313	U	C2-N1-C1'	6.27	125.22	117.70
32	a	207	C	N1-C2-O2	-6.25	115.15	118.90
32	a	1201	A	P-O3'-C3'	6.20	127.14	119.70
1	A	2506	U	N1-C2-O2	6.18	127.13	122.80
1	A	1831	G	N3-C4-N9	6.15	129.69	126.00
32	a	1140	C	N3-C2-O2	-6.14	117.60	121.90
56	9	19	G	C5-C6-O6	6.04	132.22	128.60
1	A	1831	G	N9-C4-C5	-6.04	102.99	105.40
1	A	2162	G	OP1-P-O3'	6.01	118.43	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1441	A	C5'-C4'-O4'	-5.98	101.93	109.10
32	a	475	C	C6-N1-C2	-5.94	117.92	120.30
32	a	1132	C	C6-N1-C1'	-5.94	113.67	120.80
32	a	792	A	O4'-C1'-N9	5.94	112.95	108.20
1	A	1100	C	N3-C2-O2	-5.89	117.78	121.90
1	A	481	G	O4'-C1'-N9	5.86	112.89	108.20
32	a	1028	C	C6-N1-C2	-5.83	117.97	120.30
54	x	34	U	N3-C2-O2	-5.83	118.12	122.20
32	a	1300	G	P-O3'-C3'	5.81	126.67	119.70
32	a	1028	C	N3-C2-O2	-5.78	117.86	121.90
32	a	1132	C	C2-N1-C1'	5.75	125.13	118.80
1	A	2161	C	N1-C2-O2	5.70	122.32	118.90
1	A	2506	U	C2-N1-C1'	5.70	124.53	117.70
32	a	183	C	OP1-P-O3'	5.62	117.56	105.20
32	a	1441	A	N9-C1'-C2'	-5.60	105.84	112.00
45	n	18	LYS	CB-CG-CD	5.58	126.10	111.60
32	a	474	G	C4-N9-C1'	-5.56	119.28	126.50
32	a	1190	G	OP2-P-O3'	5.55	117.42	105.20
32	a	1331	G	O4'-C1'-N9	5.54	112.63	108.20
32	a	1493	A	C4-N9-C1'	5.46	136.13	126.30
56	9	36	C	N1-C2-O2	5.46	122.17	118.90
1	A	2161	C	N3-C2-O2	-5.45	118.09	121.90
32	a	1190	G	P-O3'-C3'	5.44	126.22	119.70
32	a	1493	A	C8-N9-C1'	-5.43	117.92	127.70
32	a	1452	C	C6-N1-C2	5.42	122.47	120.30
32	a	1286	U	C5'-C4'-O4'	-5.40	102.62	109.10
32	a	250	A	O4'-C1'-N9	5.40	112.52	108.20
32	a	1332	A	O4'-C1'-N9	-5.39	103.89	108.20
32	a	142	G	C4-N9-C1'	5.39	133.50	126.50
32	a	1399	C	C2-N1-C1'	5.37	124.71	118.80
56	9	19	G	N3-C4-N9	-5.36	122.78	126.00
32	a	438	U	P-O3'-C3'	5.36	126.13	119.70
32	a	459	A	C8-N9-C4	-5.34	103.67	105.80
32	a	542	G	C4-C5-N7	5.32	112.93	110.80
32	a	1033	G	P-O3'-C3'	5.31	126.07	119.70
32	a	1452	C	O3'-P-O5'	5.29	114.06	104.00
43	l	43	LYS	C-N-CA	5.28	134.90	121.70
1	A	544	C	C2-N1-C1'	5.27	124.60	118.80
32	a	1139	G	O4'-C1'-N9	5.27	112.42	108.20
32	a	485	U	P-O3'-C3'	5.27	126.02	119.70
55	z	76	C	O4'-C1'-N1	5.26	112.41	108.20
38	g	54	SER	C-N-CA	-5.24	111.29	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	90	C	N1-C2-O2	5.23	122.04	118.90
1	A	1314	C	C2-N1-C1'	5.22	124.55	118.80
32	a	530	G	C4-N9-C1'	-5.22	119.71	126.50
32	a	1191	A	O4'-C1'-N9	5.22	112.38	108.20
32	a	142	G	C8-N9-C1'	-5.22	120.21	127.00
1	A	729	G	O4'-C1'-N9	5.17	112.34	108.20
32	a	845	A	O4'-C1'-N9	5.14	112.31	108.20
32	a	965	U	O4'-C1'-N1	5.13	112.31	108.20
56	9	33	U	C2-N1-C1'	5.12	123.85	117.70
32	a	81	A	C5'-C4'-O4'	-5.12	102.96	109.10
32	a	1227	A	C5'-C4'-O4'	5.11	115.23	109.10
32	a	542	G	N9-C4-C5	-5.09	103.36	105.40
32	a	1445	U	P-O3'-C3'	-5.08	113.61	119.70
1	A	196	A	O4'-C1'-N9	5.08	112.26	108.20
32	a	1037	C	O4'-C1'-N1	5.08	112.26	108.20
32	a	1441	A	P-O3'-C3'	5.07	125.78	119.70
1	A	1936	A	C4-N9-C1'	5.02	135.34	126.30
32	a	1497	G	N1-C6-O6	5.02	122.92	119.90
32	a	1399	C	C6-N1-C2	-5.02	118.29	120.30
1	A	704	G	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	3	31	HIS	Peptide
31	5	53	THR	Peptide
6	F	48	LYS	Mainchain
8	H	104	THR	Peptide
8	H	108	VAL	Peptide
8	H	145	ASN	Peptide
8	H	41	LYS	Peptide
8	H	66	ASN	Peptide
11	L	35	HIS	Peptide
33	b	5	SER	Peptide
41	j	27	GLU	Peptide
41	j	56	HIS	Peptide
41	j	92	LEU	Peptide
44	m	11	ASP	Peptide
44	m	45	ILE	Peptide
44	m	65	VAL	Peptide
50	s	27	ASP	Peptide

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Mol	Chain	Res	Type	Group
50	s	28	LYS	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	C	269/271 (99%)	263 (98%)	6 (2%)	0	100	100
4	D	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	29	61
5	E	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
6	F	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
7	G	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
8	H	147/149 (99%)	129 (88%)	18 (12%)	0	100	100
9	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
10	K	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
11	L	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
12	M	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
13	N	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	O	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
15	P	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
16	Q	115/117 (98%)	115 (100%)	0	0	100	100
17	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
18	S	108/110 (98%)	108 (100%)	0	0	100	100
19	T	91/93 (98%)	89 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	U	100/102 (98%)	93 (93%)	7 (7%)	0	100	100
21	V	92/94 (98%)	92 (100%)	0	0	100	100
22	W	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
23	X	75/77 (97%)	75 (100%)	0	0	100	100
24	Y	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
25	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
26	0	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
27	1	49/51 (96%)	49 (100%)	0	0	100	100
28	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
29	3	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	9	32
30	4	36/38 (95%)	36 (100%)	0	0	100	100
31	5	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
33	b	222/224 (99%)	207 (93%)	14 (6%)	1 (0%)	29	61
34	c	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
35	d	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
36	e	153/155 (99%)	145 (95%)	8 (5%)	0	100	100
37	f	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
38	g	149/151 (99%)	138 (93%)	11 (7%)	0	100	100
39	h	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
40	i	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
41	j	97/99 (98%)	90 (93%)	6 (6%)	1 (1%)	15	45
42	k	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
43	l	120/123 (98%)	111 (92%)	8 (7%)	1 (1%)	19	51
44	m	112/114 (98%)	100 (89%)	11 (10%)	1 (1%)	17	48
45	n	99/101 (98%)	85 (86%)	13 (13%)	1 (1%)	15	45
46	o	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
47	p	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
48	q	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
49	r	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
50	s	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
51	t	84/86 (98%)	82 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	u	54/56 (96%)	54 (100%)	0	0	100	100
53	v	6/8 (75%)	6 (100%)	0	0	100	100
All	All	5581/5684 (98%)	5354 (96%)	220 (4%)	7 (0%)	54	82

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	149	ASN
29	3	32	ILE
41	j	57	VAL
43	l	44	LYS
44	m	66	GLU
45	n	54	ASP
33	b	127	ASP

### 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	C	216/216 (100%)	214 (99%)	2 (1%)	78	93
4	D	163/163 (100%)	160 (98%)	3 (2%)	59	85
5	E	165/165 (100%)	162 (98%)	3 (2%)	59	85
6	F	148/148 (100%)	144 (97%)	4 (3%)	44	77
7	G	137/137 (100%)	136 (99%)	1 (1%)	84	95
8	H	114/114 (100%)	111 (97%)	3 (3%)	46	77
9	J	116/116 (100%)	116 (100%)	0	100	100
10	K	104/104 (100%)	101 (97%)	3 (3%)	42	76
11	L	103/103 (100%)	101 (98%)	2 (2%)	57	84
12	M	108/108 (100%)	108 (100%)	0	100	100
13	N	98/98 (100%)	95 (97%)	3 (3%)	40	74
14	O	87/87 (100%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	P	99/99 (100%)	99 (100%)	0	100	100
16	Q	89/89 (100%)	89 (100%)	0	100	100
17	R	84/84 (100%)	83 (99%)	1 (1%)	71	91
18	S	93/93 (100%)	93 (100%)	0	100	100
19	T	80/80 (100%)	80 (100%)	0	100	100
20	U	83/83 (100%)	83 (100%)	0	100	100
21	V	78/78 (100%)	77 (99%)	1 (1%)	69	90
22	W	57/58 (98%)	56 (98%)	1 (2%)	59	85
23	X	67/67 (100%)	66 (98%)	1 (2%)	65	87
24	Y	54/54 (100%)	54 (100%)	0	100	100
25	Z	48/48 (100%)	48 (100%)	0	100	100
26	0	47/47 (100%)	47 (100%)	0	100	100
27	1	45/46 (98%)	45 (100%)	0	100	100
28	2	38/38 (100%)	36 (95%)	2 (5%)	22	54
29	3	51/51 (100%)	49 (96%)	2 (4%)	32	66
30	4	34/34 (100%)	33 (97%)	1 (3%)	42	76
31	5	59/59 (100%)	58 (98%)	1 (2%)	60	86
33	b	186/186 (100%)	183 (98%)	3 (2%)	62	86
34	c	170/170 (100%)	170 (100%)	0	100	100
35	d	172/172 (100%)	170 (99%)	2 (1%)	71	91
36	e	118/118 (100%)	115 (98%)	3 (2%)	47	78
37	f	92/92 (100%)	92 (100%)	0	100	100
38	g	124/124 (100%)	123 (99%)	1 (1%)	81	94
39	h	104/104 (100%)	103 (99%)	1 (1%)	76	92
40	i	105/105 (100%)	103 (98%)	2 (2%)	57	84
41	j	87/87 (100%)	87 (100%)	0	100	100
42	k	90/90 (100%)	89 (99%)	1 (1%)	73	92
43	l	102/102 (100%)	102 (100%)	0	100	100
44	m	92/92 (100%)	92 (100%)	0	100	100
45	n	79/83 (95%)	79 (100%)	0	100	100
46	o	76/76 (100%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	p	65/65 (100%)	63 (97%)	2 (3%)	40	74
48	q	74/74 (100%)	74 (100%)	0	100	100
49	r	48/48 (100%)	48 (100%)	0	100	100
50	s	71/71 (100%)	70 (99%)	1 (1%)	67	89
51	t	65/65 (100%)	65 (100%)	0	100	100
52	u	48/48 (100%)	47 (98%)	1 (2%)	53	81
53	v	7/7 (100%)	7 (100%)	0	100	100
All	All	4640/4646 (100%)	4589 (99%)	51 (1%)	74	92

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	80	ARG
3	C	130	LEU
4	D	33	ARG
4	D	62	LYS
4	D	77	ARG
5	E	44	ARG
5	E	69	ARG
5	E	163	ASN
6	F	21	ASN
6	F	23	ASN
6	F	78	LYS
6	F	112	ARG
7	G	20	ASN
8	H	20	ASN
8	H	119	ASN
8	H	123	ARG
10	K	49	ARG
10	K	89	ASN
10	K	111	LYS
11	L	29	LYS
11	L	60	ARG
13	N	2	ARG
13	N	107	ASN
13	N	118	ARG
17	R	43	ASN
21	V	46	LYS
22	W	14	ARG
23	X	27	ARG

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Mol	Chain	Res	Type
28	2	25	LYS
28	2	39	ARG
29	3	32	ILE
29	3	52	LYS
30	4	12	ARG
31	5	20	ASN
33	b	7	ARG
33	b	42	ASN
33	b	222	ARG
35	d	126	ASN
35	d	151	LYS
36	e	43	ASN
36	e	70	ASN
36	e	78	ASN
38	g	5	ARG
39	h	89	LYS
40	i	106	ARG
40	i	130	ARG
42	k	14	LYS
47	p	1	MET
47	p	31	ARG
50	s	29	LYS
52	u	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	142	HIS
4	D	49	GLN
5	E	97	ASN
5	E	156	ASN
5	E	163	ASN
6	F	21	ASN
7	G	20	ASN
8	H	20	ASN
8	H	43	ASN
8	H	73	ASN
8	H	119	ASN
8	H	135	HIS
10	K	89	ASN
13	N	107	ASN
15	P	56	HIS

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Mol	Chain	Res	Type
16	Q	37	GLN
16	Q	44	GLN
17	R	43	ASN
17	R	66	HIS
19	T	48	GLN
19	T	91	GLN
24	Y	15	ASN
24	Y	39	GLN
29	3	43	HIS
31	5	48	GLN
33	b	42	ASN
33	b	58	ASN
33	b	177	ASN
35	d	120	HIS
35	d	126	ASN
35	d	152	GLN
36	e	43	ASN
36	e	70	ASN
36	e	78	ASN
37	f	52	ASN
37	f	94	HIS
38	g	86	GLN
38	g	130	ASN
38	g	142	HIS
40	i	37	GLN
40	i	126	GLN
41	j	4	GLN
42	k	119	ASN
44	m	8	ASN
46	o	35	GLN
51	t	21	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2890/2897 (99%)	448 (15%)	14 (0%)
2	B	119/120 (99%)	8 (6%)	0
32	a	1529/1533 (99%)	233 (15%)	0
54	x	76/77 (98%)	12 (15%)	0
55	z	75/76 (98%)	21 (28%)	0
56	9	74/76 (97%)	29 (39%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
57	6	10/11 (90%)	3 (30%)	0
All	All	4773/4790 (99%)	754 (15%)	15 (0%)

All (754) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	10	A
1	A	17	G
1	A	27	G
1	A	34	U
1	A	35	G
1	A	43	G
1	A	63	A
1	A	71	A
1	A	72	U
1	A	74	A
1	A	75	G
1	A	92	U
1	A	101	A
1	A	102	U
1	A	103	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	127	A
1	A	140	C
1	A	146	A
1	A	154	U
1	A	162	U
1	A	163	C
1	A	165	A
1	A	166	U
1	A	181	A
1	A	196	A
1	A	199	A
1	A	216	A
1	A	221	A
1	A	222	A
1	A	224	U
1	A	233	A

