



## Full wwPDB EM Validation Report ⓘ

Oct 14, 2021 – 10:51 pm BST

PDB ID : 7PJW  
EMDB ID : EMD-13462  
Title : Structure of the 70S-EF-G-GDP-Pi ribosome complex with tRNAs in hybrid state 2 (H2-EF-G-GDP-Pi)  
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.  
Deposited on : 2021-08-24  
Resolution : 4.00 Å (reported)  
Based on initial models : 5LZD, 5J9Z, 4AQY, 6YSS

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

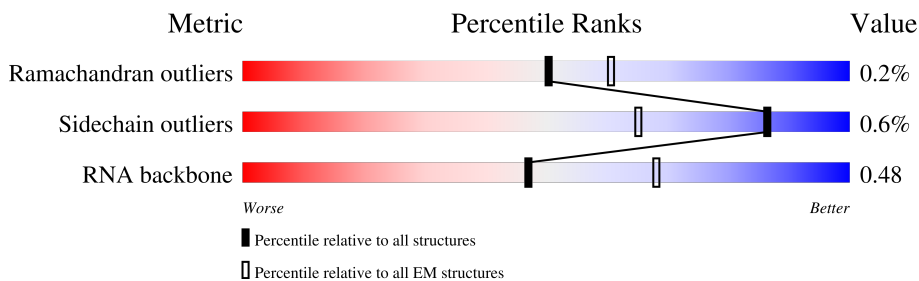
EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 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 4.00 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	0	57	77% (Upper red bar), 98% (Green), 9% (Grey)
2	1	55	73% (Upper red bar), 91% (Green), 9% (Grey)
3	2	46	65% (Upper red bar), 100% (Green)
4	3	65	77% (Upper red bar), 98% (Green), 5% (Grey)
5	4	38	66% (Upper red bar), 100% (Green)
6	5	165	79% (Upper red bar), 79% (Green), 21% (Grey)
7	6	70	94% (Upper red bar), 79% (Green), 16% (Yellow), 6% (Grey)
8	A	2903	29% (Upper red bar), 73% (Green), 26% (Yellow), 5% (Grey)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	B	120	25% 79% 21%
10	C	273	67% 99%
11	D	209	66% 100%
12	E	201	71% 100%
13	F	179	91% 99%
14	G	177	94% 99%
15	H	149	100%
16	I	142	99%
17	J	142	57% 99%
18	K	123	77% 99%
19	L	144	69% 99%
20	M	136	68% 99%
21	N	127	53% 94% 6%
22	O	117	72% 99%
23	P	115	77% 98%
24	Q	118	54% 99%
25	R	103	66% 98%
26	S	110	69% 100%
27	T	100	65% 93% 7%
28	U	104	78% 95%
29	V	94	71% 99%
30	W	85	58% 88% 12%
31	X	78	68% 97%
32	Y	63	83% 98%
33	Z	59	64% 98%


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	a	1542	49% 76% 23%
35	b	240	90% 90% 9%
36	c	233	83% 88% 12%
37	d	206	92% 100%
38	e	167	83% 94% 6%
39	f	135	72% 74% 26%
40	g	179	84% 84% 16%
41	h	130	82% 99%
42	i	130	92% 97%
43	j	103	90% 94% 5%
44	k	129	77% 89% 10%
45	l	124	83% 98%
46	m	118	96% 96%
47	n	102	91% 99%
48	o	89	78% 99%
49	p	82	74% 99%
50	q	84	75% 95% 5%
51	r	75	81% 87% 13%
52	s	92	89% 89% 11%
53	t	87	91% 98%
54	u	71	92% 90% 8%
55	v	77	94% 68% 30%
56	w	76	97% 50% 38% 12%
57	x	704	98% 98%
58	y	2	100% 50% 50%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
59	z	33	 <p>21% 15% 15% 67%</p>

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 152719 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

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

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 57 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	x	703	5444	3429	942	1048	25	0	0

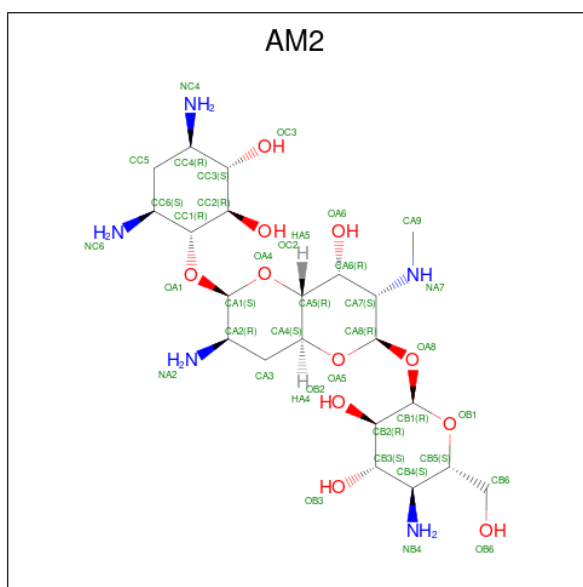
- Molecule 58 is a protein called Dipeptide (FME-PHE).

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

- Molecule 59 is a RNA chain called mRNA.

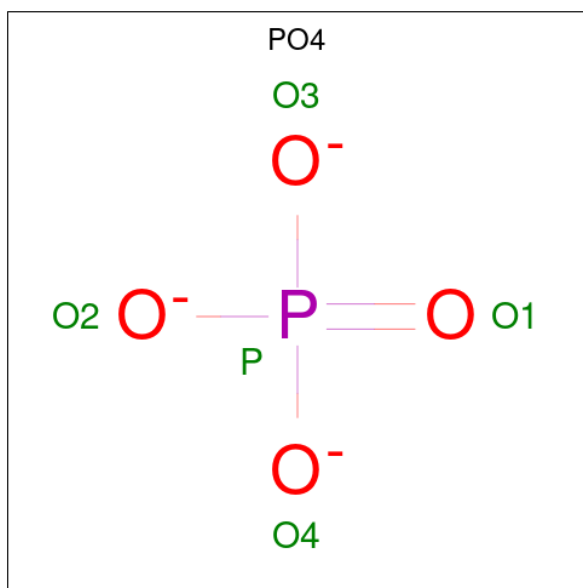
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
59	z	11	230	103	35	81	11	0	0

- Molecule 60 is APRAMYCIN (three-letter code: AM2) (formula: C<sub>21</sub>H<sub>41</sub>N<sub>5</sub>O<sub>11</sub>).



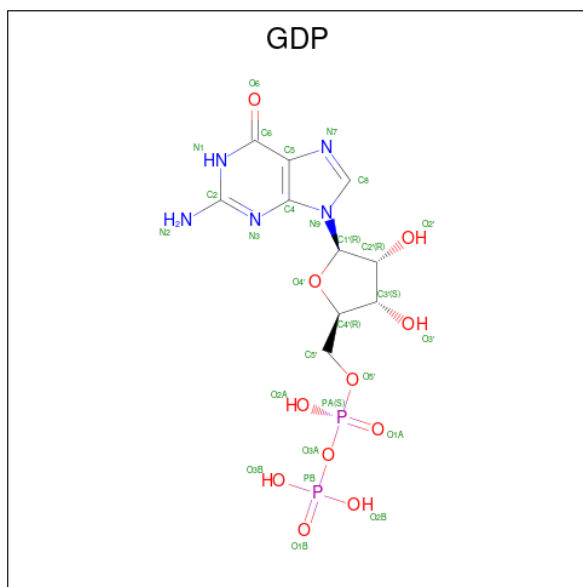
Mol	Chain	Residues	Atoms				AltConf
60	a	1	Total	C	N	O	0
			37	21	5	11	

- Molecule 61 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			AltConf
61	x	1	Total	O	P	0
			5	4	1	

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



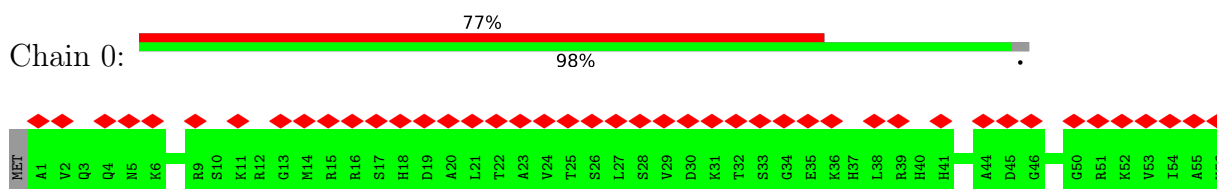
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
62	x	1	28	10	5	11	2	0



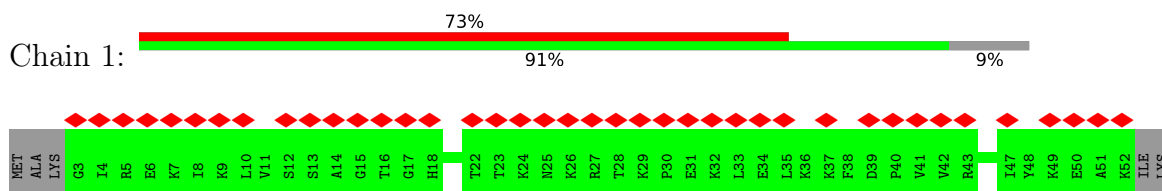
### 3 Residue-property plots [i](#)

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

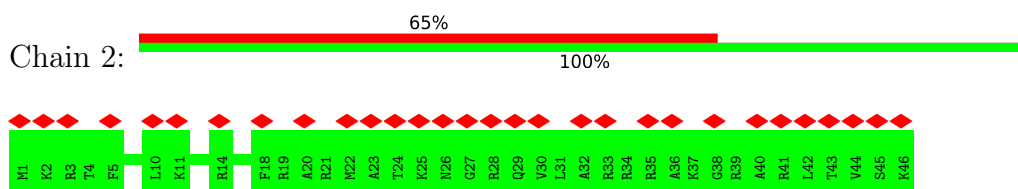
- Molecule 1: 50S ribosomal protein L32



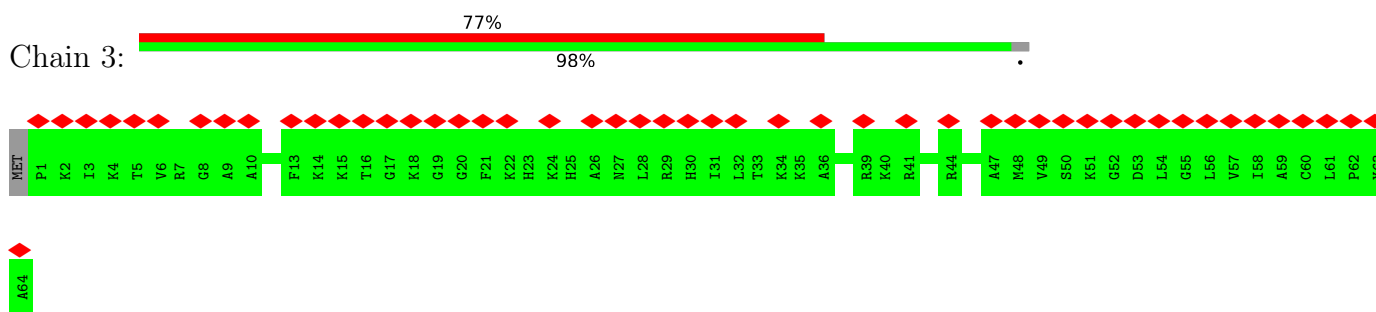
- Molecule 2: 50S ribosomal protein L33



- Molecule 3: 50S ribosomal protein L34

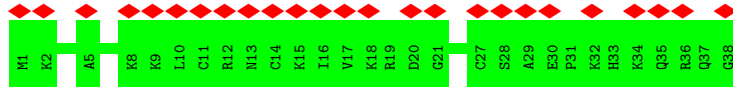


- Molecule 4: 50S ribosomal protein L35

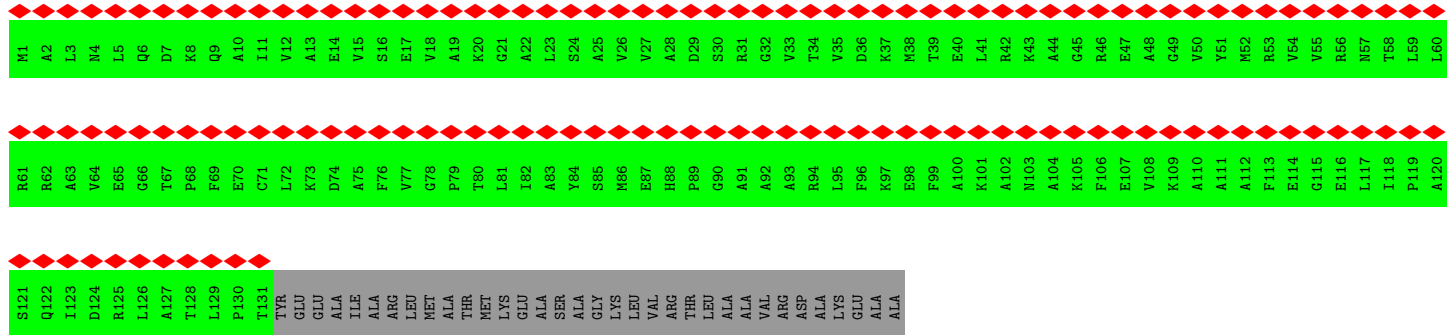
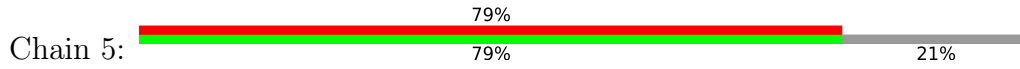


- Molecule 5: 50S ribosomal protein L36

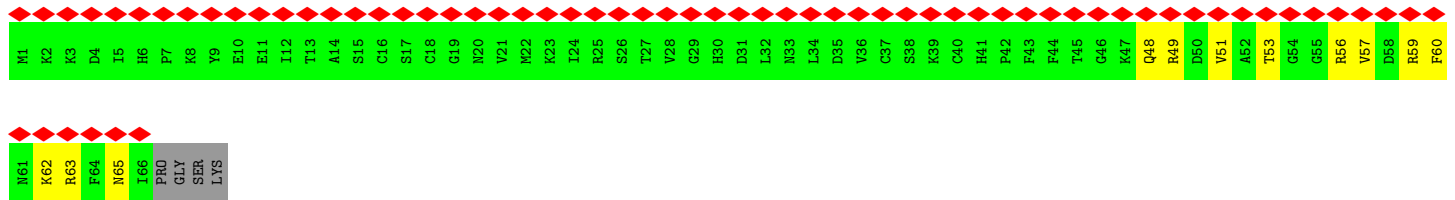
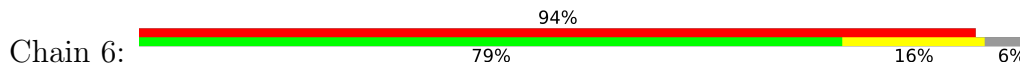




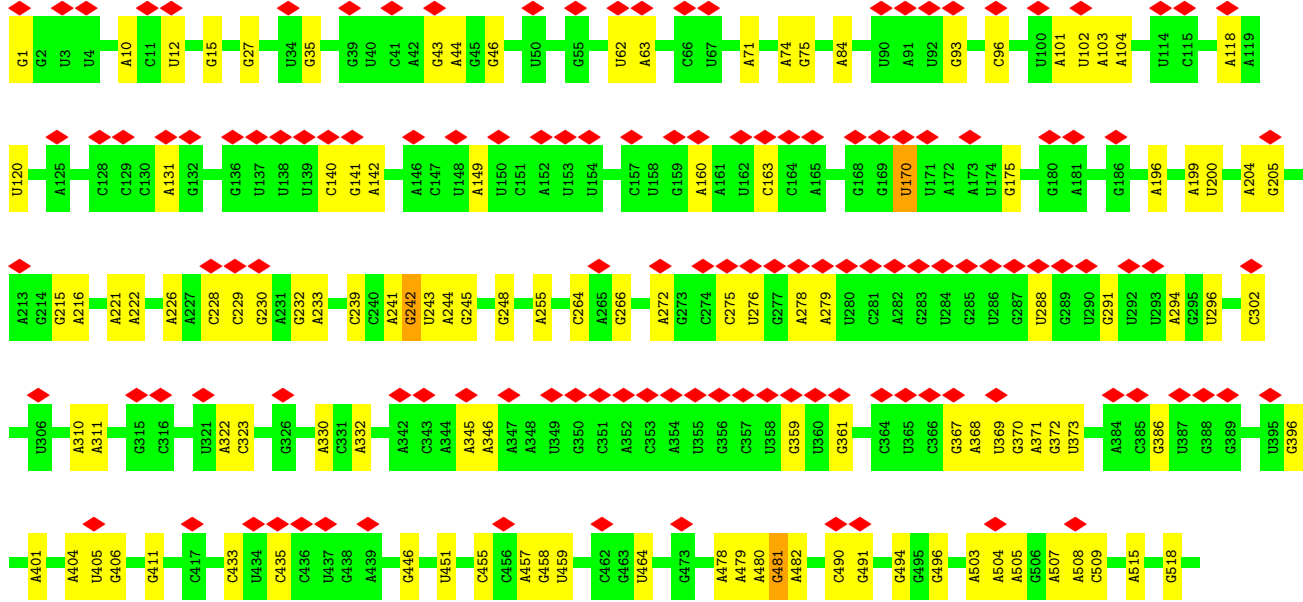
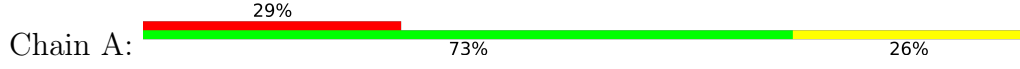
• Molecule 6: 50S ribosomal protein L10