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Mol	Chain	Res	Type
1	A	248	G
1	A	264	C
1	A	265	A
1	A	276	U
1	A	277	G
1	A	278	A
1	A	279	A
1	A	280	U
1	A	282	A
1	A	284	U
1	A	290	U
1	A	302	C
1	A	303	G
1	A	311	A
1	A	330	A
1	A	334	C
1	A	352	A
1	A	357	C
1	A	359	G
1	A	386	G
1	A	396	G
1	A	404	A
1	A	406	G
1	A	407	G
1	A	411	G
1	A	435	C
1	A	454	A
1	A	475	C
1	A	481	G
1	A	484	C
1	A	491	G
1	A	498	G
1	A	505	A
1	A	508	A
1	A	509	C
1	A	510	C
1	A	518	G
1	A	529	A
1	A	532	A
1	A	544	C
1	A	546	U
1	A	547	A

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Mol	Chain	Res	Type
1	A	548	G
1	A	549	G
1	A	550	C
1	A	563	A
1	A	573	U
1	A	575	A
1	A	603	A
1	A	613	A
1	A	614	A
1	A	621	A
1	A	637	A
1	A	643	A
1	A	645	C
1	A	646	U
1	A	647	G
1	A	653	U
1	A	654	A
1	A	664	G
1	A	677	A
1	A	685	A
1	A	686	U
1	A	711	G
1	A	717	C
1	A	726	G
1	A	730	A
1	A	738	G
1	A	747	5MU
1	A	764	A
1	A	765	C
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	791	C
1	A	792	A
1	A	805	G
1	A	812	C
1	A	827	U
1	A	828	U
1	A	846	U

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Mol	Chain	Res	Type
1	A	858	G
1	A	866	A
1	A	878	A
1	A	879	G
1	A	880	G
1	A	883	G
1	A	884	U
1	A	885	C
1	A	893	C
1	A	896	A
1	A	897	C
1	A	901	C
1	A	905	A
1	A	910	A
1	A	915	C
1	A	931	U
1	A	934	U
1	A	941	A
1	A	945	A
1	A	946	C
1	A	961	C
1	A	968	C
1	A	974	G
1	A	982	C
1	A	983	A
1	A	996	A
1	A	1012	U
1	A	1013	C
1	A	1026	G
1	A	1033	U
1	A	1040	A
1	A	1044	C
1	A	1045	C
1	A	1052	C
1	A	1053	C
1	A	1054	A
1	A	1055	G
1	A	1060	U
1	A	1062	G
1	A	1065	U
1	A	1066	U
1	A	1067	A

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Mol	Chain	Res	Type
1	A	1070	A
1	A	1071	G
1	A	1073	A
1	A	1078	U
1	A	1083	U
1	A	1084	A
1	A	1086	A
1	A	1088	A
1	A	1089	A
1	A	1090	A
1	A	1097	U
1	A	1098	A
1	A	1099	G
1	A	1107	G
1	A	1108	U
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1119	U
1	A	1122	G
1	A	1128	G
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1141	U
1	A	1142	A
1	A	1172	C
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1180	U
1	A	1199	U
1	A	1206	G
1	A	1212	G
1	A	1236	G
1	A	1242	U
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1257	C
1	A	1262	A

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Mol	Chain	Res	Type
1	A	1268	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1300	G
1	A	1301	A
1	A	1318	U
1	A	1321	A
1	A	1332	G
1	A	1338	G
1	A	1343	G
1	A	1352	U
1	A	1365	A
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1395	A
1	A	1416	G
1	A	1423	G
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1444	G
1	A	1449	G
1	A	1452	G
1	A	1460	U
1	A	1461	C
1	A	1474	U
1	A	1478	G
1	A	1482	G
1	A	1494	A
1	A	1495	A
1	A	1509	A
1	A	1515	A
1	A	1531	C
1	A	1533	C
1	A	1536	C
1	A	1540	G
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1583	A

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Mol	Chain	Res	Type
1	A	1584	U
1	A	1606	C
1	A	1608	A
1	A	1634	A
1	A	1636	U
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1654	A
1	A	1665	A
1	A	1674	G
1	A	1677	A
1	A	1725	U
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1733	G
1	A	1739	A
1	A	1764	C
1	A	1773	A
1	A	1782	U
1	A	1800	C
1	A	1808	A
1	A	1811	G
1	A	1816	C
1	A	1829	A
1	A	1847	A
1	A	1855	U
1	A	1866	A
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1888	G
1	A	1906	G
1	A	1907	G
1	A	1914	C
1	A	1929	G
1	A	1930	G
1	A	1935	G
1	A	1937	A
1	A	1938	A

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Mol	Chain	Res	Type
1	A	1955	U
1	A	1963	U
1	A	1964	G
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1989	G
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	2021	C
1	A	2023	C
1	A	2027	G
1	A	2033	A
1	A	2036	C
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2069	G7M
1	A	2099	U
1	A	2106	U
1	A	2107	G
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2115	G
1	A	2116	G
1	A	2117	A
1	A	2119	A
1	A	2125	G
1	A	2126	A
1	A	2127	G
1	A	2128	G
1	A	2129	C
1	A	2131	U
1	A	2132	U
1	A	2134	A
1	A	2135	A
1	A	2138	G

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Mol	Chain	Res	Type
1	A	2142	A
1	A	2143	C
1	A	2146	C
1	A	2147	A
1	A	2149	U
1	A	2151	U
1	A	2152	G
1	A	2154	A
1	A	2155	U
1	A	2158	A
1	A	2159	G
1	A	2160	C
1	A	2161	C
1	A	2163	A
1	A	2164	C
1	A	2165	C
1	A	2169	A
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2183	A
1	A	2186	G
1	A	2189	U
1	A	2190	G
1	A	2198	A
1	A	2203	U
1	A	2204	G
1	A	2211	A
1	A	2223	G
1	A	2225	A
1	A	2238	G
1	A	2249	U
1	A	2259	U
1	A	2268	A
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2288	A
1	A	2305	U
1	A	2307	G
1	A	2308	G
1	A	2309	A

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Mol	Chain	Res	Type
1	A	2310	C
1	A	2321	U
1	A	2322	A
1	A	2325	G
1	A	2333	A
1	A	2341	G
1	A	2345	G
1	A	2347	C
1	A	2383	G
1	A	2385	C
1	A	2391	G
1	A	2396	G
1	A	2398	U
1	A	2399	G
1	A	2406	A
1	A	2425	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2441	U
1	A	2448	A
1	A	2475	C
1	A	2476	A
1	A	2478	A
1	A	2491	U
1	A	2502	G
1	A	2505	G
1	A	2506	U
1	A	2508	G
1	A	2518	A
1	A	2520	C
1	A	2529	G
1	A	2547	A
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2578	G
1	A	2580	PSU
1	A	2602	A
1	A	2609	U
1	A	2613	U

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Mol	Chain	Res	Type
1	A	2629	U
1	A	2646	C
1	A	2654	A
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2716	C
1	A	2724	U
1	A	2726	A
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2750	A
1	A	2751	G
1	A	2758	A
1	A	2759	G
1	A	2778	A
1	A	2791	G
1	A	2799	A
1	A	2805	C
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2835	A
1	A	2836	U
1	A	2849	U
1	A	2861	U
1	A	2873	A
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2891	U
1	A	2901	C
2	B	16	G
2	B	35	C
2	B	44	G
2	B	56	G
2	B	89	U
2	B	90	C
2	B	105	G
2	B	109	A

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Mol	Chain	Res	Type
32	a	4	U
32	a	5	U
32	a	6	G
32	a	7	A
32	a	9	G
32	a	32	A
32	a	39	G
32	a	47	C
32	a	48	C
32	a	50	A
32	a	51	A
32	a	71	A
32	a	72	A
32	a	78	A
32	a	79	G
32	a	81	A
32	a	82	G
32	a	83	C
32	a	84	U
32	a	85	U
32	a	86	G
32	a	88	U
32	a	89	U
32	a	94	G
32	a	95	C
32	a	98	A
32	a	116	A
32	a	120	A
32	a	121	U
32	a	122	G
32	a	127	G
32	a	130	A
32	a	131	A
32	a	142	G
32	a	163	C
32	a	164	G
32	a	166	U
32	a	181	A
32	a	183	C
32	a	184	G
32	a	187	G
32	a	197	A

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Mol	Chain	Res	Type
32	a	207	C
32	a	208	U
32	a	209	U
32	a	210	C
32	a	211	G
32	a	212	G
32	a	226	G
32	a	245	U
32	a	246	A
32	a	247	G
32	a	250	A
32	a	251	G
32	a	258	G
32	a	266	G
32	a	267	C
32	a	281	G
32	a	282	A
32	a	289	G
32	a	301	G
32	a	321	A
32	a	328	C
32	a	347	G
32	a	352	C
32	a	354	G
32	a	367	U
32	a	372	C
32	a	373	A
32	a	384	G
32	a	397	A
32	a	404	G
32	a	406	G
32	a	409	U
32	a	411	A
32	a	413	G
32	a	414	A
32	a	422	C
32	a	424	G
32	a	429	U
32	a	435	A
32	a	439	U
32	a	459	A
32	a	467	U

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Mol	Chain	Res	Type
32	a	468	A
32	a	470	C
32	a	473	U
32	a	478	A
32	a	479	U
32	a	481	G
32	a	484	G
32	a	486	U
32	a	497	G
32	a	500	G
32	a	509	A
32	a	511	C
32	a	513	C
32	a	515	G
32	a	516	PSU
32	a	518	C
32	a	519	C
32	a	527	G7M
32	a	532	A
32	a	535	A
32	a	547	A
32	a	562	U
32	a	572	A
32	a	573	A
32	a	575	G
32	a	576	C
32	a	577	G
32	a	579	A
32	a	596	A
32	a	633	G
32	a	650	G
32	a	653	U
32	a	665	A
32	a	718	A
32	a	721	G
32	a	722	G
32	a	724	G
32	a	731	G
32	a	748	G
32	a	755	G
32	a	777	A
32	a	793	U

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Mol	Chain	Res	Type
32	a	794	A
32	a	815	A
32	a	817	C
32	a	821	G
32	a	832	G
32	a	841	C
32	a	842	U
32	a	843	U
32	a	844	G
32	a	845	A
32	a	846	G
32	a	902	G
32	a	926	G
32	a	934	C
32	a	960	U
32	a	961	U
32	a	966	2MG
32	a	967	5MC
32	a	968	A
32	a	969	A
32	a	975	A
32	a	976	G
32	a	977	A
32	a	993	G
32	a	1004	A
32	a	1005	A
32	a	1026	G
32	a	1030	U
32	a	1031	C
32	a	1033	G
32	a	1034	G
32	a	1035	A
32	a	1053	G
32	a	1065	U
32	a	1094	G
32	a	1095	U
32	a	1101	A
32	a	1132	C
32	a	1138	G
32	a	1139	G
32	a	1140	C
32	a	1141	C

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Mol	Chain	Res	Type
32	a	1142	G
32	a	1157	A
32	a	1158	C
32	a	1159	U
32	a	1166	G
32	a	1168	U
32	a	1169	A
32	a	1171	A
32	a	1182	G
32	a	1184	G
32	a	1191	A
32	a	1196	A
32	a	1197	A
32	a	1202	U
32	a	1212	U
32	a	1213	A
32	a	1225	A
32	a	1226	C
32	a	1227	A
32	a	1238	A
32	a	1256	A
32	a	1257	A
32	a	1260	G
32	a	1275	A
32	a	1279	G
32	a	1280	A
32	a	1285	A
32	a	1286	U
32	a	1287	A
32	a	1299	A
32	a	1300	G
32	a	1301	U
32	a	1302	C
32	a	1303	C
32	a	1317	C
32	a	1320	C
32	a	1340	A
32	a	1345	U
32	a	1346	A
32	a	1353	G
32	a	1363	A
32	a	1364	U

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Mol	Chain	Res	Type
32	a	1370	G
32	a	1394	A
32	a	1398	A
32	a	1399	C
32	a	1400	C
32	a	1419	G
32	a	1429	A
32	a	1432	G
32	a	1441	A
32	a	1446	A
32	a	1451	U
32	a	1452	C
32	a	1487	G
32	a	1492	A
32	a	1493	A
32	a	1497	G
32	a	1499	A
32	a	1502	A
32	a	1503	A
32	a	1506	U
32	a	1517	G
32	a	1529	G
32	a	1530	G
54	x	8	U
54	x	9	A
54	x	17	U
54	x	20	U
54	x	23	G
54	x	43	U
54	x	47	G
54	x	48	U
54	x	49	C
54	x	55	U
54	x	60	G
54	x	76	C
55	z	3	G
55	z	10	G
55	z	11	G
55	z	13	U
55	z	14	C
55	z	17	A
55	z	18	A

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Mol	Chain	Res	Type
55	z	19	G
55	z	20	G
55	z	21	G
55	z	22	A
55	z	43	G
55	z	49	C
55	z	50	G
55	z	51	G
55	z	58	G
55	z	63	C
55	z	69	G
55	z	74	A
55	z	76	C
55	z	77	A
56	9	5	G
56	9	6	A
56	9	8	U
56	9	10	G
56	9	13	C
56	9	14	A
56	9	18	G
56	9	19	G
56	9	20	G
56	9	21	A
56	9	22	G
56	9	26	A
56	9	27	C
56	9	34	U
56	9	35	A
56	9	36	C
56	9	45	G
56	9	47	U
56	9	48	C
56	9	49	G
56	9	57	G
56	9	58	A
56	9	59	U
56	9	61	C
56	9	63	G
56	9	64	U
56	9	69	A
56	9	70	C

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Mol	Chain	Res	Type
56	9	76	A
57	6	26	U
57	6	28	U
57	6	32	C

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	183	C
1	A	784	G
1	A	845	A
1	A	1111	A
1	A	1138	G
1	A	1183	U
1	A	1190	G
1	A	1300	G
1	A	1399	C
1	A	1738	G
1	A	1913	A
1	A	2124	G
1	A	2162	G
1	A	2189	U
56	9	63	G