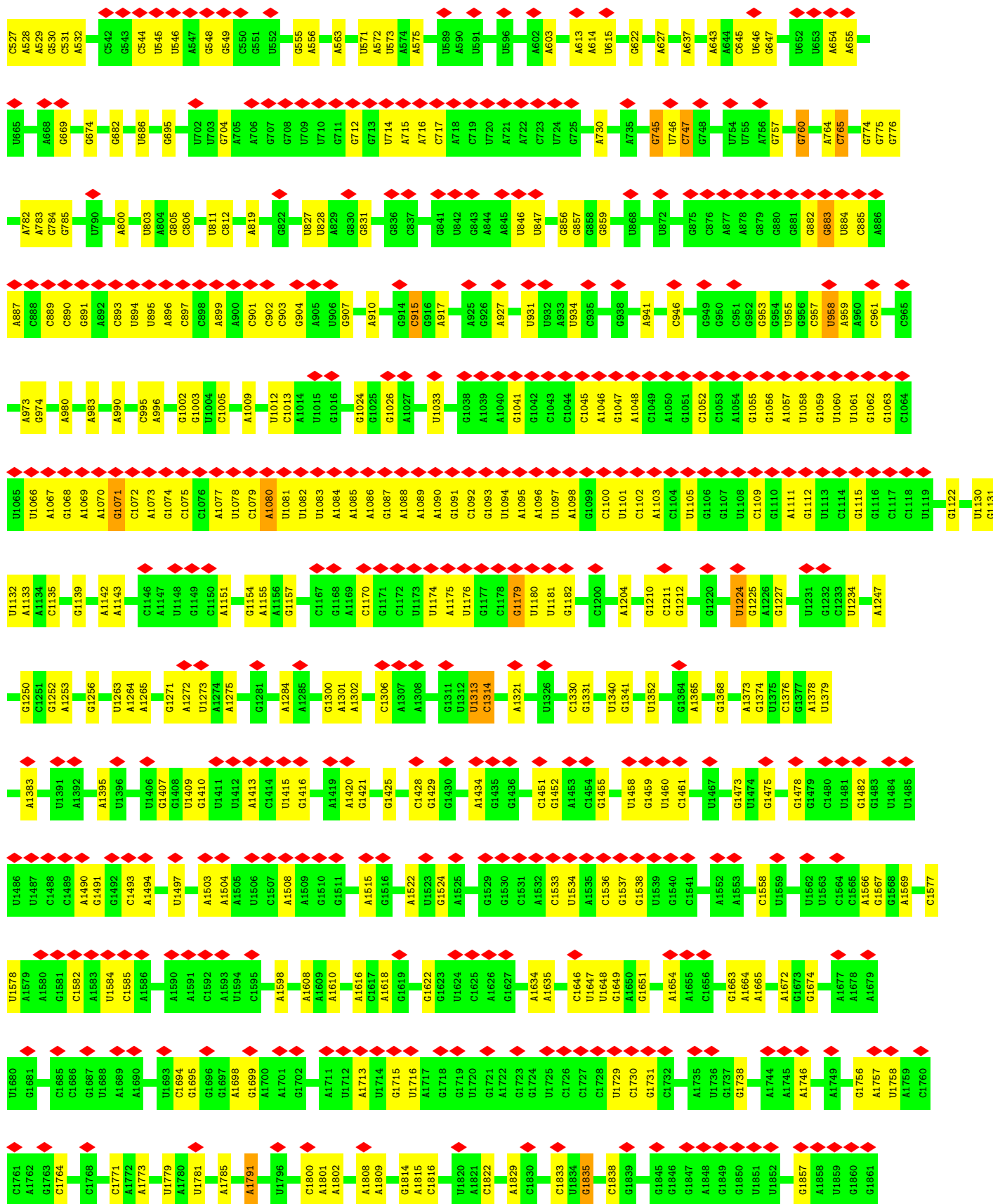


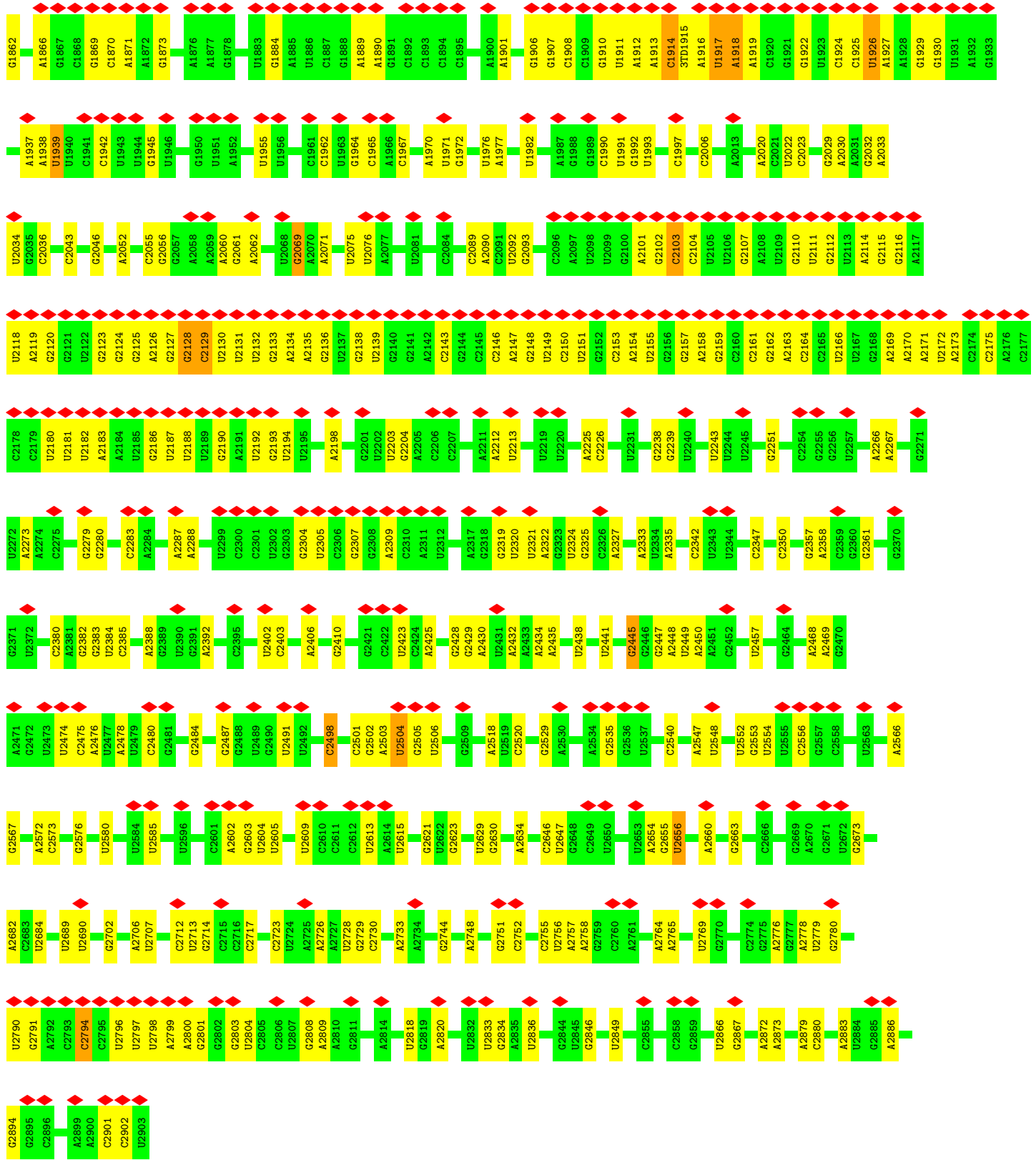
• Molecule 7: 50S ribosomal protein L31



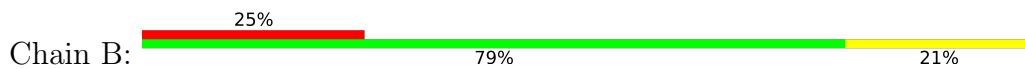
• Molecule 8: 23S ribosomal RNA

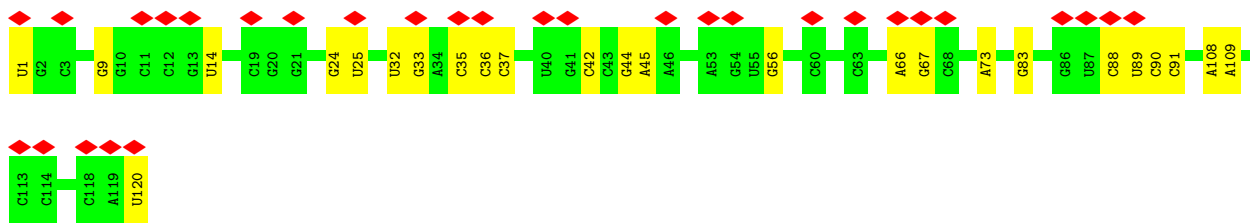






• Molecule 9: 5S ribosomal RNA





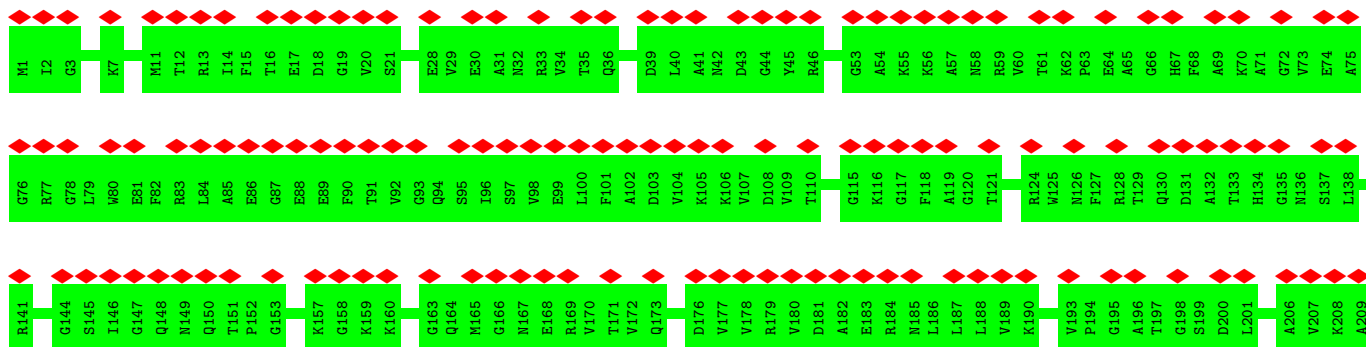
- Molecule 10: 50S ribosomal protein L2

Chain C: 67%  
99%



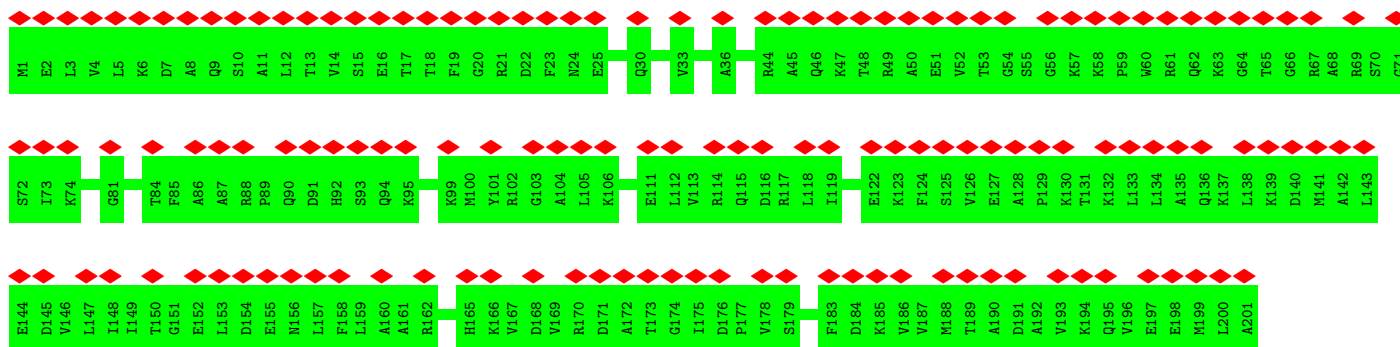
- Molecule 11: 50S ribosomal protein L3

Chain D: 66%  
100%

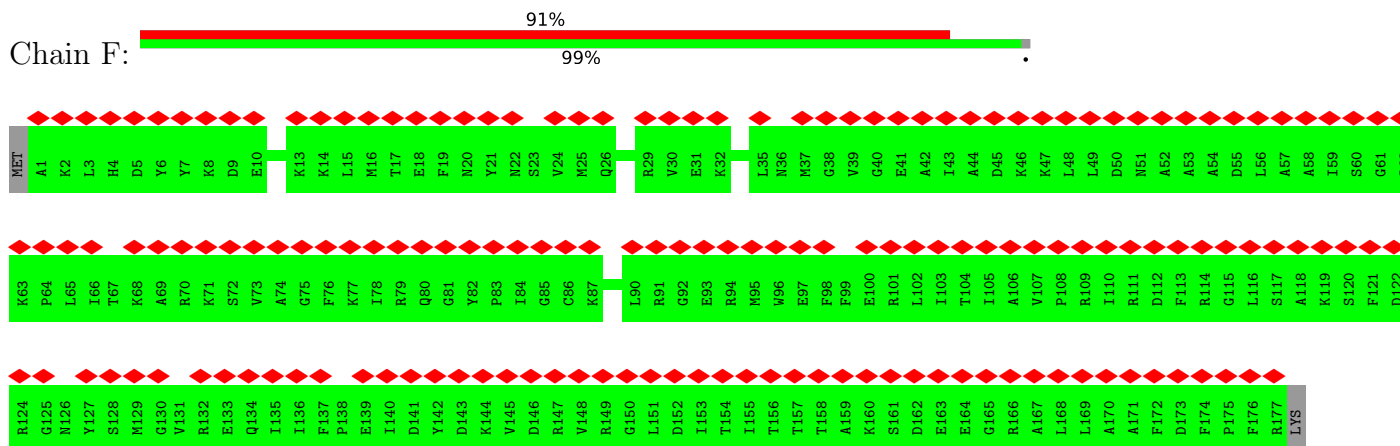


- Molecule 12: 50S ribosomal protein L4

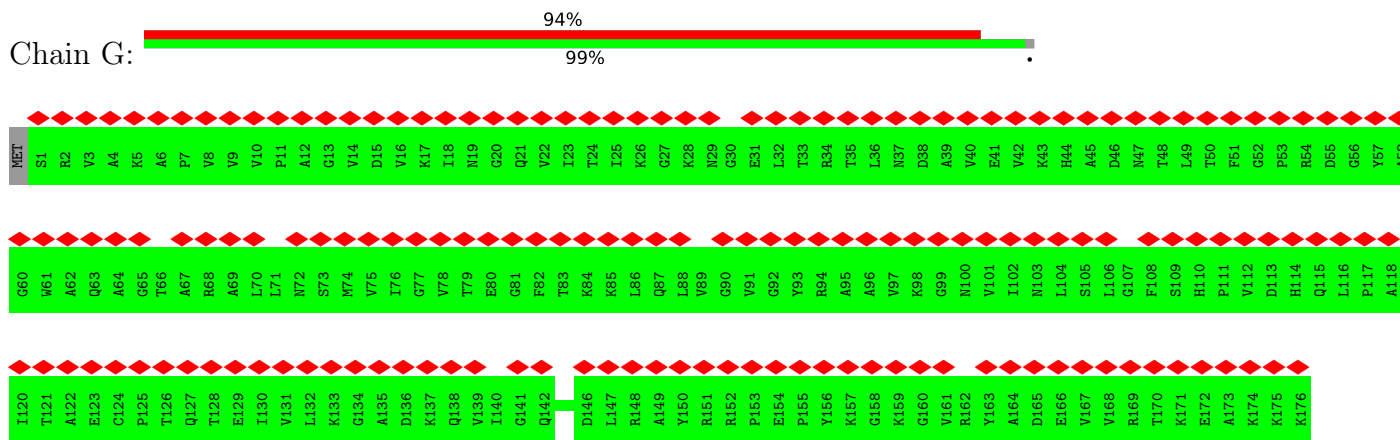
Chain E: 71%  
100%



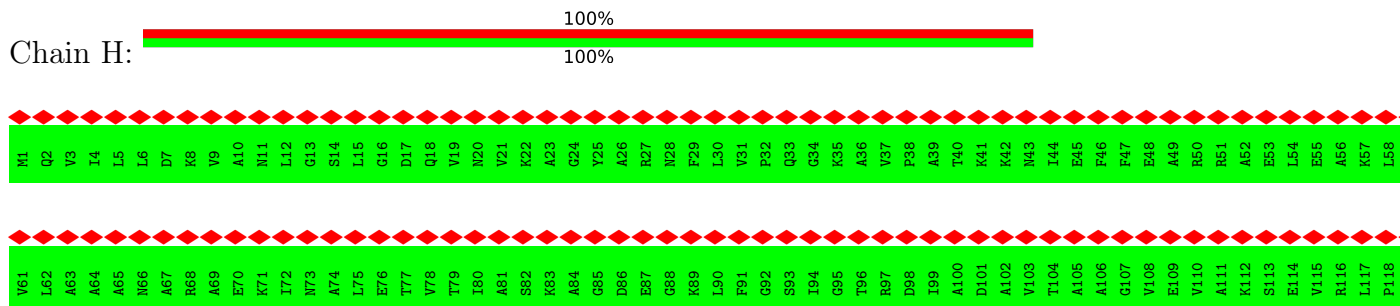
• Molecule 13: 50S ribosomal protein L5

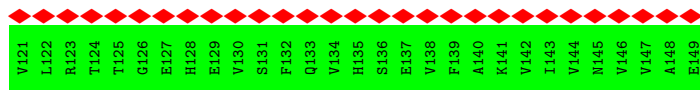


• Molecule 14: 50S ribosomal protein L6

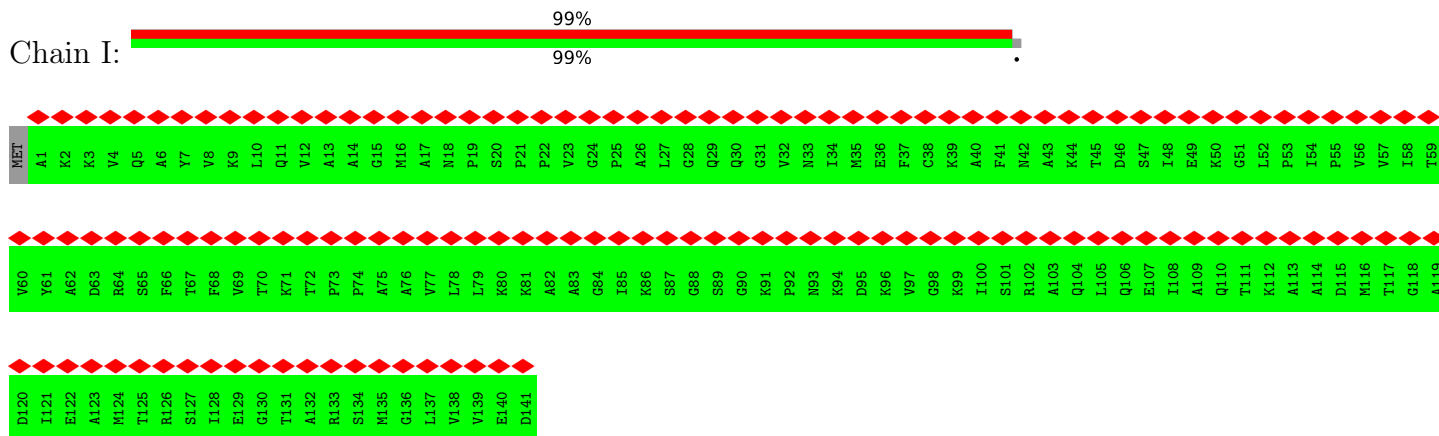


• Molecule 15: 50S ribosomal protein L9

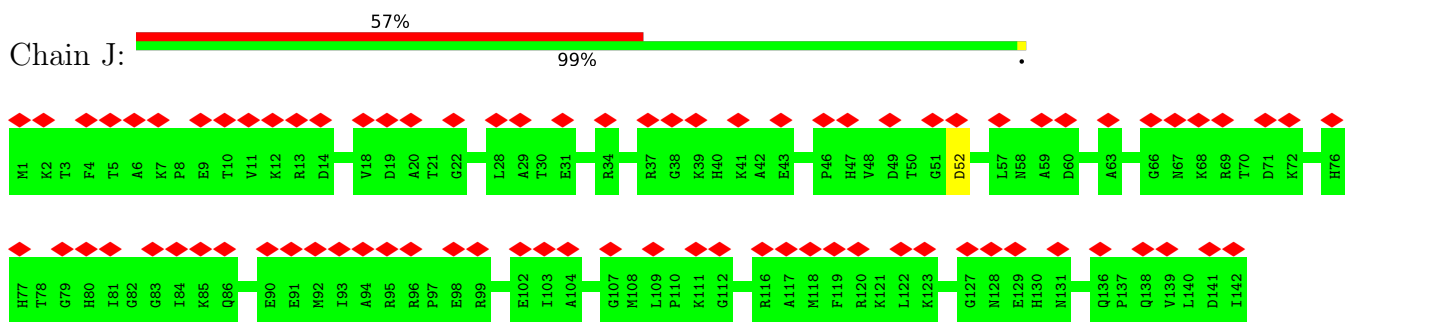




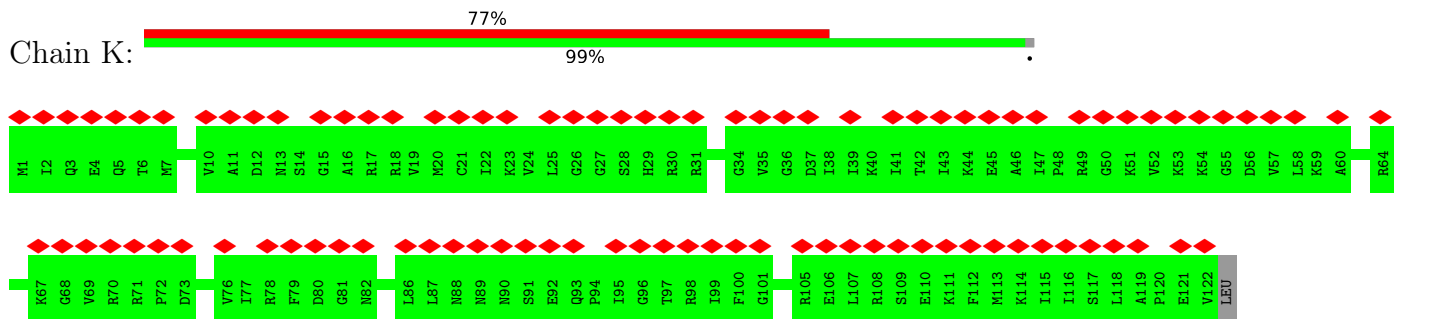
• Molecule 16: 50S ribosomal protein L11



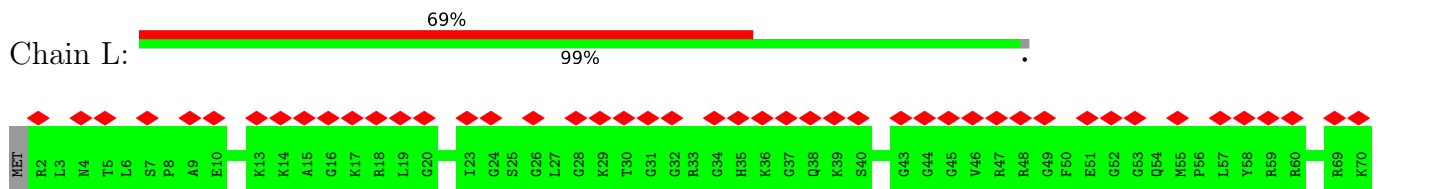
• Molecule 17: 50S ribosomal protein L13

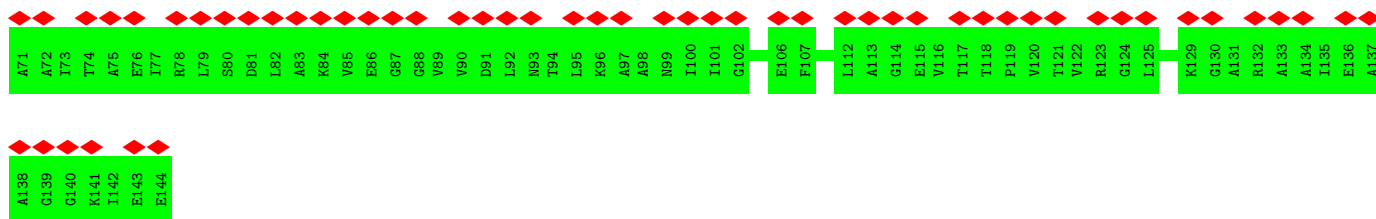


• Molecule 18: 50S ribosomal protein L14

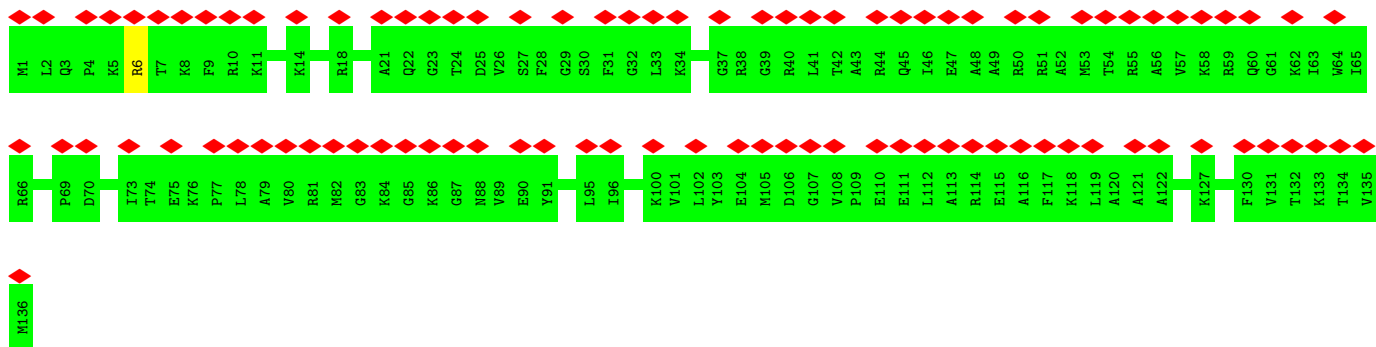


• Molecule 19: 50S ribosomal protein L15

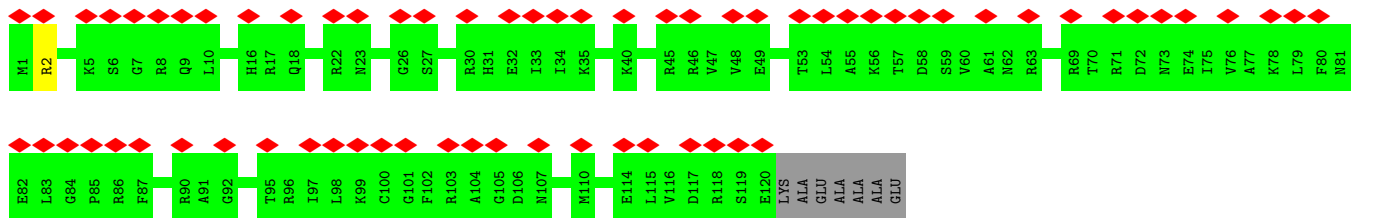
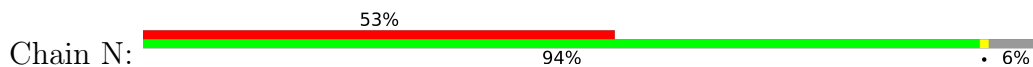