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

37 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	OMC	A	2498	1,58	19,22,23	2.85	8 (42%)	26,31,34	0.87	1 (3%)
1	PSU	A	2580	1	18,21,22	1.14	3 (16%)	22,30,33	2.06	6 (27%)
32	MA6	a	1518	32	19,26,27	1.09	1 (5%)	18,38,41	3.97	2 (11%)
1	OMU	A	2552	1,58	19,22,23	2.95	7 (36%)	26,31,34	1.78	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MA	A	2503	1,58	17,25,26	2.66	6 (35%)	17,37,40	1.42	3 (17%)
32	5MC	a	1407	32	18,22,23	3.36	7 (38%)	26,32,35	1.03	2 (7%)
1	1MG	A	745	1	18,26,27	2.63	5 (27%)	19,39,42	1.46	3 (15%)
1	PSU	A	2605	1	18,21,22	1.07	2 (11%)	22,30,33	1.76	4 (18%)
32	5MC	a	967	32	18,22,23	3.44	7 (38%)	26,32,35	0.99	3 (11%)
43	D2T	l	89	43	7,9,10	1.01	0	6,11,13	2.58	3 (50%)
32	G7M	a	527	32	20,26,27	2.39	7 (35%)	17,39,42	1.16	1 (5%)
32	4OC	a	1402	32	20,23,24	2.99	8 (40%)	26,32,35	0.96	2 (7%)
32	UR3	a	1498	32	19,22,23	2.74	6 (31%)	26,32,35	1.36	3 (11%)
32	2MG	a	1516	32	18,26,27	2.41	7 (38%)	16,38,41	1.65	4 (25%)
1	5MU	A	1939	1	19,22,23	4.83	6 (31%)	28,32,35	3.70	11 (39%)
1	OMG	A	2251	1,54	18,26,27	2.42	7 (38%)	19,38,41	1.68	5 (26%)
1	5MC	A	1962	1	18,22,23	3.34	7 (38%)	26,32,35	1.04	2 (7%)
1	PSU	A	955	1	18,21,22	1.04	2 (11%)	22,30,33	1.80	4 (18%)
1	6MZ	A	1618	1	18,25,26	1.95	2 (11%)	16,36,39	2.39	3 (18%)
32	2MG	a	966	32	18,26,27	2.44	7 (38%)	16,38,41	1.48	3 (18%)
4	MEQ	D	150	4	8,9,10	0.88	0	5,10,12	0.54	0
1	5MU	A	747	1	19,22,23	4.88	6 (31%)	28,32,35	3.90	10 (35%)
32	2MG	a	1207	32	18,26,27	2.49	7 (38%)	16,38,41	1.40	3 (18%)
1	2MG	A	1835	1	18,26,27	2.38	7 (38%)	16,38,41	1.60	4 (25%)
1	G7M	A	2069	1	20,26,27	2.23	6 (30%)	17,39,42	1.16	1 (5%)
12	4D4	M	81	12	9,11,12	2.46	3 (33%)	8,13,15	1.01	0
1	PSU	A	2457	1	18,21,22	1.03	2 (11%)	22,30,33	1.89	4 (18%)
32	MA6	a	1519	32	19,26,27	1.30	3 (15%)	18,38,41	3.23	2 (11%)
1	PSU	A	1917	1	18,21,22	1.06	2 (11%)	22,30,33	1.74	4 (18%)
1	PSU	A	2504	1,58	18,21,22	1.00	2 (11%)	22,30,33	1.86	4 (18%)
32	PSU	a	516	32,58	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
1	PSU	A	746	1,58	18,21,22	1.21	2 (11%)	22,30,33	1.83	3 (13%)
1	2MG	A	2445	1	18,26,27	2.34	7 (38%)	16,38,41	1.57	4 (25%)
1	PSU	A	1911	1	18,21,22	1.00	2 (11%)	22,30,33	1.72	4 (18%)
1	6MZ	A	2030	1	18,25,26	1.98	2 (11%)	16,36,39	2.23	3 (18%)
1	PSU	A	2604	1	18,21,22	1.04	2 (11%)	22,30,33	1.84	4 (18%)
1	3TD	A	1915	1	18,22,23	4.25	9 (50%)	22,32,35	1.72	2 (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
1	OMC	A	2498	1,58	-	1/9/27/28	0/2/2/2
1	PSU	A	2580	1	-	2/7/25/26	0/2/2/2
32	MA6	a	1518	32	-	0/7/29/30	0/3/3/3
1	OMU	A	2552	1,58	-	0/9/27/28	0/2/2/2
1	2MA	A	2503	1,58	-	2/3/25/26	0/3/3/3
32	5MC	a	1407	32	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	a	967	32	-	2/7/25/26	0/2/2/2
43	D2T	l	89	43	-	4/7/12/14	-
32	G7M	a	527	32	-	2/3/25/26	0/3/3/3
32	4OC	a	1402	32	-	2/9/29/30	0/2/2/2
32	UR3	a	1498	32	-	0/7/25/26	0/2/2/2
32	2MG	a	1516	32	-	0/5/27/28	0/3/3/3
1	5MU	A	1939	1	-	0/7/25/26	0/2/2/2
1	OMG	A	2251	1,54	-	1/5/27/28	0/3/3/3
1	5MC	A	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	0/5/27/28	0/3/3/3
32	2MG	a	966	32	-	2/5/27/28	0/3/3/3
4	MEQ	D	150	4	-	3/8/9/11	-
1	5MU	A	747	1	-	0/7/25/26	0/2/2/2
32	2MG	a	1207	32	-	0/5/27/28	0/3/3/3
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
1	G7M	A	2069	1	-	3/3/25/26	0/3/3/3
12	4D4	M	81	12	-	1/11/12/14	-
1	PSU	A	2457	1	-	0/7/25/26	0/2/2/2
32	MA6	a	1519	32	-	2/7/29/30	0/3/3/3
1	PSU	A	1917	1	-	1/7/25/26	0/2/2/2
1	PSU	A	2504	1,58	-	0/7/25/26	0/2/2/2
32	PSU	a	516	32,58	-	0/7/25/26	0/2/2/2
1	PSU	A	746	1,58	-	1/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	2/5/27/28	0/3/3/3
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	0/7/25/26	0/2/2/2

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	C6-C5	12.19	1.49	1.35
1	A	747	5MU	C6-N1	11.67	1.58	1.38
1	A	1939	5MU	C6-N1	11.34	1.57	1.38
1	A	1939	5MU	C2-N1	10.03	1.54	1.38
1	A	747	5MU	C4-C5	9.89	1.61	1.44
1	A	747	5MU	C2-N1	9.77	1.54	1.38
1	A	1939	5MU	C4-C5	9.48	1.60	1.44
32	a	967	5MC	C6-C5	8.82	1.49	1.34
32	a	1407	5MC	C6-C5	8.76	1.49	1.34
1	A	1915	3TD	C2-N1	8.56	1.48	1.37
1	A	1962	5MC	C6-C5	8.55	1.48	1.34
1	A	1939	5MU	C4-N3	-7.89	1.24	1.38
1	A	747	5MU	C4-N3	-7.85	1.24	1.38
32	a	1498	UR3	C2-N1	7.49	1.49	1.38
1	A	2503	2MA	C2-N3	7.41	1.46	1.31
1	A	1618	6MZ	C6-N6	6.87	1.46	1.35
1	A	2030	6MZ	C6-N6	6.74	1.46	1.35
1	A	2552	OMU	C2-N3	6.71	1.49	1.38
1	A	1915	3TD	C6-N1	6.61	1.47	1.36
1	A	747	5MU	C6-C5	6.54	1.45	1.34
1	A	1939	5MU	C6-C5	6.40	1.45	1.34
32	a	1402	4OC	C4-N3	6.40	1.43	1.32
1	A	745	1MG	C2-N3	6.30	1.46	1.34
32	a	1402	4OC	C6-C5	6.27	1.49	1.35
32	a	967	5MC	C2-N3	6.16	1.48	1.36
1	A	745	1MG	C2-N2	6.14	1.45	1.34
32	a	967	5MC	C4-N3	6.05	1.44	1.34
1	A	1962	5MC	C4-N3	5.99	1.44	1.34
1	A	2498	OMC	C2-N3	5.97	1.48	1.36
1	A	2552	OMU	C2-N1	5.97	1.48	1.38
32	a	1498	UR3	C6-C5	5.90	1.48	1.35
1	A	2503	2MA	C4-N3	5.87	1.51	1.37
32	a	1407	5MC	C4-N3	5.72	1.43	1.34
1	A	1962	5MC	C2-N3	5.69	1.47	1.36
1	A	2498	OMC	C6-C5	5.66	1.48	1.35
32	a	1407	5MC	C2-N3	5.60	1.47	1.36
32	a	1402	4OC	C2-N3	5.60	1.47	1.36
12	M	81	4D4	CZ-NE	5.57	1.44	1.33
1	A	2552	OMU	C6-C5	5.57	1.48	1.35
32	a	1207	2MG	C2-N2	5.36	1.45	1.33
32	a	966	2MG	C2-N2	5.33	1.45	1.33
32	a	527	G7M	C2-N3	5.29	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	1516	2MG	C2-N2	5.04	1.44	1.33
1	A	1835	2MG	C2-N2	5.01	1.44	1.33
1	A	2445	2MG	C2-N2	4.92	1.44	1.33
1	A	2069	G7M	C2-N3	4.87	1.45	1.33
32	a	1207	2MG	C4-N3	4.87	1.49	1.37
1	A	745	1MG	C4-N3	4.77	1.48	1.37
1	A	2445	2MG	C4-N3	4.77	1.48	1.37
1	A	2498	OMC	C4-N4	4.76	1.45	1.33
32	a	527	G7M	C4-N3	4.74	1.48	1.37
1	A	2251	OMG	O6-C6	-4.71	1.13	1.23
1	A	1835	2MG	C4-N3	4.70	1.48	1.37
32	a	966	2MG	C4-N3	4.66	1.48	1.37
32	a	966	2MG	C2-N1	4.65	1.44	1.36
32	a	1207	2MG	C2-N1	4.59	1.44	1.36
32	a	527	G7M	C2-N2	4.58	1.45	1.34
1	A	2069	G7M	C4-N3	4.56	1.48	1.37
1	A	2498	OMC	C4-N3	4.56	1.43	1.34
32	a	1498	UR3	C2-N3	4.52	1.47	1.39
32	a	1516	2MG	C2-N1	4.51	1.43	1.36
1	A	2251	OMG	C2-N3	4.51	1.44	1.33
1	A	2069	G7M	C2-N2	4.41	1.44	1.34
32	a	1407	5MC	C6-N1	4.35	1.45	1.38
32	a	1516	2MG	C4-N3	4.32	1.47	1.37
1	A	2251	OMG	C2-N2	4.30	1.44	1.34
32	a	1402	4OC	C4-N4	4.30	1.44	1.35
1	A	2498	OMC	C2-N1	4.27	1.49	1.40
1	A	1835	2MG	C2-N1	4.26	1.43	1.36
1	A	1915	3TD	C2-N3	4.19	1.47	1.38
32	a	967	5MC	C6-N1	4.16	1.45	1.38
1	A	1962	5MC	C6-N1	4.13	1.45	1.38
32	a	967	5MC	C4-N4	4.08	1.44	1.34
1	A	1962	5MC	C4-N4	4.06	1.44	1.34
32	a	1407	5MC	C4-N4	4.05	1.44	1.34
32	a	1402	4OC	C5-C4	3.97	1.49	1.40
1	A	2251	OMG	C4-N3	3.92	1.46	1.37
32	a	1207	2MG	C6-N1	3.88	1.43	1.37
32	a	967	5MC	C2-N1	3.88	1.48	1.40
1	A	2552	OMU	O2-C2	-3.79	1.16	1.23
1	A	1962	5MC	C2-N1	3.76	1.48	1.40
1	A	2445	2MG	C2-N1	3.71	1.42	1.36
32	a	1402	4OC	C2-N1	3.68	1.48	1.40
1	A	2552	OMU	C4-N3	3.64	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	1407	5MC	C2-N1	3.61	1.47	1.40
1	A	1939	5MU	O2-C2	-3.52	1.16	1.23
32	a	527	G7M	C6-N1	3.48	1.43	1.37
32	a	966	2MG	C6-N1	3.43	1.43	1.37
1	A	2552	OMU	O4-C4	-3.38	1.17	1.24
32	a	1516	2MG	C5-C4	-3.38	1.34	1.43
32	a	1516	2MG	C6-N1	3.36	1.42	1.37
1	A	1835	2MG	C6-N1	3.33	1.42	1.37
32	a	1498	UR3	C6-N1	3.32	1.46	1.38
1	A	2030	6MZ	C5-C4	-3.30	1.32	1.40
1	A	747	5MU	O2-C2	-3.30	1.17	1.23
32	a	1407	5MC	O2-C2	-3.29	1.17	1.23
12	M	81	4D4	CZ-NH2	3.29	1.45	1.32
1	A	746	PSU	C6-C5	3.28	1.39	1.35
1	A	2445	2MG	C5-C4	-3.21	1.34	1.43
1	A	1915	3TD	O2-C2	-3.20	1.17	1.23
32	a	516	PSU	C6-C5	3.15	1.39	1.35
1	A	2445	2MG	C6-N1	3.12	1.42	1.37
1	A	1962	5MC	O2-C2	-3.11	1.17	1.23
32	a	527	G7M	C5-C6	3.09	1.53	1.45
1	A	2580	PSU	C6-C5	3.03	1.38	1.35
1	A	2503	2MA	C6-N1	3.03	1.44	1.38
32	a	1402	4OC	O2-C2	-3.01	1.18	1.23
1	A	1915	3TD	C1'-C5	3.01	1.57	1.50
32	a	1402	4OC	C6-N1	2.99	1.45	1.38
32	a	966	2MG	C5-C4	-2.97	1.35	1.43
1	A	2498	OMC	C6-N1	2.96	1.45	1.38
1	A	1917	PSU	C6-C5	2.96	1.38	1.35
1	A	2498	OMC	O2-C2	-2.95	1.18	1.23
1	A	745	1MG	C5-C4	-2.95	1.35	1.43
1	A	2552	OMU	C6-N1	2.95	1.45	1.38
1	A	1835	2MG	C5-C6	2.94	1.53	1.47
1	A	1835	2MG	C5-C4	-2.92	1.35	1.43
1	A	1915	3TD	C4-N3	2.90	1.46	1.40
1	A	1618	6MZ	C5-C4	-2.90	1.33	1.40
1	A	1911	PSU	C6-C5	2.89	1.38	1.35
1	A	2445	2MG	O6-C6	-2.87	1.17	1.23
32	a	1207	2MG	C5-C4	-2.85	1.35	1.43
1	A	2069	G7M	O6-C6	-2.85	1.17	1.23
1	A	2251	OMG	C5-C4	-2.83	1.35	1.43
32	a	967	5MC	O2-C2	-2.83	1.18	1.23
1	A	2251	OMG	C2-N1	2.82	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	1519	MA6	C2-N3	2.82	1.36	1.32
1	A	2503	2MA	C5-C4	-2.81	1.35	1.43
32	a	1516	2MG	C5-C6	2.78	1.53	1.47
1	A	955	PSU	C6-C5	2.78	1.38	1.35
1	A	2069	G7M	C6-N1	2.77	1.42	1.37
1	A	746	PSU	O4'-C1'	-2.75	1.40	1.43
32	a	1207	2MG	C5-C6	2.71	1.52	1.47
32	a	966	2MG	C5-C6	2.66	1.52	1.47
32	a	1498	UR3	C5-C4	2.65	1.50	1.43
1	A	2069	G7M	C5-C6	2.61	1.52	1.45
32	a	1516	2MG	O6-C6	-2.60	1.18	1.23
1	A	2605	PSU	C6-C5	2.58	1.38	1.35
1	A	2251	OMG	C5-C6	2.57	1.52	1.47
1	A	2457	PSU	C6-C5	2.55	1.38	1.35
1	A	2604	PSU	C6-C5	2.54	1.38	1.35
32	a	527	G7M	O6-C6	-2.52	1.18	1.23
1	A	1835	2MG	O6-C6	-2.52	1.18	1.23
1	A	2445	2MG	C5-C6	2.51	1.52	1.47
32	a	527	G7M	C2-N1	2.48	1.43	1.37
32	a	966	2MG	O6-C6	-2.47	1.18	1.23
32	a	1518	MA6	C5-C4	-2.44	1.34	1.40
32	a	1207	2MG	O6-C6	-2.41	1.18	1.23
32	a	1519	MA6	C4-N3	2.39	1.39	1.35
1	A	745	1MG	C5-C6	2.33	1.54	1.47
12	M	81	4D4	CZ-NH1	-2.28	1.25	1.34
1	A	2504	PSU	C6-C5	2.27	1.38	1.35
1	A	1915	3TD	C10-N3	-2.27	1.42	1.47
1	A	2498	OMC	C5-C4	2.24	1.48	1.42
1	A	2580	PSU	O4'-C1'	-2.23	1.40	1.43
1	A	2503	2MA	C2-N1	2.22	1.43	1.36
1	A	2605	PSU	C4-C5	-2.22	1.37	1.44
32	a	1498	UR3	C4-N3	2.19	1.45	1.40
32	a	1519	MA6	C5-C4	-2.17	1.35	1.40
1	A	2503	2MA	CM2-C2	2.16	1.55	1.49
1	A	1915	3TD	O4-C4	-2.13	1.18	1.23
1	A	2604	PSU	C4-C5	-2.13	1.38	1.44
1	A	1917	PSU	C4-C5	-2.12	1.38	1.44
1	A	2457	PSU	C4-C5	-2.06	1.38	1.44
1	A	2580	PSU	C4-C5	-2.04	1.38	1.44
1	A	1911	PSU	C4-C5	-2.03	1.38	1.44
1	A	955	PSU	C4-C5	-2.02	1.38	1.44
1	A	2504	PSU	C4-C5	-2.01	1.38	1.44