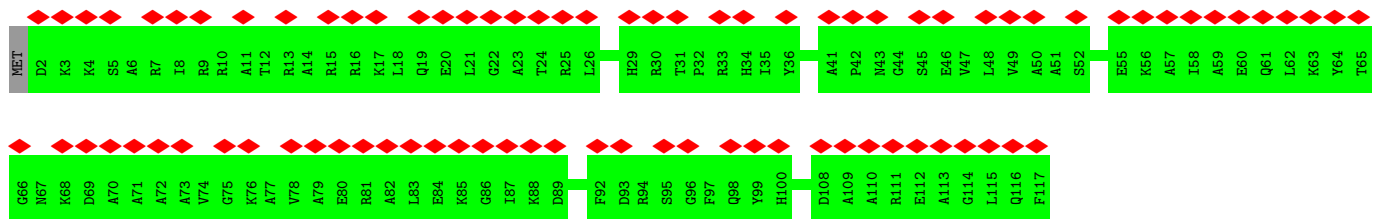
• Molecule 20: 50S ribosomal protein L16



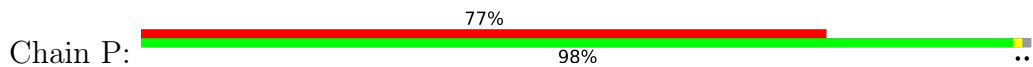
• Molecule 21: 50S ribosomal protein L17



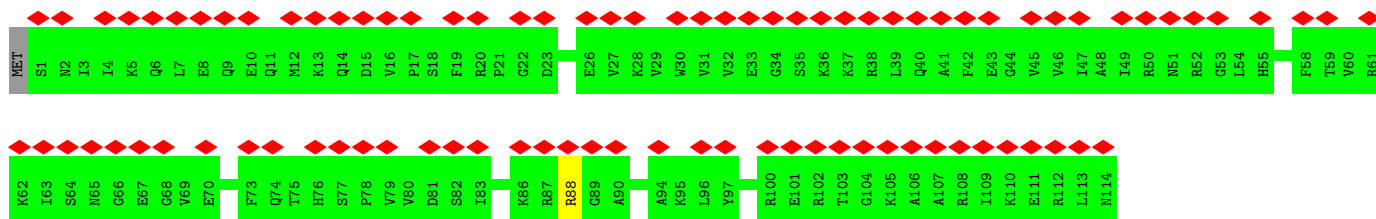
• Molecule 22: 50S ribosomal protein L18



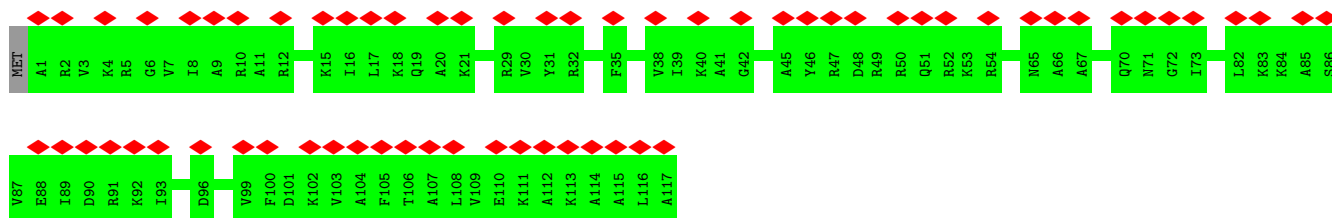
• Molecule 23: 50S ribosomal protein L19



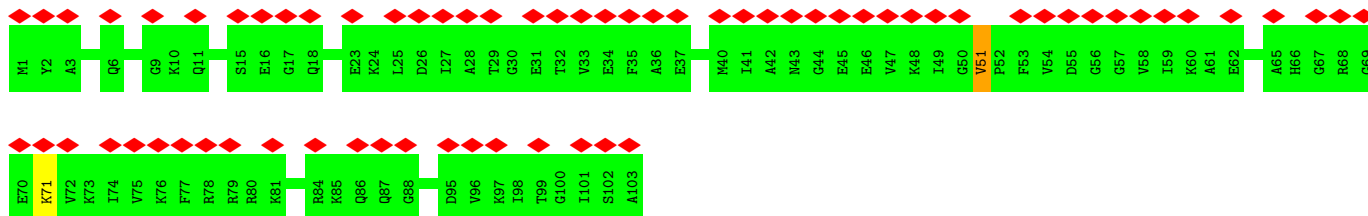




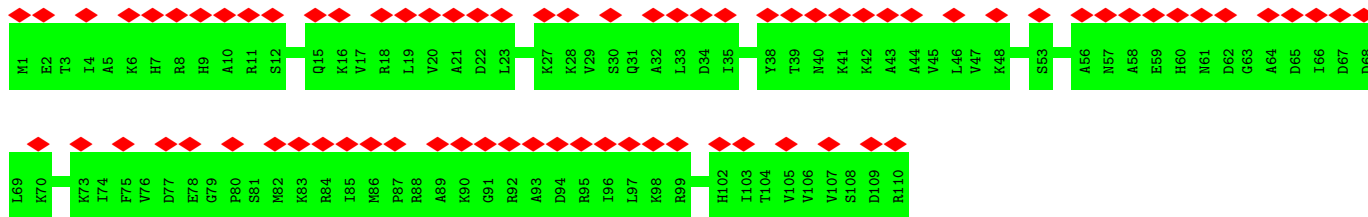
• Molecule 24: 50S ribosomal protein L20



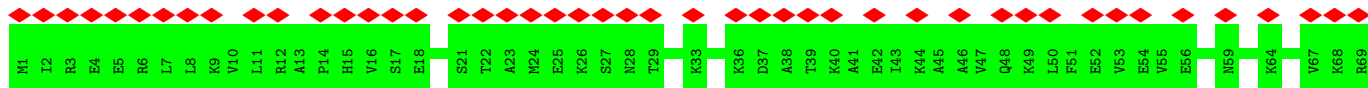
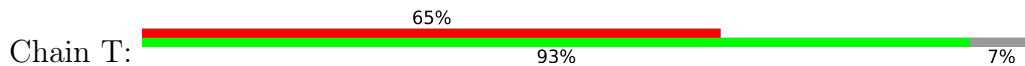
• Molecule 25: 50S ribosomal protein L21

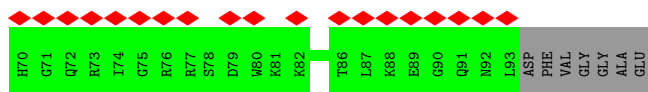


• Molecule 26: 50S ribosomal protein L22

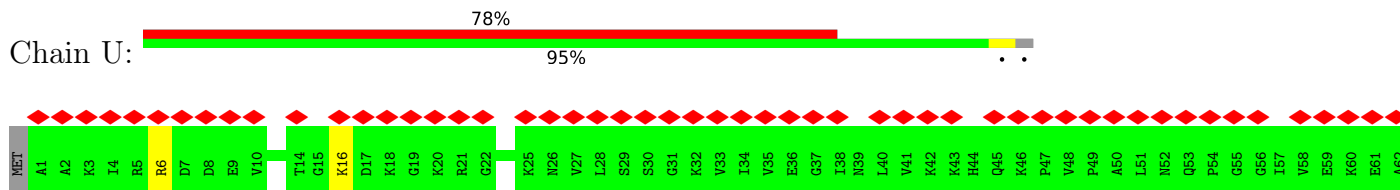


• Molecule 27: 50S ribosomal protein L23

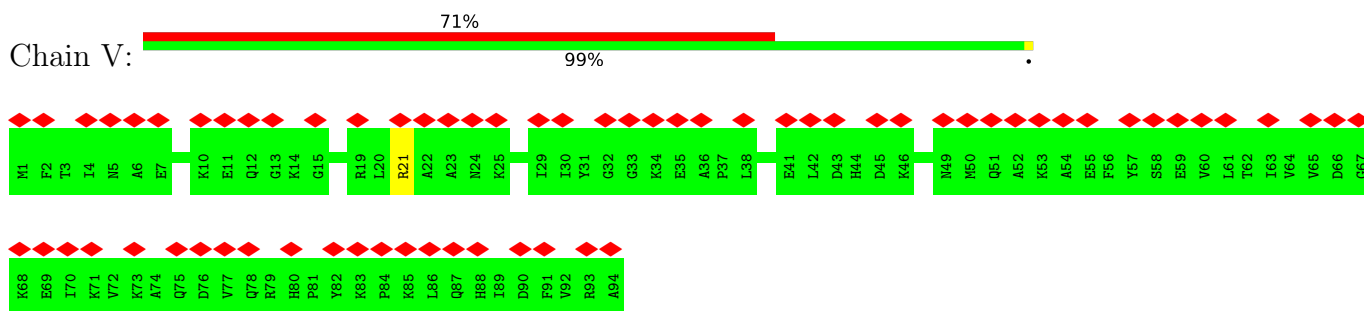




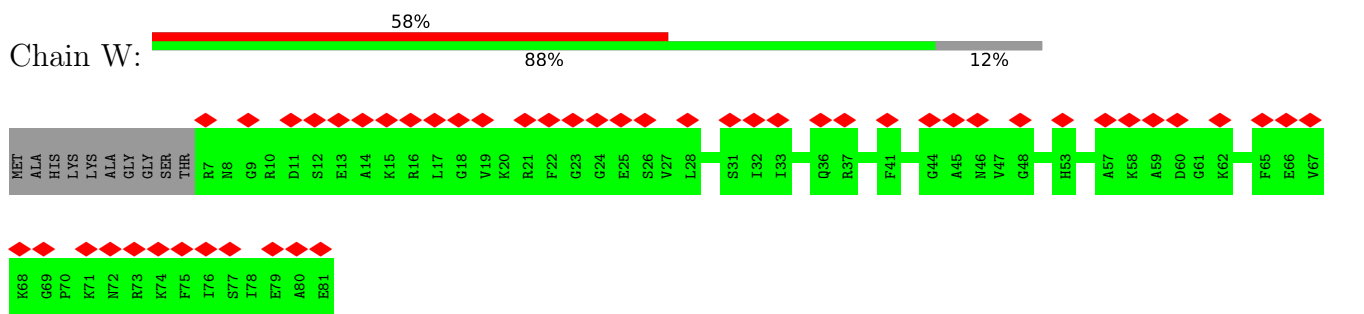
- Molecule 28: 50S ribosomal protein L24



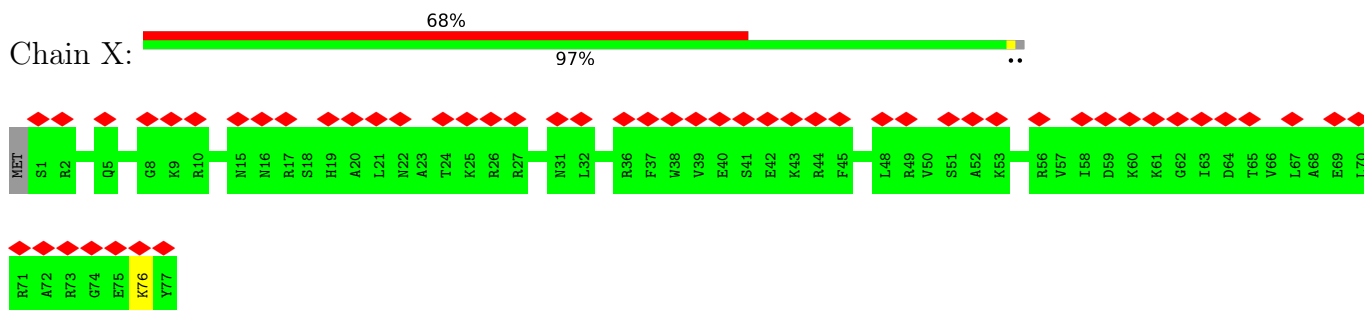
- Molecule 29: 50S ribosomal protein L25



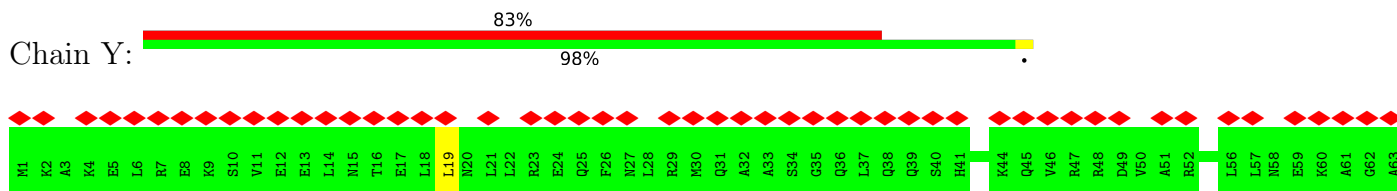
- Molecule 30: 50S ribosomal protein L27



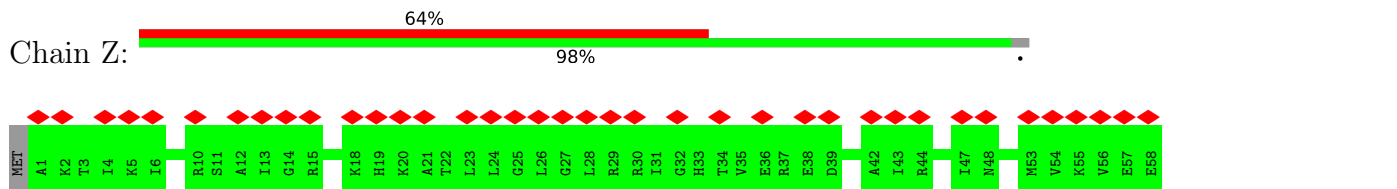
- Molecule 31: 50S ribosomal protein L28



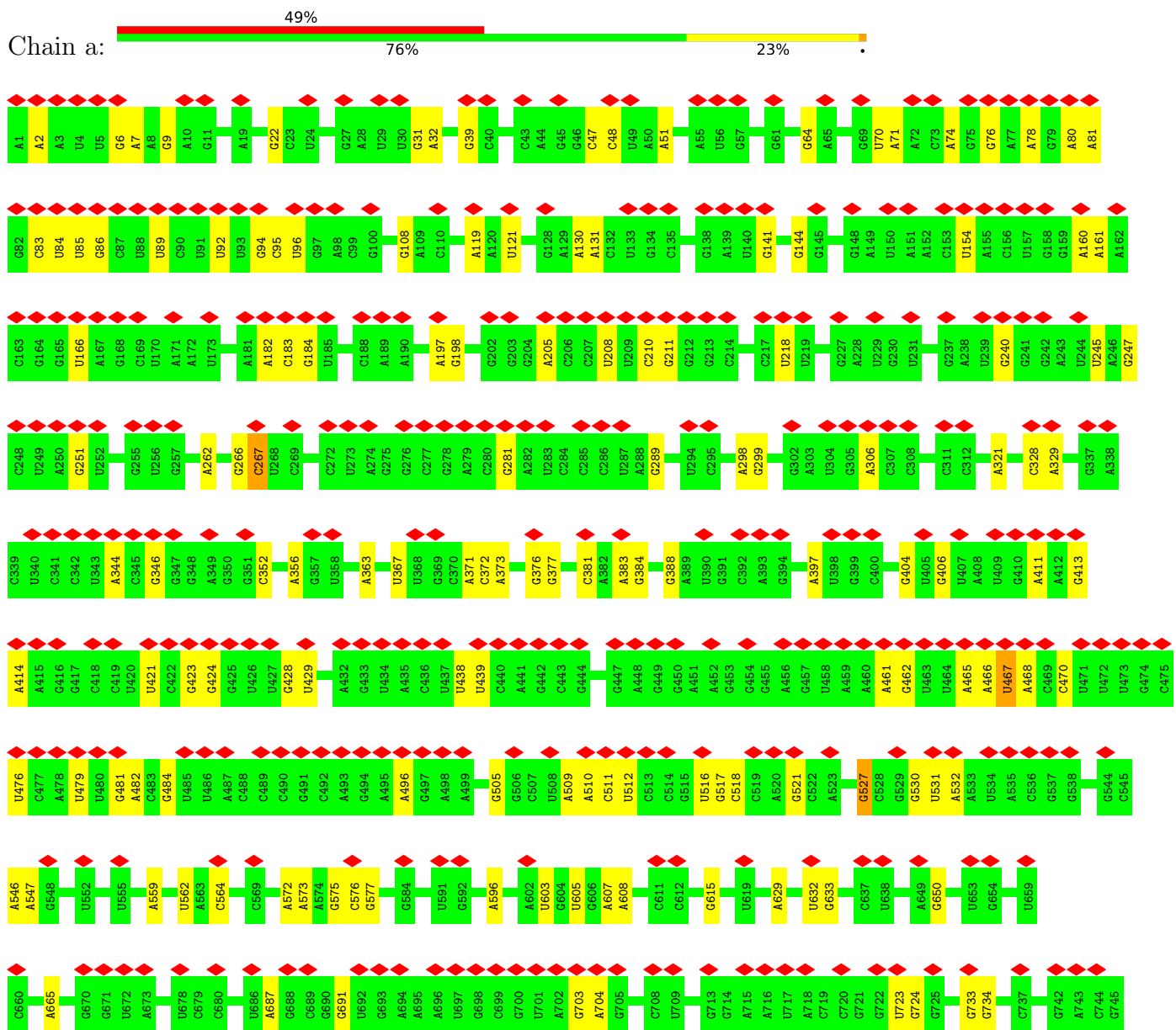
- Molecule 32: 50S ribosomal protein L29