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1518	MA6	N1-C6-N6	-15.73	100.50	117.06
32	a	1519	MA6	N1-C6-N6	-13.13	103.23	117.06
1	A	747	5MU	C5-C4-N3	12.82	126.25	115.31
1	A	1939	5MU	C5-C4-N3	11.61	125.22	115.31
1	A	747	5MU	C5-C6-N1	-11.22	111.79	123.34
1	A	1939	5MU	C5-C6-N1	-10.15	112.90	123.34
1	A	2030	6MZ	N3-C2-N1	-6.00	119.30	128.68
1	A	1618	6MZ	N3-C2-N1	-5.83	119.57	128.68
1	A	1618	6MZ	C9-N6-C6	-5.78	117.89	122.87
1	A	1915	3TD	N1-C2-N3	5.72	120.65	116.14
1	A	2552	OMU	C4-N3-C2	-5.58	119.22	126.58
32	a	1518	MA6	N3-C2-N1	-5.57	119.98	128.68
1	A	2580	PSU	N1-C2-N3	5.33	121.17	115.13
1	A	747	5MU	C4-N3-C2	-5.25	120.56	127.35
1	A	2605	PSU	C4-N3-C2	-5.13	118.94	126.34
1	A	2504	PSU	C4-N3-C2	-5.08	119.02	126.34
1	A	1939	5MU	N3-C2-N1	5.01	121.54	114.89
1	A	1939	5MU	C4-N3-C2	-5.00	120.88	127.35
1	A	747	5MU	O4-C4-C5	-4.91	119.21	124.90
1	A	2457	PSU	C4-N3-C2	-4.90	119.28	126.34
1	A	1939	5MU	C5M-C5-C6	-4.89	116.32	122.85
1	A	955	PSU	C4-N3-C2	-4.81	119.41	126.34
1	A	2457	PSU	N1-C2-N3	4.79	120.55	115.13
1	A	2604	PSU	C4-N3-C2	-4.75	119.49	126.34
1	A	2580	PSU	C4-N3-C2	-4.70	119.57	126.34
1	A	1911	PSU	C4-N3-C2	-4.68	119.60	126.34
32	a	516	PSU	C4-N3-C2	-4.65	119.64	126.34
1	A	2504	PSU	N1-C2-N3	4.63	120.37	115.13
1	A	746	PSU	C4-N3-C2	-4.62	119.68	126.34
1	A	955	PSU	N1-C2-N3	4.59	120.33	115.13
32	a	1498	UR3	C4-N3-C2	-4.54	120.29	124.56
1	A	2604	PSU	N1-C2-N3	4.53	120.26	115.13
1	A	1917	PSU	C4-N3-C2	-4.52	119.82	126.34
1	A	747	5MU	C5M-C5-C6	-4.48	116.87	122.85
1	A	746	PSU	N1-C2-N3	4.43	120.15	115.13
1	A	747	5MU	N3-C2-N1	4.37	120.69	114.89
1	A	1939	5MU	O4-C4-C5	-4.32	119.89	124.90
1	A	2030	6MZ	C2-N1-C6	4.32	120.30	116.59
1	A	1939	5MU	C5M-C5-C4	4.30	123.50	118.77
1	A	1911	PSU	N1-C2-N3	4.26	119.96	115.13
1	A	1917	PSU	N1-C2-N3	4.25	119.95	115.13
32	a	516	PSU	N1-C2-N3	4.23	119.93	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	5MU	C5M-C5-C4	4.23	123.42	118.77
1	A	745	1MG	C5-C6-N1	4.21	120.23	113.90
1	A	1618	6MZ	C2-N1-C6	4.13	120.13	116.59
1	A	2030	6MZ	C9-N6-C6	-4.07	119.36	122.87
1	A	2552	OMU	N3-C2-N1	4.07	120.29	114.89
1	A	2605	PSU	N1-C2-N3	3.95	119.60	115.13
1	A	2445	2MG	C5-C6-N1	3.91	120.85	113.95
43	l	89	D2T	CB1-SB-CB	3.87	109.45	102.44
1	A	2251	OMG	C5-C6-N1	3.81	120.69	113.95
43	l	89	D2T	OD2-CG-CB	3.80	121.37	113.15
1	A	1915	3TD	C4-N3-C2	-3.77	120.51	124.61
1	A	1835	2MG	C5-C6-N1	3.77	120.61	113.95
32	a	1516	2MG	C5-C6-N1	3.75	120.57	113.95
1	A	2503	2MA	C5-C6-N1	3.72	120.44	114.02
1	A	2552	OMU	C5-C4-N3	3.71	120.40	114.84
32	a	966	2MG	C5-C6-N1	3.71	120.50	113.95
32	a	1407	5MC	C5-C6-N1	-3.57	119.67	123.34
32	a	1207	2MG	C5-C6-N1	3.54	120.20	113.95
1	A	2580	PSU	O2-C2-N1	-3.38	119.06	122.79
1	A	1962	5MC	C5-C6-N1	-3.35	119.89	123.34
32	a	527	G7M	C2-N1-C6	-3.32	118.99	125.10
1	A	2251	OMG	C2-N1-C6	-3.19	119.23	125.10
1	A	2069	G7M	C2-N1-C6	-3.17	119.27	125.10
1	A	2251	OMG	C8-N7-C5	3.12	108.94	102.99
32	a	1516	2MG	C8-N7-C5	3.09	108.89	102.99
1	A	1835	2MG	C8-N7-C5	3.09	108.87	102.99
1	A	2503	2MA	C8-N7-C5	3.04	108.78	102.99
32	a	1519	MA6	N3-C2-N1	-2.99	124.00	128.68
1	A	747	5MU	O4-C4-N3	-2.91	114.54	120.12
32	a	1516	2MG	CM2-N2-C2	-2.91	117.43	123.86
1	A	1917	PSU	O2-C2-N1	-2.89	119.61	122.79
1	A	2552	OMU	O4-C4-C5	-2.85	120.14	125.16
1	A	2580	PSU	C6-N1-C2	-2.84	119.78	122.68
1	A	955	PSU	O2-C2-N1	-2.82	119.69	122.79
32	a	1498	UR3	C6-N1-C2	-2.81	119.27	121.79
1	A	2457	PSU	O2-C2-N1	-2.81	119.70	122.79
1	A	2445	2MG	CM2-N2-C2	-2.81	117.67	123.86
32	a	966	2MG	C8-N7-C5	2.77	108.26	102.99
1	A	1835	2MG	CM2-N2-C2	-2.77	117.75	123.86
1	A	2580	PSU	C6-C5-C4	2.75	120.12	118.20
1	A	1939	5MU	O4-C4-N3	-2.73	114.89	120.12
32	a	1207	2MG	C8-N7-C5	2.64	108.03	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2445	2MG	C8-N7-C5	2.59	107.93	102.99
32	a	966	2MG	O6-C6-C5	-2.59	119.32	124.37
1	A	1939	5MU	C6-C5-C4	2.57	120.18	118.03
1	A	745	1MG	C8-N7-C5	2.56	107.87	102.99
1	A	1939	5MU	O2-C2-N1	-2.55	119.40	122.79
32	a	967	5MC	C5-C6-N1	-2.52	120.75	123.34
1	A	2580	PSU	O4'-C1'-C2'	2.46	108.61	105.14
1	A	747	5MU	O2-C2-N1	-2.44	119.54	122.79
1	A	2445	2MG	O6-C6-C5	-2.41	119.66	124.37
1	A	1962	5MC	CM5-C5-C6	-2.41	119.63	122.85
1	A	2457	PSU	C6-N1-C2	-2.40	120.23	122.68
32	a	1207	2MG	O6-C6-C5	-2.39	119.70	124.37
32	a	1516	2MG	O6-C6-C5	-2.39	119.71	124.37
1	A	1835	2MG	O6-C6-C5	-2.37	119.74	124.37
32	a	1498	UR3	C1'-N1-C2	2.35	120.96	116.99
32	a	516	PSU	O4'-C1'-C2'	2.33	108.43	105.14
1	A	2604	PSU	O2-C2-N1	-2.33	120.23	122.79
32	a	516	PSU	O2-C2-N1	-2.31	120.25	122.79
1	A	2504	PSU	O2-C2-N1	-2.27	120.29	122.79
1	A	2251	OMG	O6-C6-C5	-2.27	119.94	124.37
1	A	1917	PSU	C6-N1-C2	-2.26	120.37	122.68
32	a	1407	5MC	CM5-C5-C6	-2.25	119.84	122.85
1	A	2605	PSU	C5-C4-N3	2.24	121.66	116.58
1	A	2503	2MA	N1-C2-N3	-2.24	119.34	123.06
32	a	1402	4OC	C6-C5-C4	2.23	119.69	116.96
1	A	746	PSU	C6-C5-C4	2.20	119.74	118.20
1	A	2504	PSU	C6-C5-C4	2.19	119.73	118.20
1	A	2552	OMU	O2-C2-N1	-2.16	119.92	122.79
43	l	89	D2T	OD2-CG-OD1	-2.14	119.22	124.09
1	A	2498	OMC	C6-C5-C4	2.14	120.96	117.50
1	A	1911	PSU	C6-N1-C2	-2.14	120.50	122.68
32	a	967	5MC	C5-C4-N3	-2.08	119.43	121.67
1	A	2251	OMG	N2-C2-N1	2.08	121.13	116.71
32	a	967	5MC	CM5-C5-C6	-2.07	120.08	122.85
1	A	2604	PSU	C6-N1-C2	-2.06	120.58	122.68
1	A	2605	PSU	O4-C4-C5	-2.06	118.66	124.05
1	A	1939	5MU	C1'-N1-C2	2.06	121.30	117.57
1	A	745	1MG	CM1-N1-C6	2.03	120.32	117.55
32	a	1402	4OC	CM4-N4-C4	-2.01	118.52	122.45
1	A	747	5MU	C6-C5-C4	2.01	119.71	118.03
1	A	1911	PSU	O2-C2-N1	-2.01	120.58	122.79
1	A	955	PSU	C6-N1-C2	-2.00	120.63	122.68