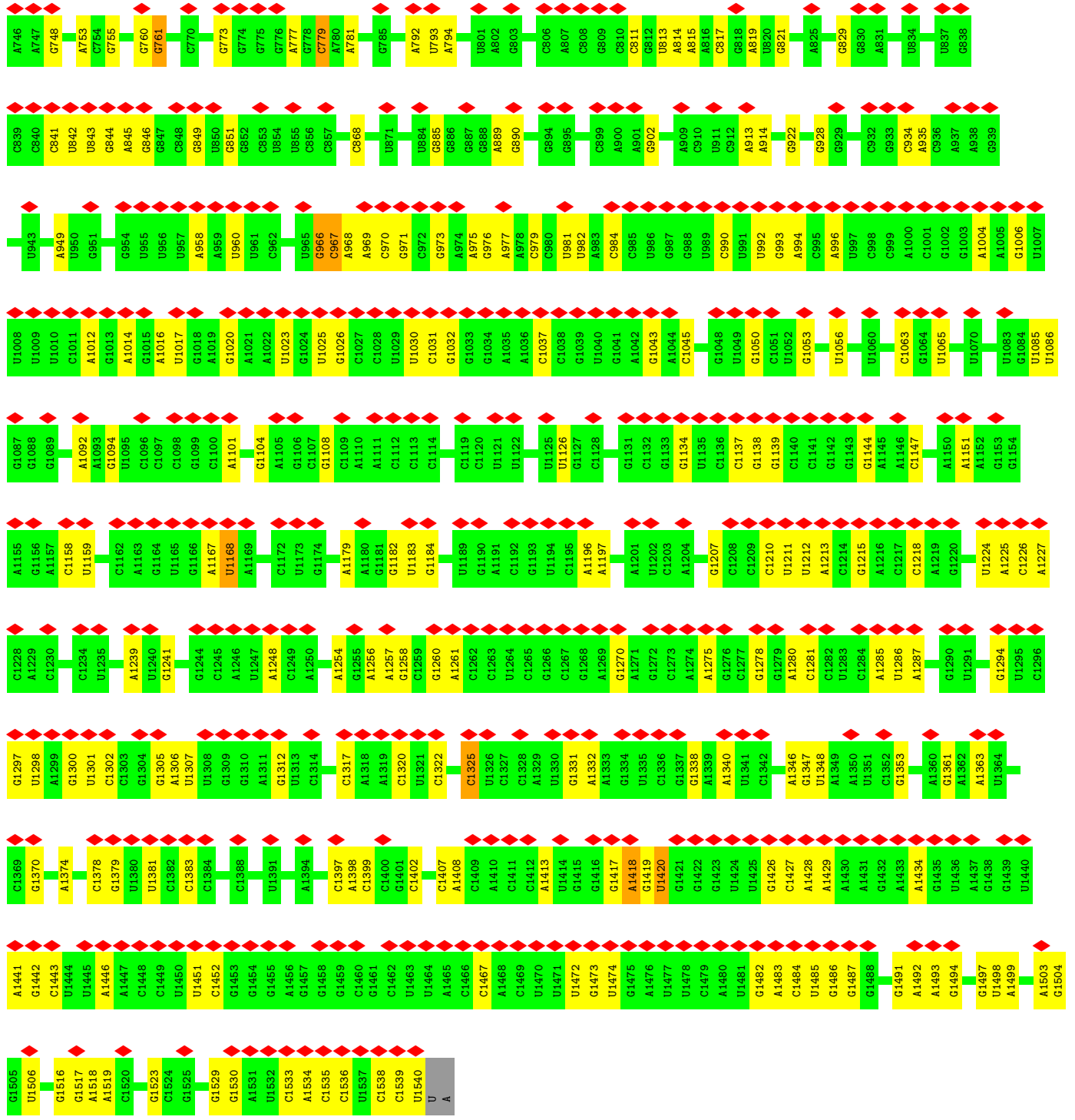


• Molecule 33: 50S ribosomal protein L30

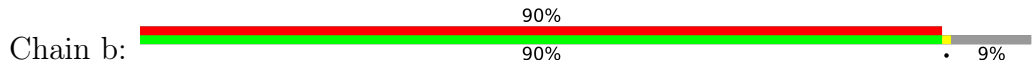


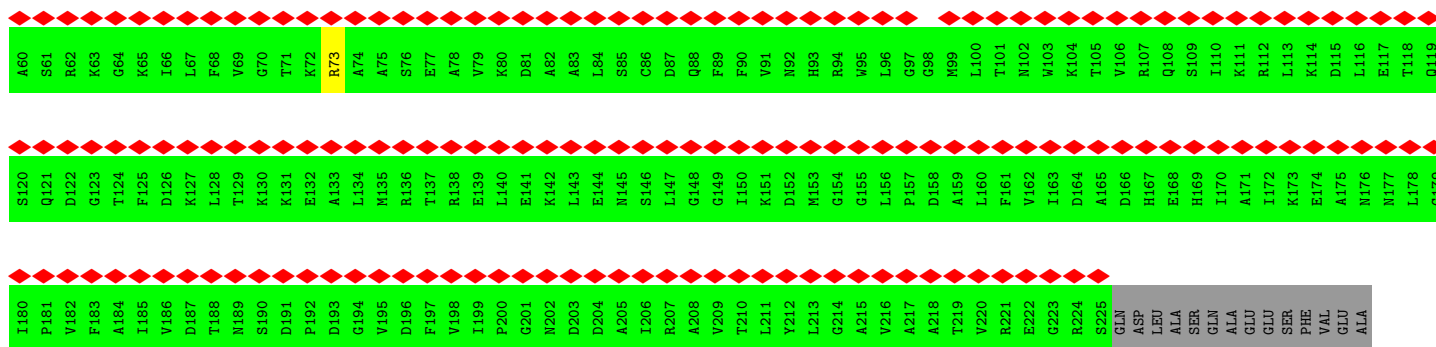
• Molecule 34: 16S ribosomal RNA



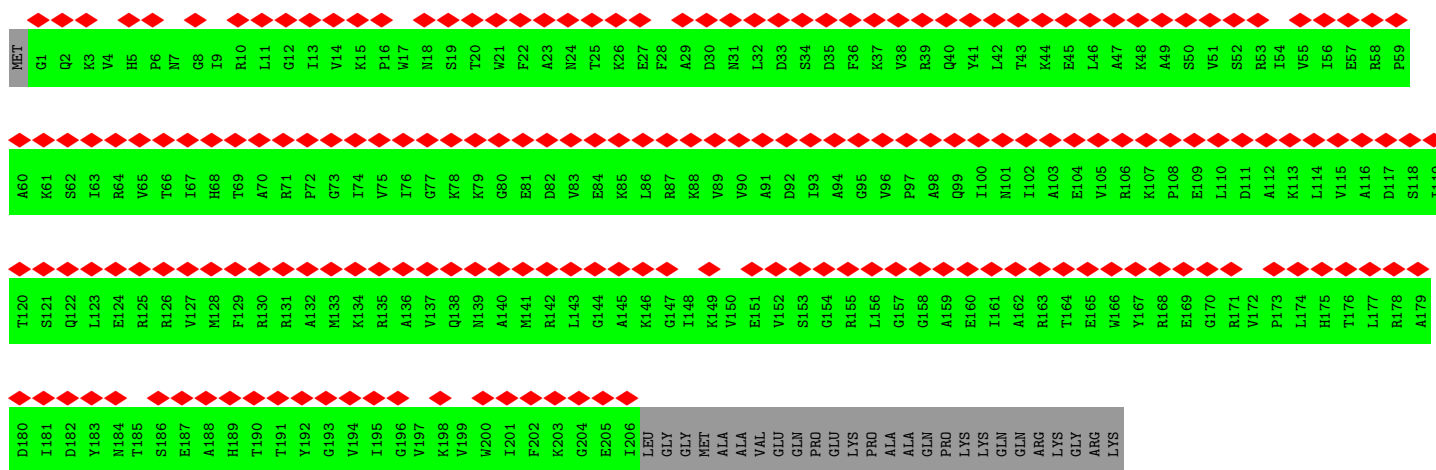
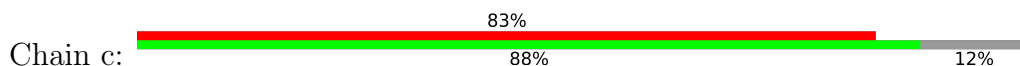


• Molecule 35: 30S ribosomal protein S2

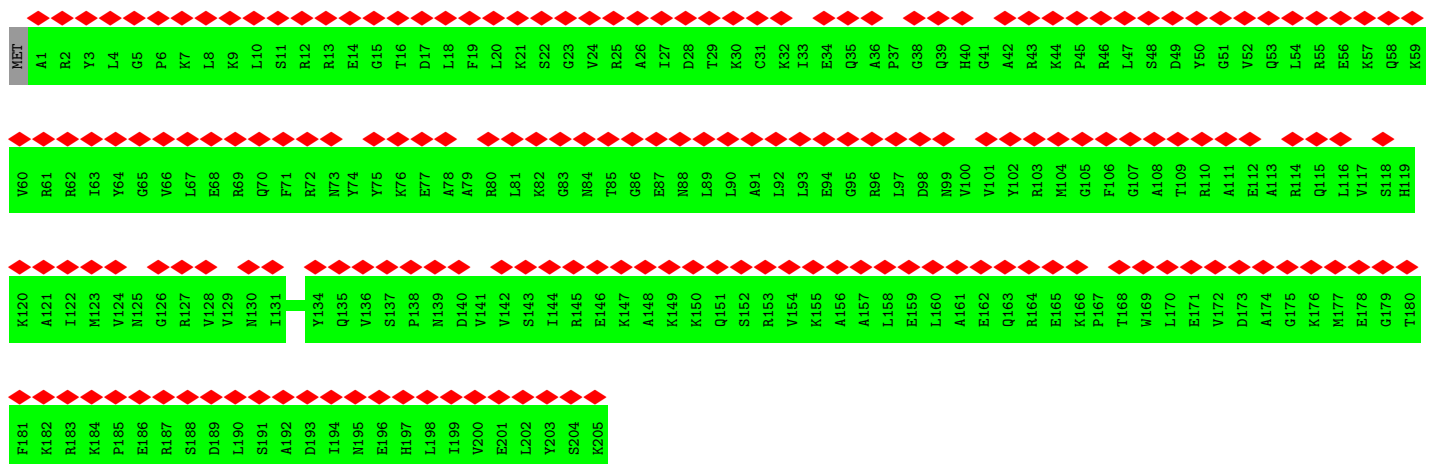
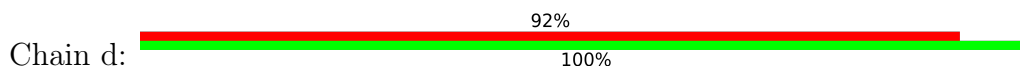




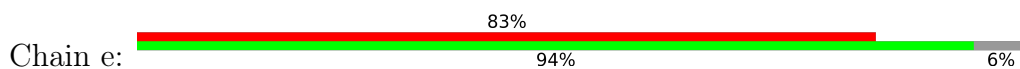
• Molecule 36: 30S ribosomal protein S3

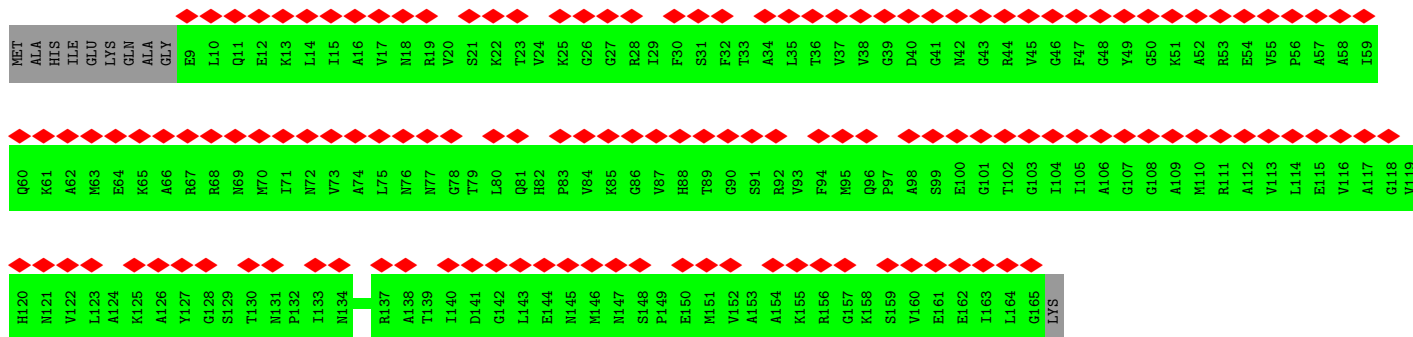


• Molecule 37: 30S ribosomal protein S4

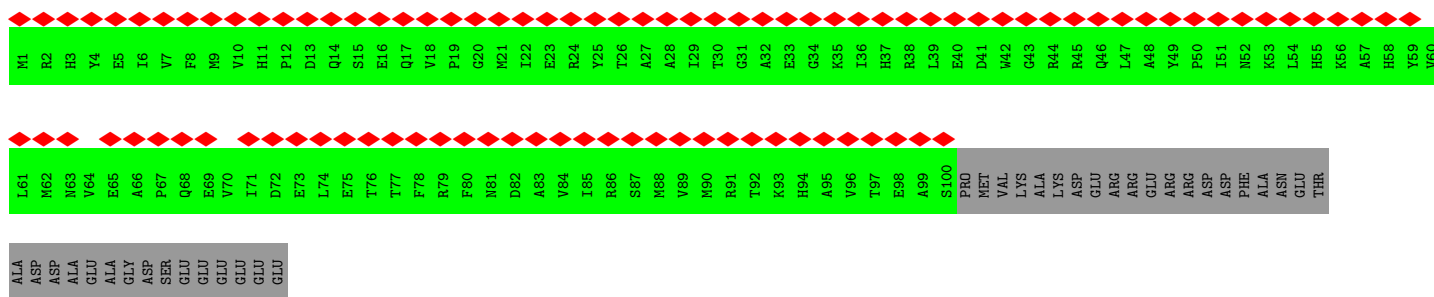
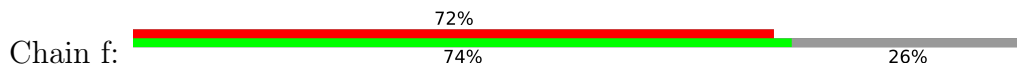


• Molecule 38: 30S ribosomal protein S5

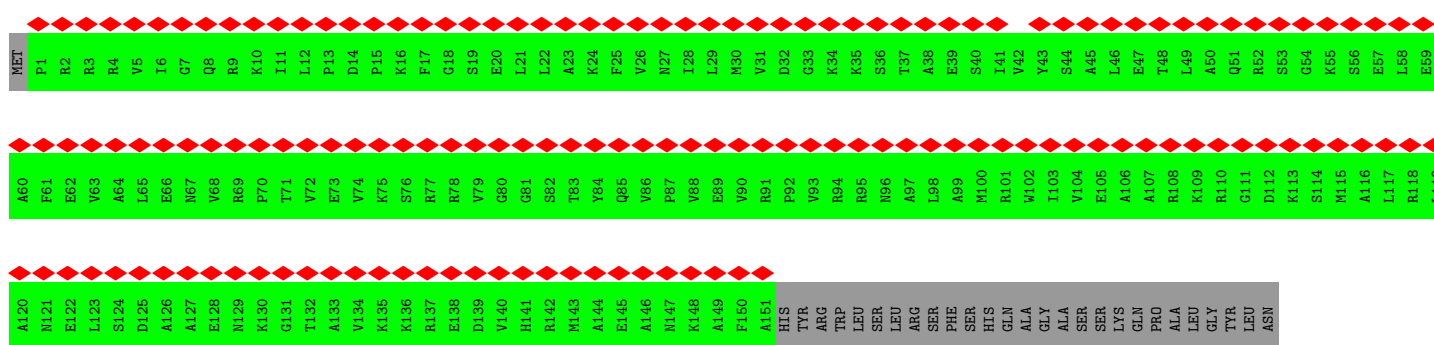
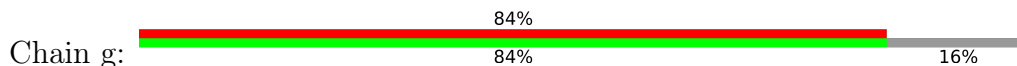