There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	150	MEQ	N-CA-CB-CG
4	D	150	MEQ	C-CA-CB-CG
4	D	150	MEQ	O-C-CA-CB
43	l	89	D2T	CG-CB-SB-CB1
1	A	2030	6MZ	O4'-C4'-C5'-O5'
1	A	2251	OMG	C1'-C2'-O2'-CM2
32	a	527	G7M	O4'-C4'-C5'-O5'
32	a	527	G7M	C3'-C4'-C5'-O5'
32	a	966	2MG	C3'-C4'-C5'-O5'
32	a	967	5MC	O4'-C4'-C5'-O5'
32	a	967	5MC	C3'-C4'-C5'-O5'
32	a	1519	MA6	O4'-C4'-C5'-O5'
1	A	2580	PSU	O4'-C4'-C5'-O5'
32	a	966	2MG	O4'-C4'-C5'-O5'
32	a	1519	MA6	C3'-C4'-C5'-O5'
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2580	PSU	C3'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
32	a	1402	4OC	O4'-C4'-C5'-O5'
1	A	2069	G7M	O4'-C4'-C5'-O5'
1	A	2069	G7M	C3'-C4'-C5'-O5'
1	A	2445	2MG	O4'-C4'-C5'-O5'
43	l	89	D2T	SB-CB-CG-OD1
43	l	89	D2T	CA-CB-CG-OD1
1	A	2503	2MA	C4'-C5'-O5'-P
1	A	2069	G7M	C4'-C5'-O5'-P
1	A	746	PSU	O4'-C1'-C5'-C4
43	l	89	D2T	CA-CB-SB-CB1
32	a	1402	4OC	C3'-C4'-C5'-O5'
1	A	1917	PSU	O4'-C4'-C5'-O5'
1	A	2498	OMC	C3'-C2'-O2'-CM2
1	A	2503	2MA	O4'-C4'-C5'-O5'
12	M	81	4D4	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 362 ligands modelled in this entry, 359 are monoatomic - leaving 3 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$
59	ERY	A	3237	-	53,53,53	1.78	14 (26%)	82,82,82	5.01	36 (43%)
60	SY5	a	1714	58	18,20,20	2.65	2 (11%)	16,24,24	1.91	4 (25%)
60	SY5	a	1715	-	18,20,20	2.62	4 (22%)	16,24,24	1.71	2 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	ERY	A	3237	-	3/3/21/21	25/72/107/107	0/3/3/3
60	SY5	a	1714	58	-	15/22/22/22	-
60	SY5	a	1715	-	-	9/22/22/22	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	a	1714	SY5	C14-N06	9.94	1.48	1.35
60	a	1715	SY5	C14-N06	9.83	1.48	1.35
59	A	3237	ERY	O2-C1	7.18	1.51	1.34
59	A	3237	ERY	O10-C6	-3.11	1.39	1.44
59	A	3237	ERY	O4-C14	3.05	1.49	1.42
60	a	1714	SY5	O02-C14	-2.81	1.17	1.23
59	A	3237	ERY	C19-C16	2.78	1.58	1.52
59	A	3237	ERY	O2-C13	-2.74	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	A	3237	ERY	C2-C1	2.73	1.57	1.51
59	A	3237	ERY	O9-C22	2.66	1.48	1.41
59	A	3237	ERY	C2-C3	-2.53	1.49	1.55
59	A	3237	ERY	C23-C24	-2.48	1.48	1.53
60	a	1715	SY5	O02-C14	-2.40	1.18	1.23
59	A	3237	ERY	O12-C11	-2.38	1.38	1.42
60	a	1715	SY5	C15-N07	-2.25	1.45	1.48
59	A	3237	ERY	O11-C9	-2.23	1.18	1.21
59	A	3237	ERY	C7-C8	2.19	1.57	1.54
59	A	3237	ERY	C25-C24	-2.10	1.49	1.53
60	a	1715	SY5	O01-C11	-2.05	1.37	1.43
59	A	3237	ERY	C10-C11	2.02	1.57	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	A	3237	ERY	O5-C16-C15	-16.62	86.33	112.96
59	A	3237	ERY	O13-C12-C13	-15.12	82.97	107.28
59	A	3237	ERY	O5-C16-C19	-13.80	87.92	110.92
59	A	3237	ERY	O5-C16-C17	-13.51	83.79	103.81
59	A	3237	ERY	O13-C12-C11	-12.88	82.92	108.90
59	A	3237	ERY	O10-C6-C32	-12.10	80.59	108.47
59	A	3237	ERY	O13-C12-C35	-10.79	85.48	107.78
59	A	3237	ERY	O3-C3-C4	10.02	120.29	108.22
59	A	3237	ERY	O10-C6-C7	-9.60	83.66	108.40
59	A	3237	ERY	O10-C6-C5	-9.07	90.39	107.59
59	A	3237	ERY	C15-C16-C17	8.42	122.75	107.67
59	A	3237	ERY	O7-C5-C4	-6.21	102.25	111.54
59	A	3237	ERY	C13-C12-C11	6.16	120.45	108.28
59	A	3237	ERY	C32-C6-C5	5.56	119.89	110.12
59	A	3237	ERY	C32-C6-C7	5.44	120.30	111.09
59	A	3237	ERY	C35-C12-C13	5.13	118.53	111.31
59	A	3237	ERY	C34-C10-C11	-5.08	108.06	114.38
59	A	3237	ERY	C13-O2-C1	-4.82	109.61	118.18
60	a	1715	SY5	C16-N07-N06	4.36	113.23	109.12
59	A	3237	ERY	C19-C16-C15	4.35	118.25	110.49
60	a	1714	SY5	C16-N07-N06	4.03	112.92	109.12
59	A	3237	ERY	C12-C11-C10	-3.89	111.56	116.43
59	A	3237	ERY	C7-C6-C5	3.54	117.40	110.48
60	a	1714	SY5	C15-N07-N06	3.41	114.47	109.50
60	a	1715	SY5	C14-N06-N07	3.32	123.60	120.29
60	a	1714	SY5	O02-C14-C12	-3.14	116.90	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	A	3237	ERY	C19-C16-C17	3.08	117.54	111.24
59	A	3237	ERY	C14-O3-C3	2.91	120.54	114.66
59	A	3237	ERY	O3-C3-C2	-2.91	106.08	111.14
59	A	3237	ERY	C3-C4-C5	2.81	117.24	111.19
59	A	3237	ERY	C36-C13-C12	-2.76	109.97	115.20
59	A	3237	ERY	C35-C12-C11	2.55	117.53	113.05
59	A	3237	ERY	C8-C9-C10	-2.54	114.69	119.10
59	A	3237	ERY	C27-C26-C25	-2.53	109.42	113.40
59	A	3237	ERY	C22-O9-C26	-2.47	109.00	112.91
59	A	3237	ERY	C7-C8-C9	-2.44	109.13	113.32
59	A	3237	ERY	C2-C3-C4	-2.38	106.17	113.05
59	A	3237	ERY	C14-O4-C18	-2.33	107.56	113.84
59	A	3237	ERY	C16-C17-C18	2.22	114.55	111.14
59	A	3237	ERY	O12-C11-C10	-2.18	107.45	110.71
60	a	1714	SY5	C14-N06-N07	2.14	122.42	120.29
59	A	3237	ERY	C11-C10-C9	-2.07	106.21	109.57

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
59	A	3237	ERY	C14
59	A	3237	ERY	C12
59	A	3237	ERY	C6

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	A	3237	ERY	C10-C11-C12-C13
59	A	3237	ERY	C10-C11-C12-C35
59	A	3237	ERY	C10-C11-C12-O13
59	A	3237	ERY	O12-C11-C12-C13
59	A	3237	ERY	O12-C11-C12-C35
59	A	3237	ERY	C35-C12-C13-O2
59	A	3237	ERY	C35-C12-C13-C36
59	A	3237	ERY	O13-C12-C13-C36
59	A	3237	ERY	C4-C3-O3-C14
59	A	3237	ERY	C4-C5-C6-C7
59	A	3237	ERY	C4-C5-C6-C32
59	A	3237	ERY	O7-C5-C6-C7
59	A	3237	ERY	O7-C5-C6-C32
59	A	3237	ERY	C32-C6-C7-C8
59	A	3237	ERY	C6-C7-C8-C9

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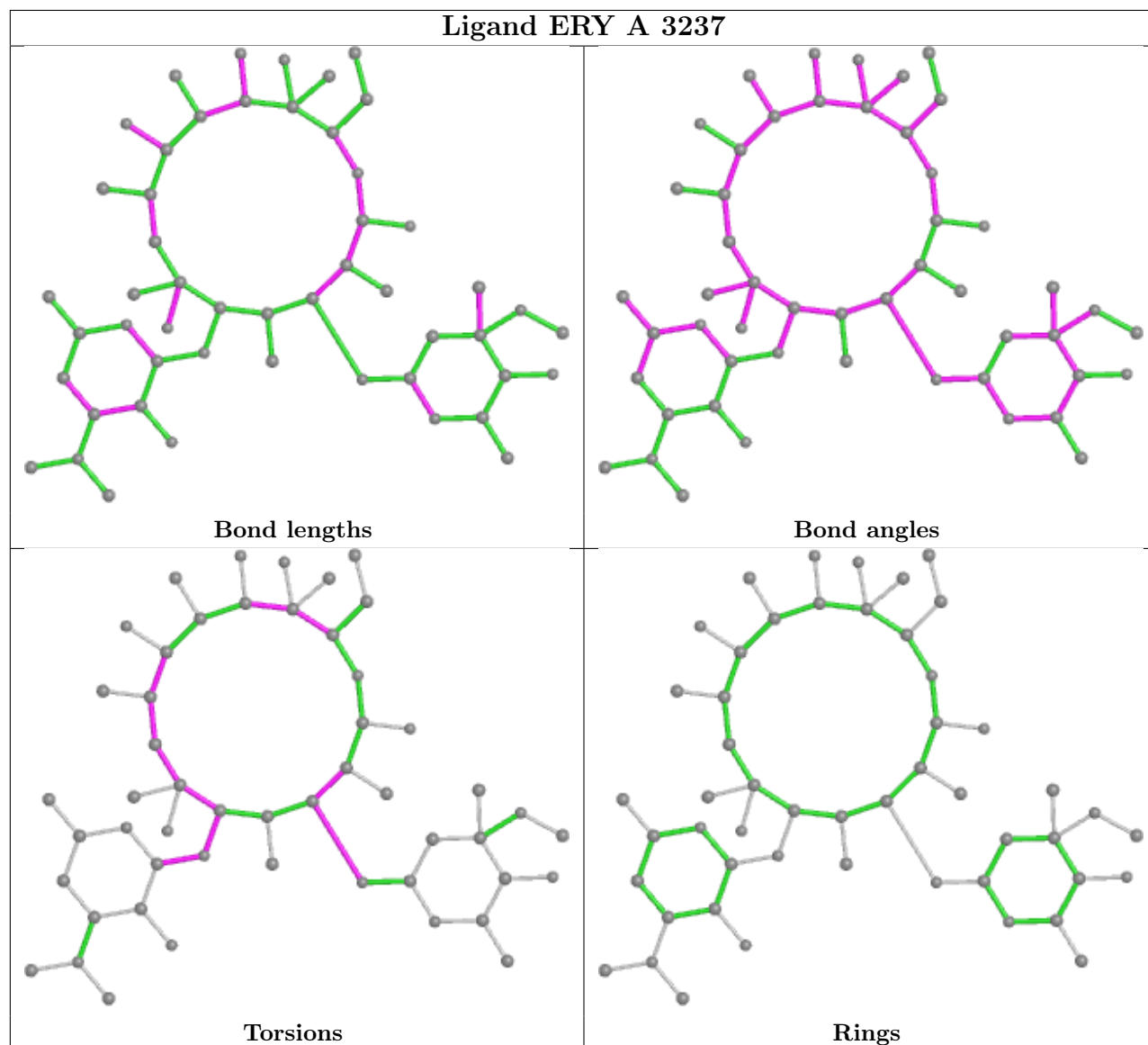
Mol	Chain	Res	Type	Atoms
59	A	3237	ERY	C6-C7-C8-C33
59	A	3237	ERY	C7-C8-C9-C10
59	A	3237	ERY	C7-C8-C9-O11
60	a	1714	SY5	C09-C10-C11-O01
60	a	1714	SY5	C10-C11-C13-N08
60	a	1714	SY5	O01-C11-C13-N08
60	a	1714	SY5	C11-C13-N08-C18
60	a	1714	SY5	N07-C15-C17-O03
60	a	1714	SY5	N07-C15-C17-O04
60	a	1714	SY5	C17-C15-N07-N06
60	a	1714	SY5	C14-N06-N07-C15
60	a	1714	SY5	C14-N06-N07-C16
60	a	1715	SY5	C18-C19-C20-N21
60	a	1715	SY5	C14-N06-N07-C16
60	a	1714	SY5	N08-C18-C19-C20
59	A	3237	ERY	O9-C22-O7-C5
59	A	3237	ERY	C4-C5-O7-C22
59	A	3237	ERY	O10-C6-C7-C8
59	A	3237	ERY	O12-C11-C12-O13
60	a	1715	SY5	N07-C15-C17-O03
60	a	1715	SY5	N07-C15-C17-O04
59	A	3237	ERY	C6-C5-O7-C22
60	a	1715	SY5	C14-N06-N07-C15
60	a	1715	SY5	C11-C13-N08-C18
60	a	1714	SY5	N05-C09-C12-C14
60	a	1714	SY5	C09-C10-C11-C13
60	a	1714	SY5	C10-C09-C12-C14
60	a	1714	SY5	C19-C18-N08-C13
60	a	1715	SY5	C19-C18-N08-C13
60	a	1714	SY5	C17-C15-N07-C16
59	A	3237	ERY	C30-C2-C3-C4
60	a	1715	SY5	C09-C12-C14-N06
60	a	1715	SY5	C09-C12-C14-O02
59	A	3237	ERY	C33-C8-C9-C10

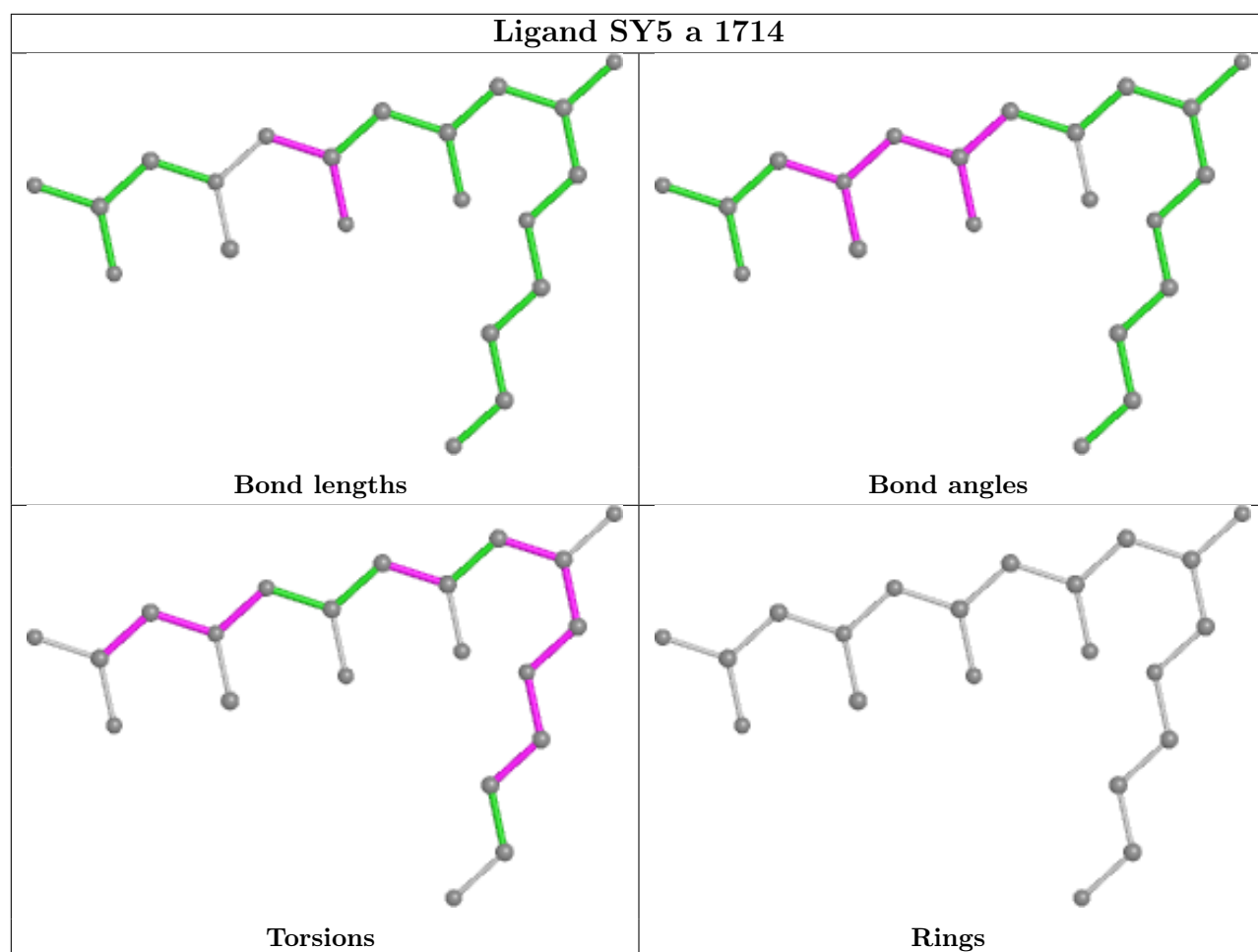
There are no ring outliers.

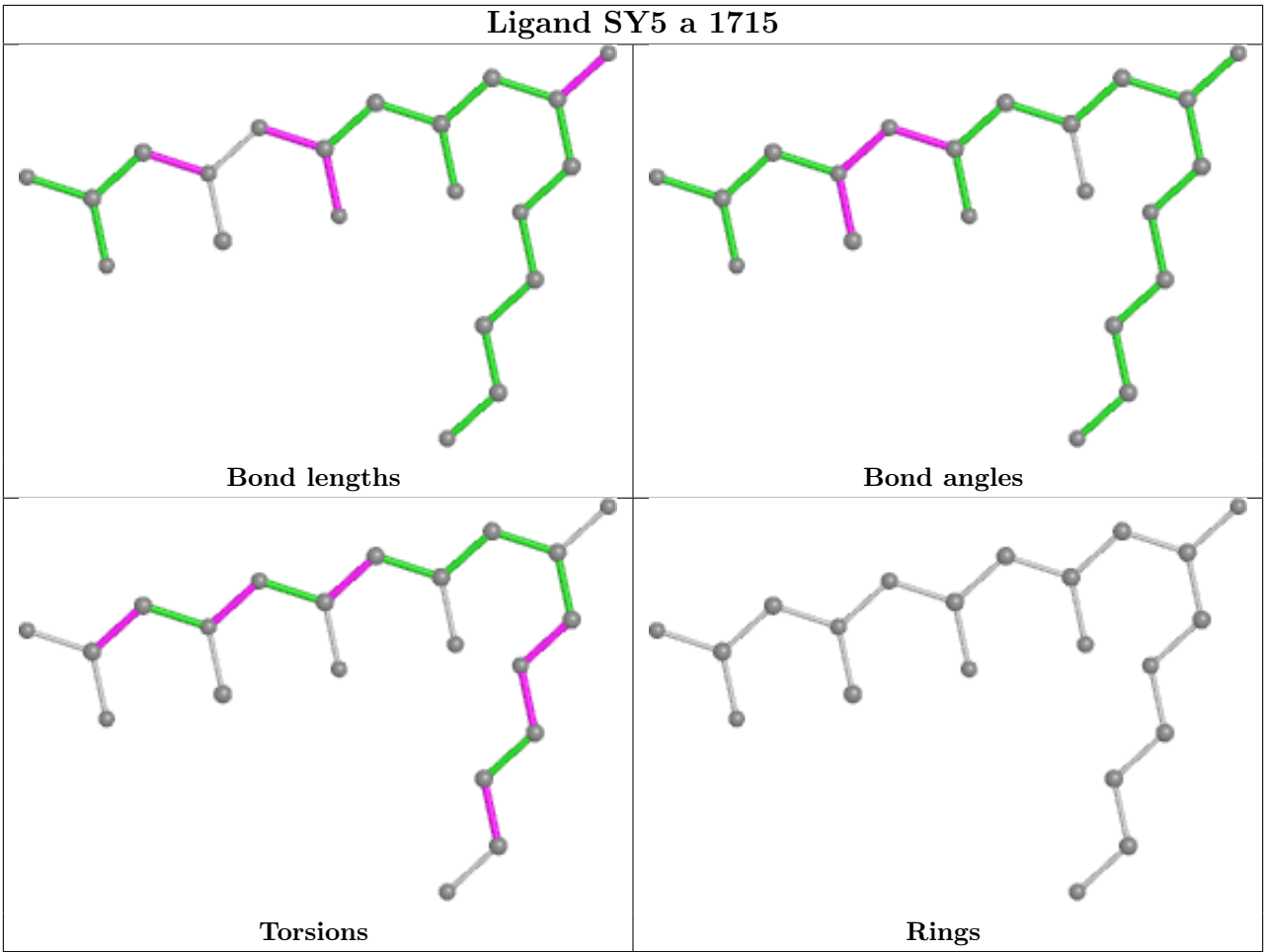
No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
56	9	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	885:C	O3'	892:A	P	13.17
1	9	15:G	O3'	16:C	P	3.32
1	A	2099:U	O3'	2100:G	P	3.04



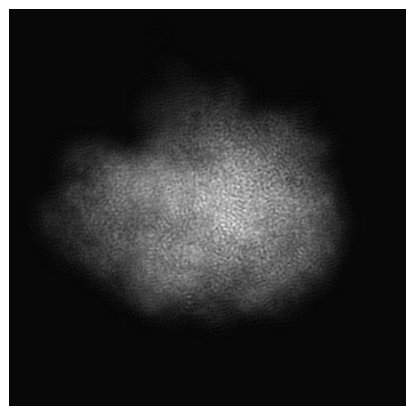
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12035. These allow visual inspection of the internal detail of the map and identification of artifacts.

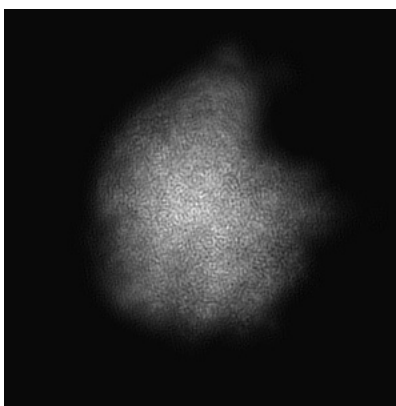
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

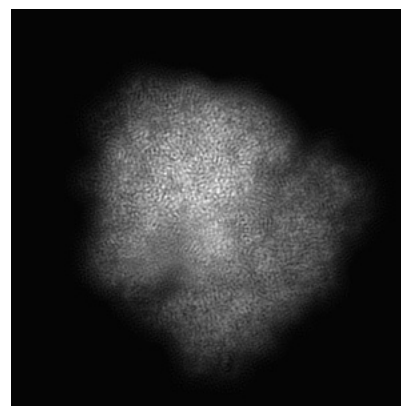
#### 6.1.1 Primary map



X

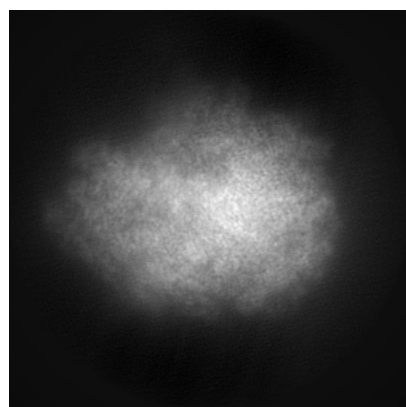


Y

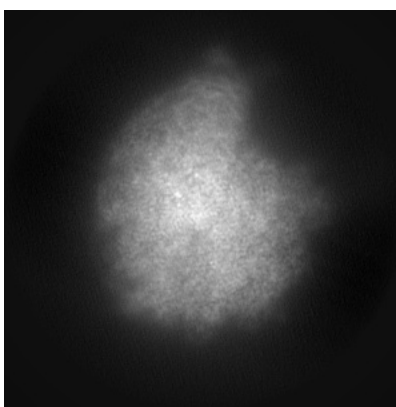


Z

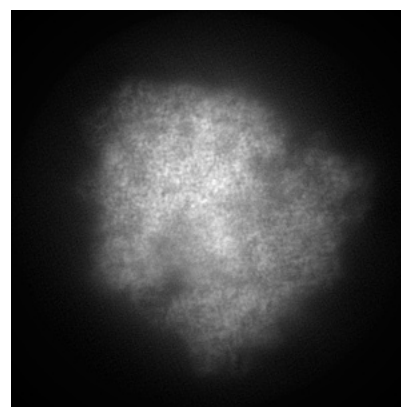
#### 6.1.2 Raw map



X



Y

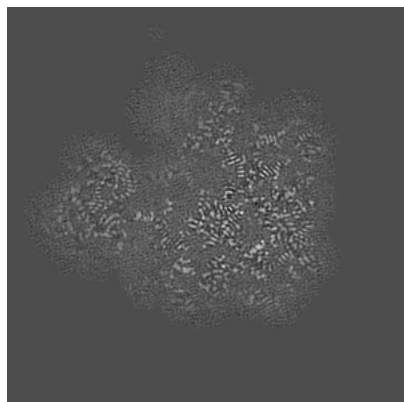


Z

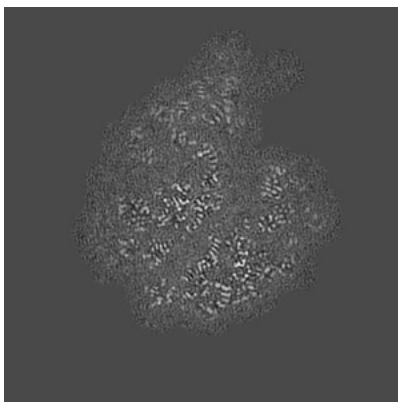
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

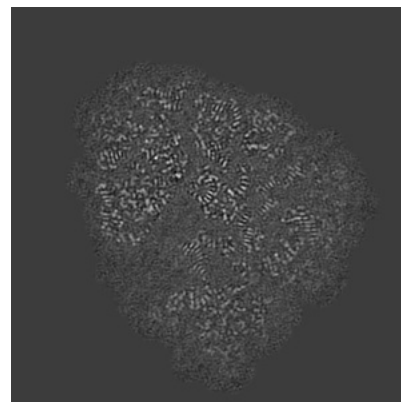
### 6.2.1 Primary map



X Index: 180

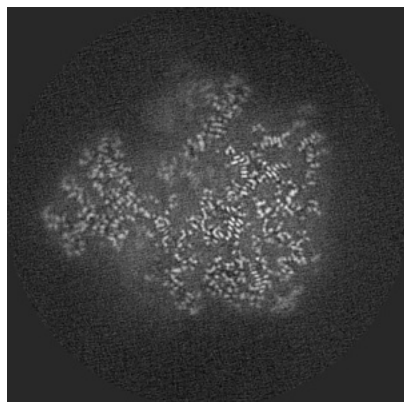


Y Index: 180

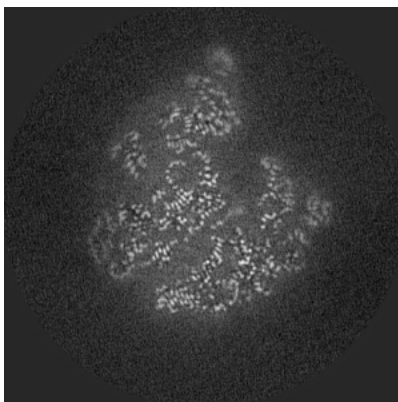


Z Index: 180

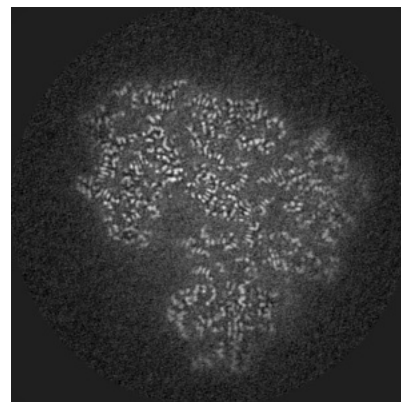
### 6.2.2 Raw map



X Index: 180



Y Index: 180

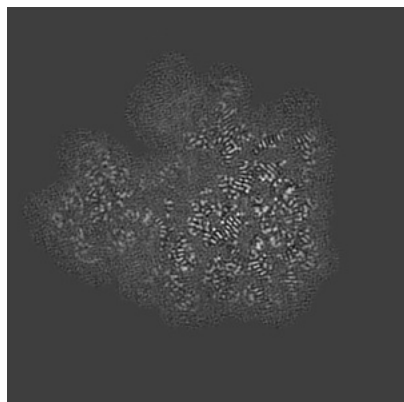


Z Index: 180

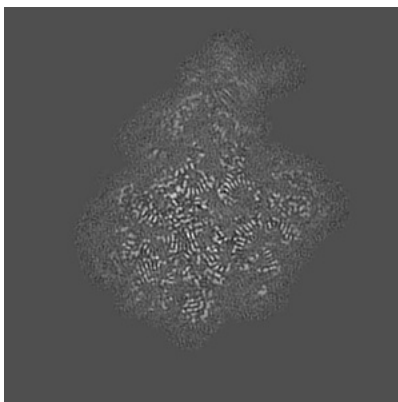
The images above show central slices of the map in three orthogonal directions.

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

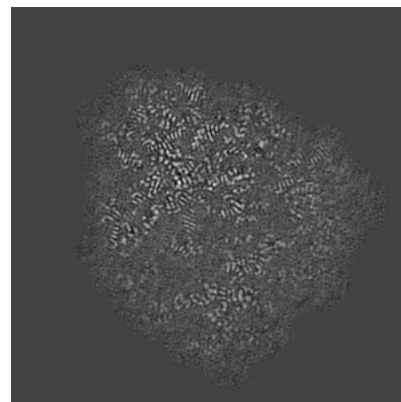
### 6.3.1 Primary map



X Index: 184

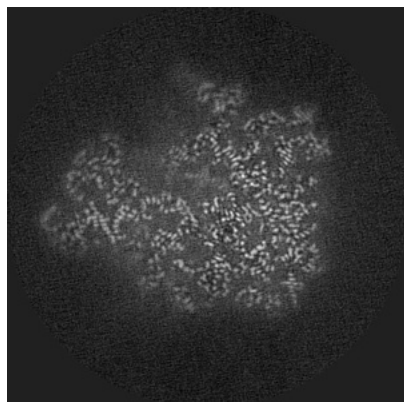


Y Index: 192

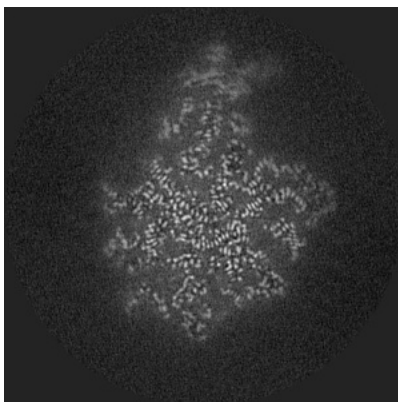


Z Index: 189

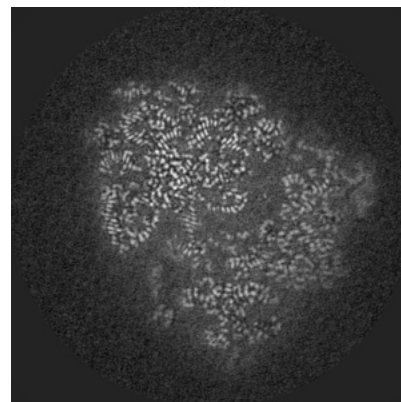
### 6.3.2 Raw map



X Index: 174



Y Index: 206

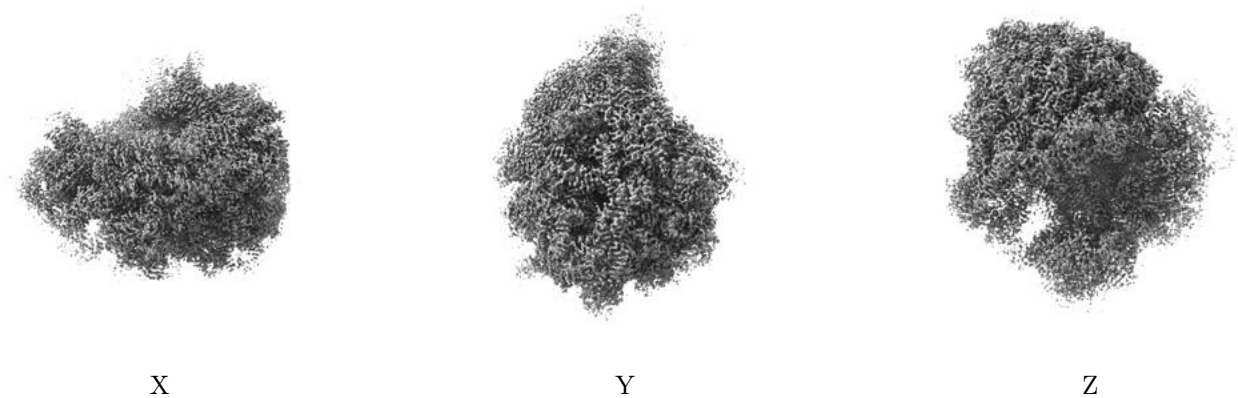


Z Index: 190

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

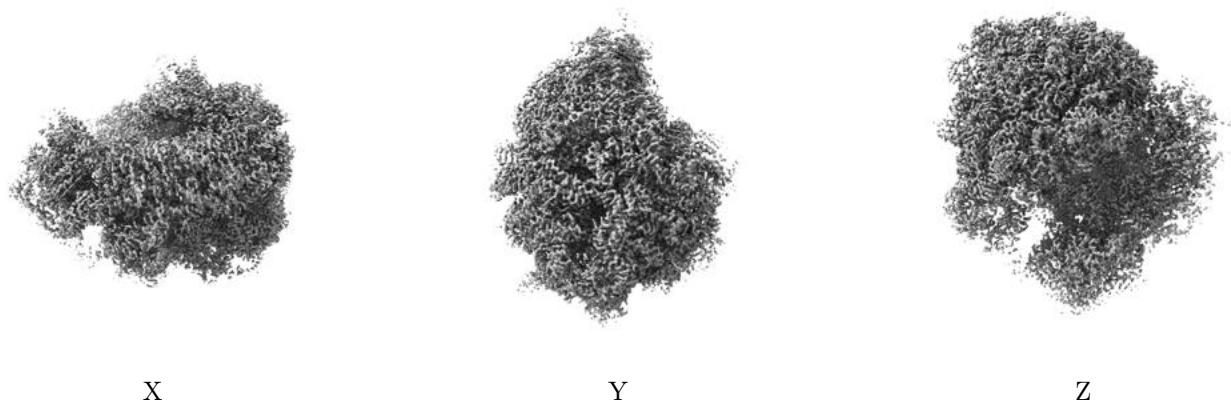
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.083. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

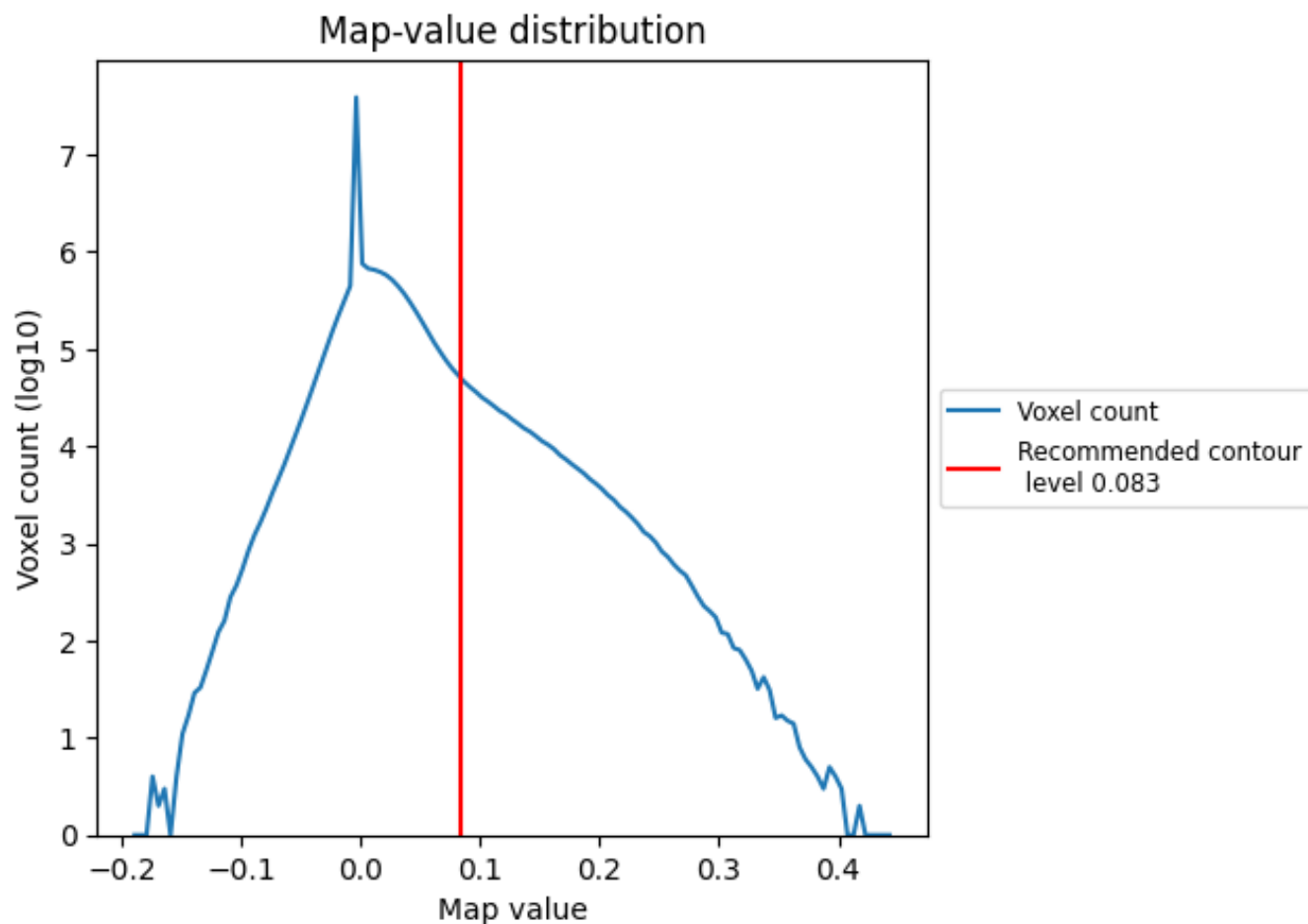
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

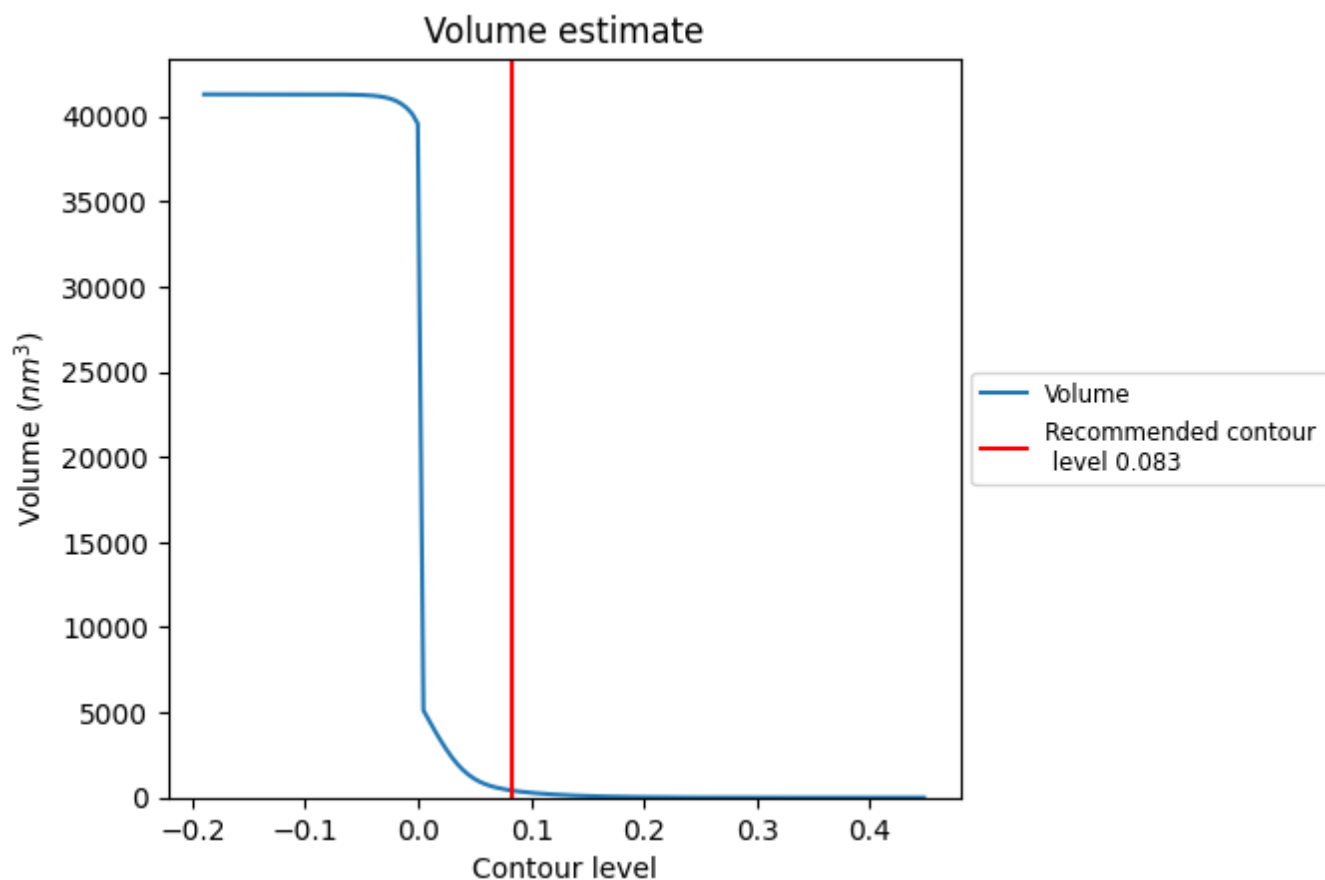
This section contains the results of statistical analysis of the map.

### 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.

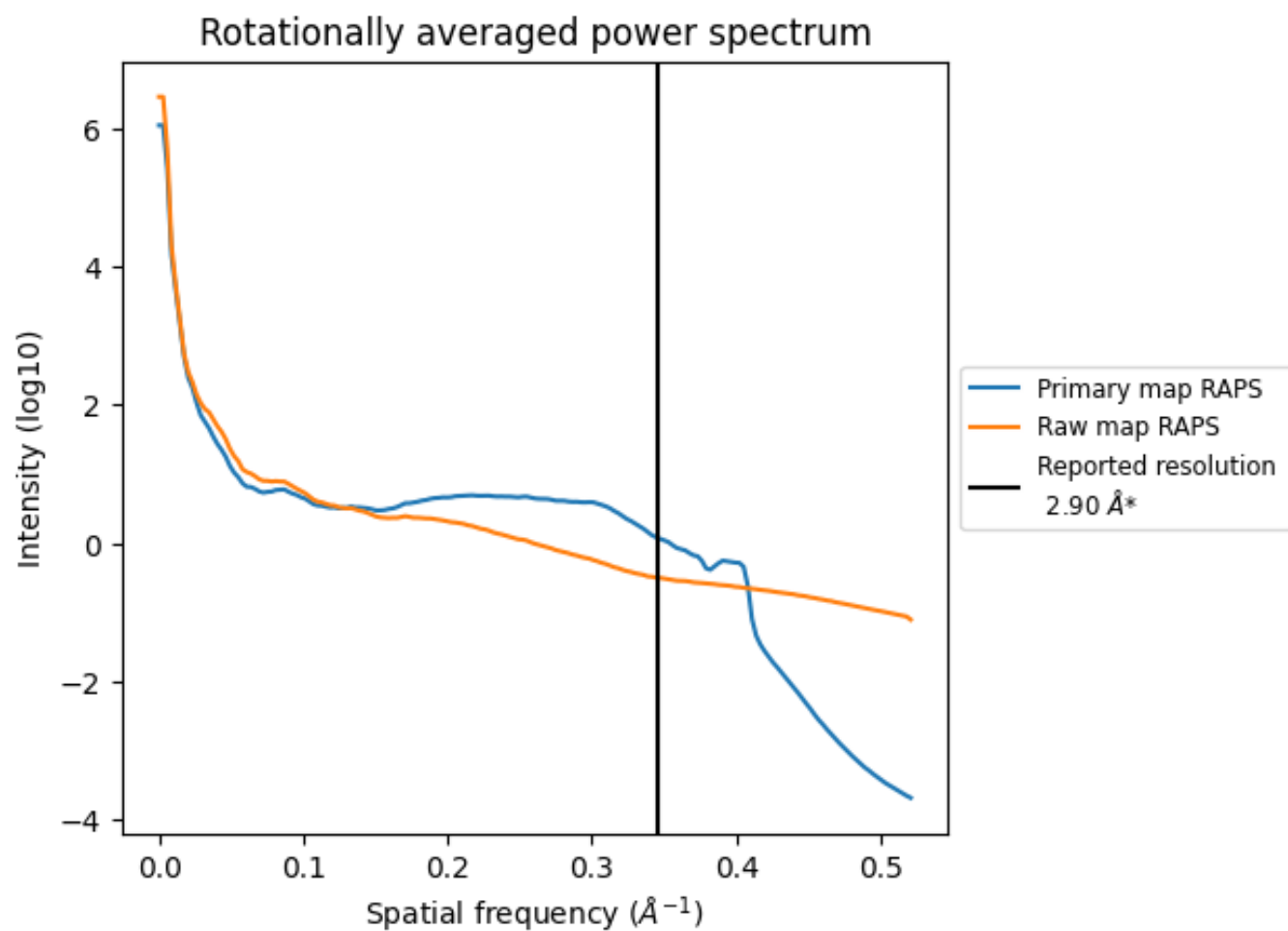
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 414 nm<sup>3</sup>; this corresponds to an approximate mass of 374 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 ⓘ

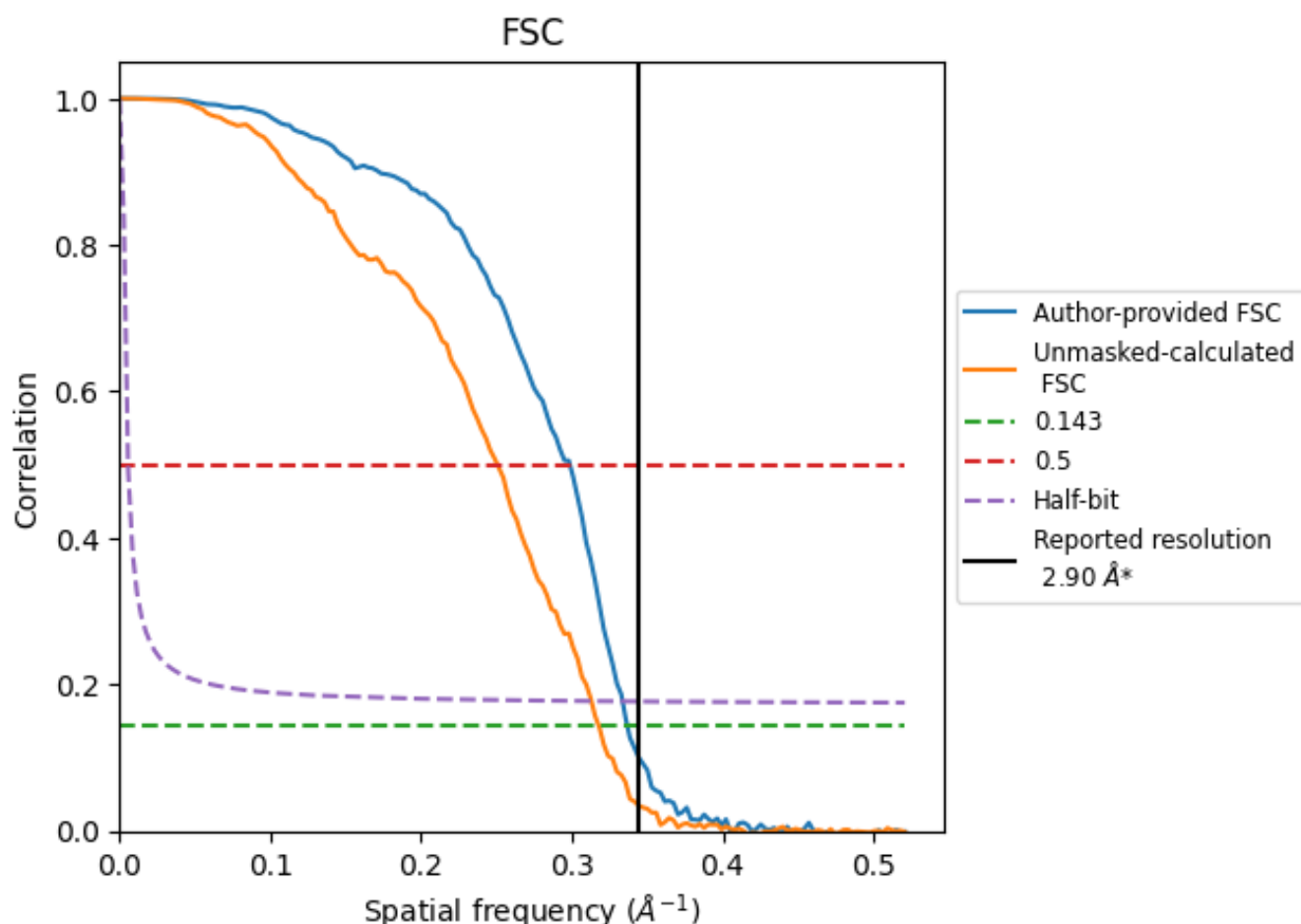


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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 0.345 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

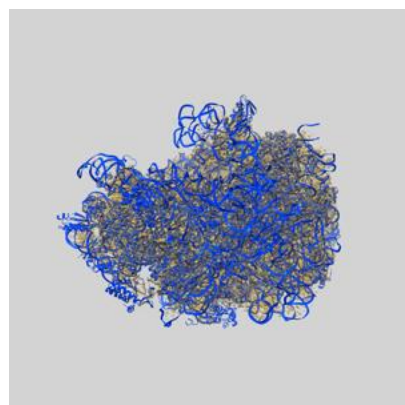
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.97	3.35	3.00
Unmasked-calculated*	3.15	3.99	3.20

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

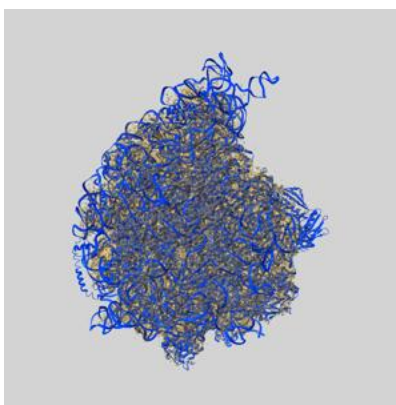
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12035 and PDB model 7B5K. Per-residue inclusion information can be found in section 3 on page 17.

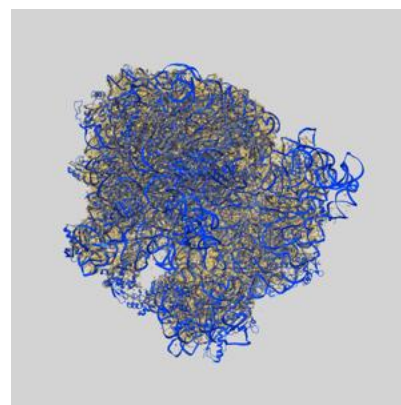
### 9.1 Map-model overlay [i](#)



X



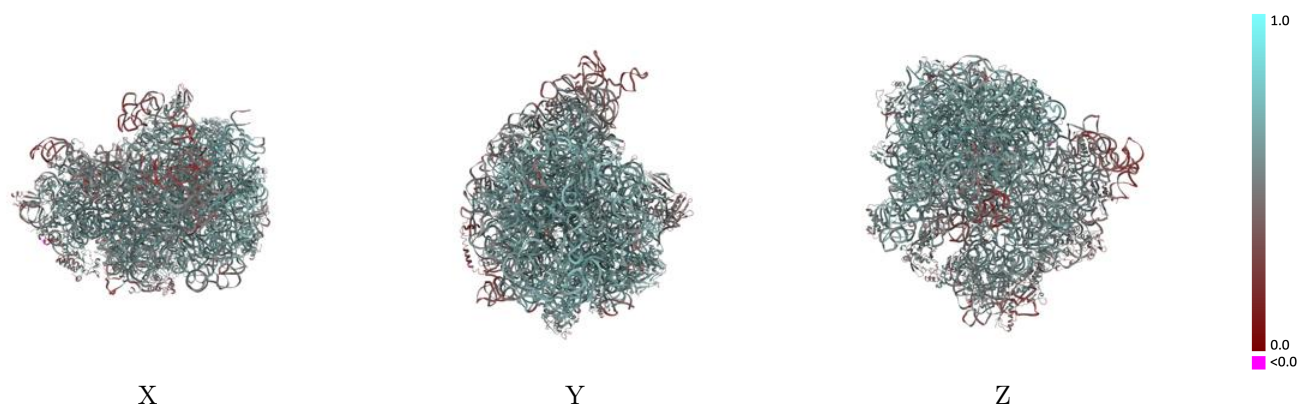
Y



Z

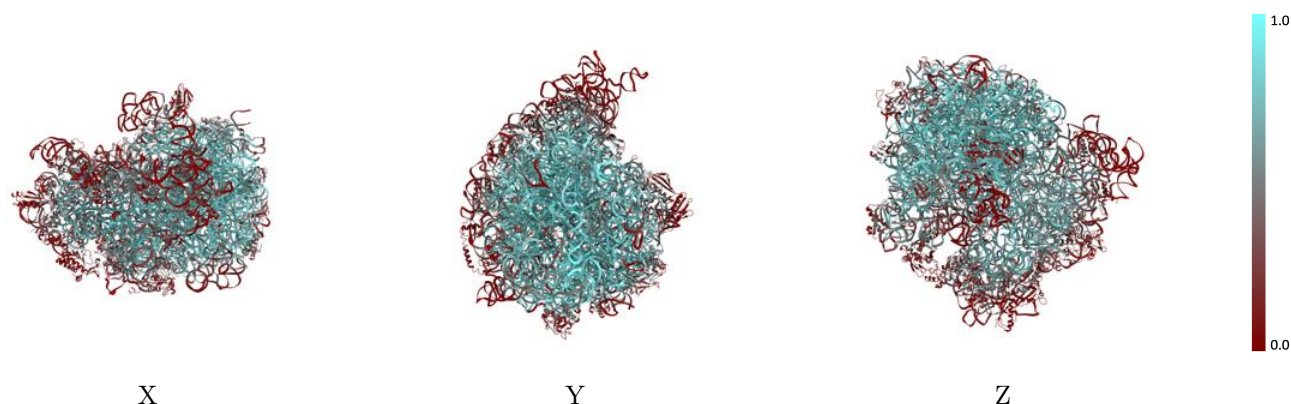
The images above show the 3D surface view of the map at the recommended contour level 0.083 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



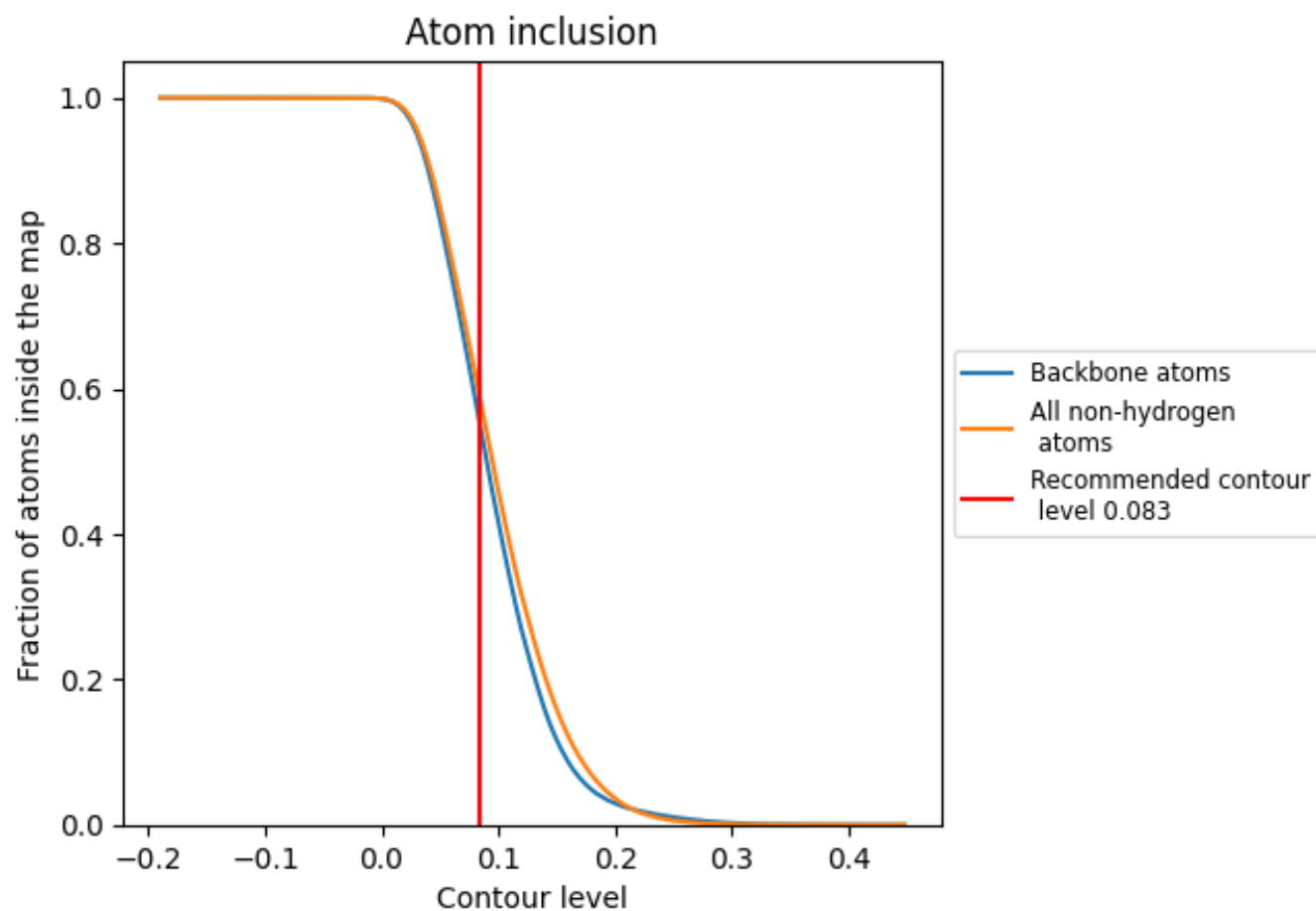
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.083).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 60% 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 (0.083) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5960	 0.5640
0	 0.6410	 0.5850
1	 0.5246	 0.5620
2	 0.8451	 0.6300
3	 0.8269	 0.6300
4	 0.6267	 0.5820
5	 0.0352	 0.3610
6	 0.6838	 0.5710
9	 0.1269	 0.3960
A	 0.7499	 0.6040
B	 0.5381	 0.5680
C	 0.7572	 0.6180
D	 0.6422	 0.6090
E	 0.4760	 0.5630
F	 0.2542	 0.4950
G	 0.1627	 0.4600
H	 0.0685	 0.3640
J	 0.6227	 0.6010
K	 0.6547	 0.5990
L	 0.6025	 0.5940
M	 0.6731	 0.6040
N	 0.7244	 0.6220
O	 0.3536	 0.5420
P	 0.5968	 0.5830
Q	 0.6975	 0.6250
R	 0.4718	 0.5830
S	 0.6340	 0.5950
T	 0.4903	 0.5600
U	 0.2986	 0.5240
V	 0.3686	 0.5510
W	 0.7252	 0.6110
X	 0.6772	 0.5980
Y	 0.2863	 0.5160
Z	 0.5858	 0.5950
a	 0.5659	 0.5410



*Continued on next page...*

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Chain	Atom inclusion	Q-score
b	 0.1376	 0.4570
c	 0.3954	 0.5330
d	 0.1214	 0.4240
e	 0.5205	 0.5530
f	 0.2509	 0.4790
g	 0.2247	 0.4580
h	 0.4281	 0.5410
i	 0.2707	 0.4900
j	 0.2156	 0.4580
k	 0.4490	 0.5370
l	 0.4865	 0.5470
m	 0.2664	 0.4900
n	 0.3581	 0.5070
o	 0.3928	 0.5290
p	 0.2026	 0.4530
q	 0.3259	 0.5000
r	 0.4587	 0.5490
s	 0.2578	 0.4950
t	 0.2153	 0.4670
u	 0.2590	 0.4810
v	 0.8571	 0.6460
x	 0.6355	 0.5640
z	 0.3650	 0.5020