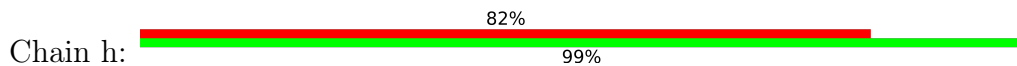
• Molecule 39: 30S ribosomal protein S6



• Molecule 40: 30S ribosomal protein S7

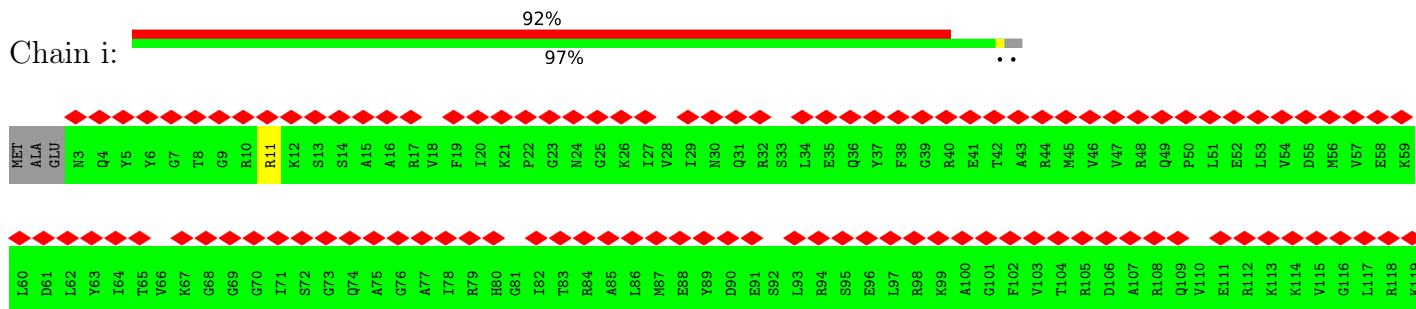


• Molecule 41: 30S ribosomal protein S8



E123  
I124  
I125  
C126  
Y127  
V128  
A129

• Molecule 42: 30S ribosomal protein S9

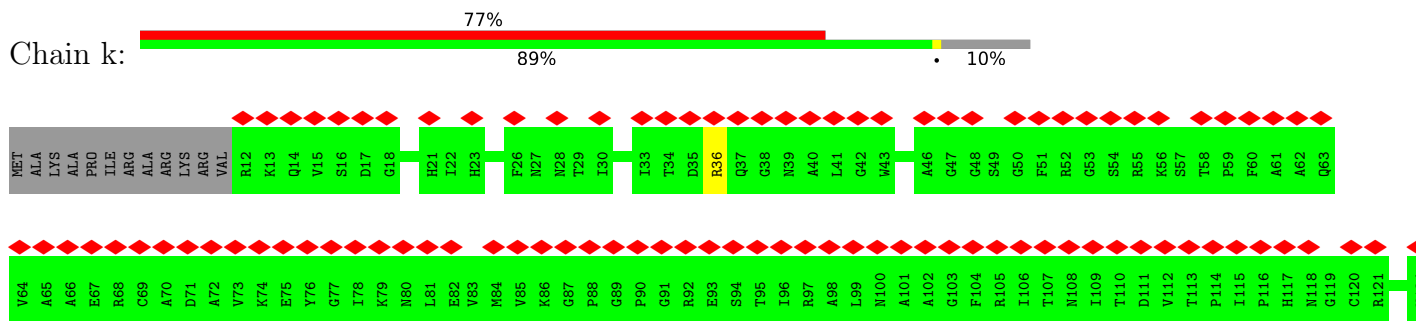


A120  
R121  
R122  
R123  
P124  
Q125  
F126  
S127  
K128  
R129

• Molecule 43: 30S ribosomal protein S10



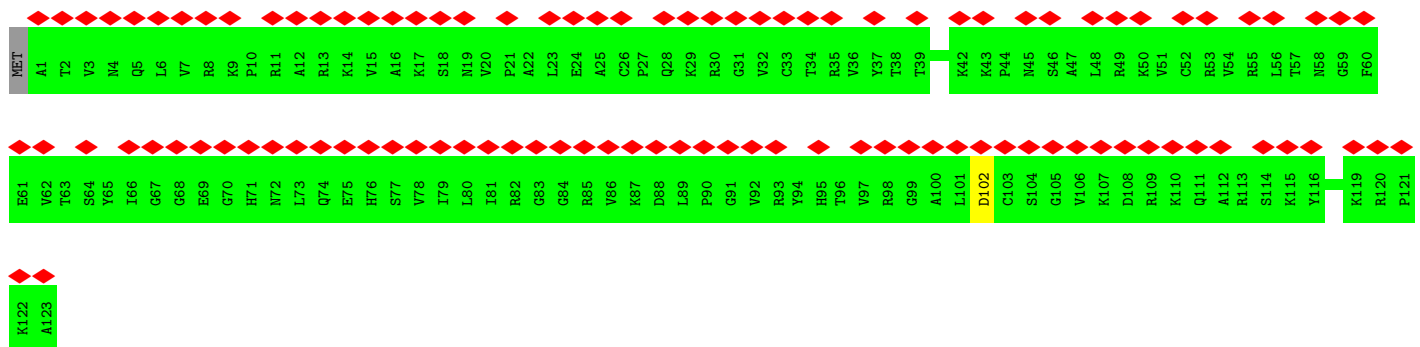
• Molecule 44: 30S ribosomal protein S11



K125  
R126  
R127  
VAL

• Molecule 45: 30S ribosomal protein S12





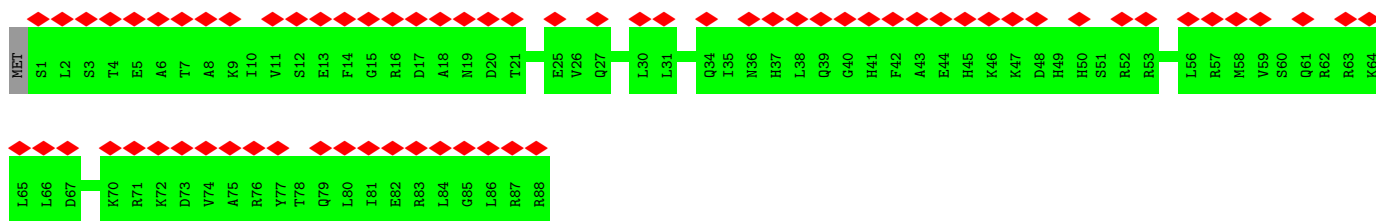
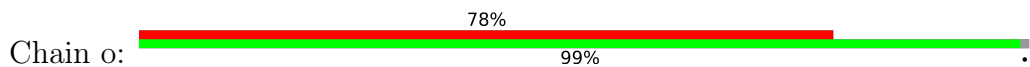
• Molecule 46: 30S ribosomal protein S13



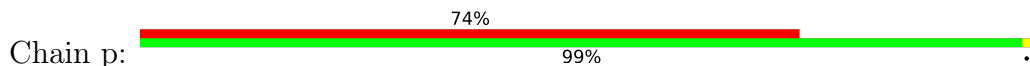
• Molecule 47: 30S ribosomal protein S14



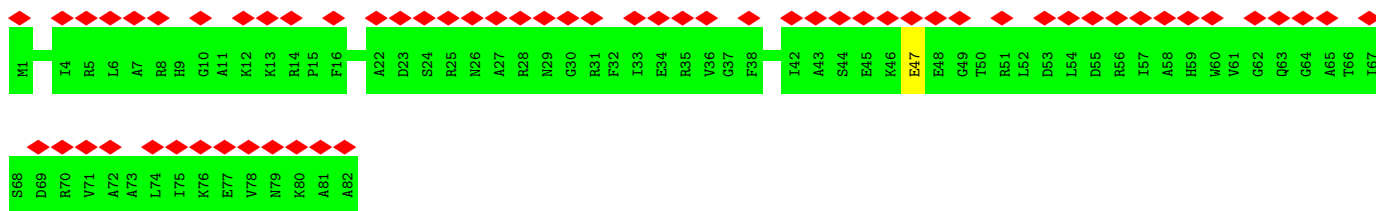
• Molecule 48: 30S ribosomal protein S15



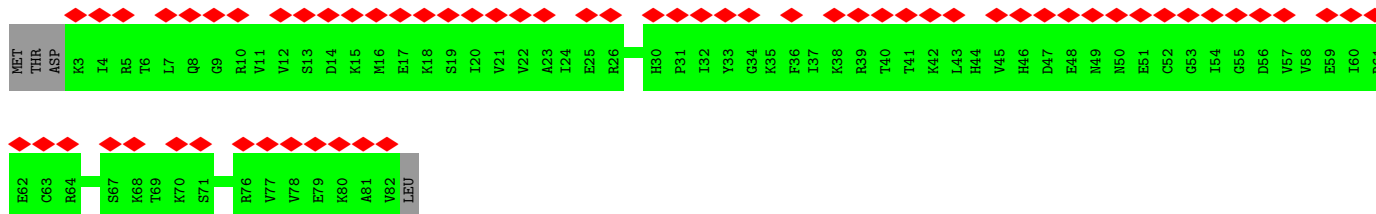
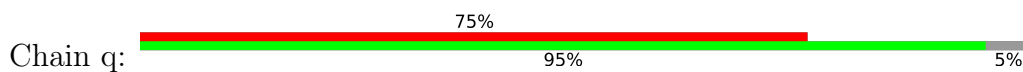
• Molecule 49: 30S ribosomal protein S16



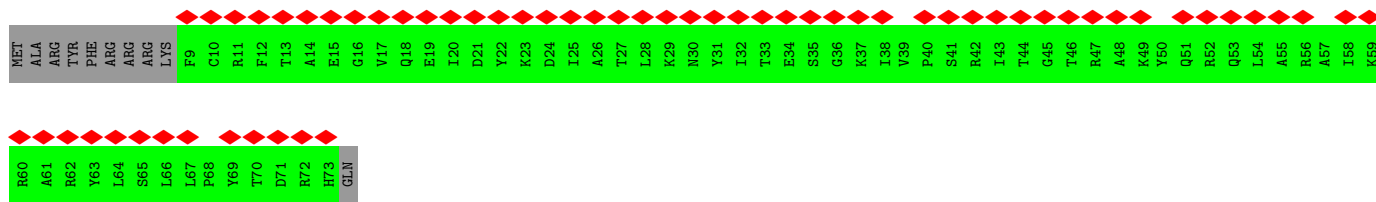
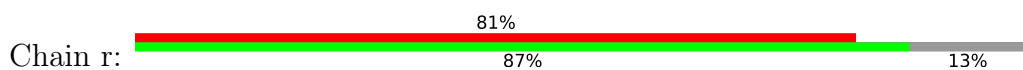




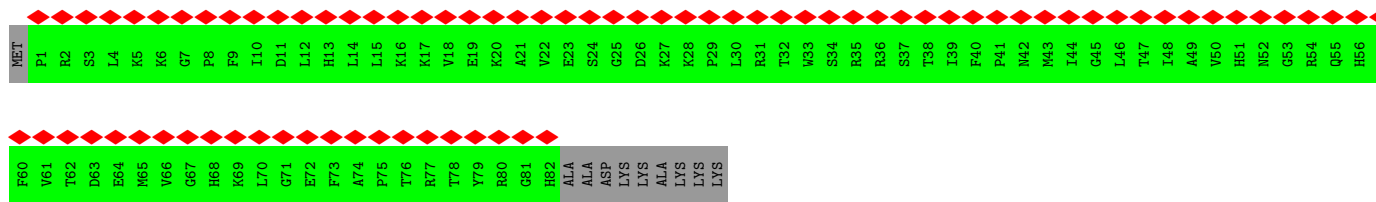
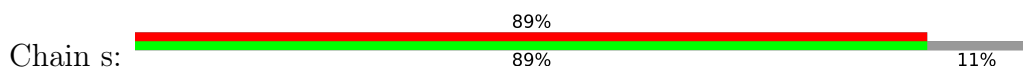
• Molecule 50: 30S ribosomal protein S17



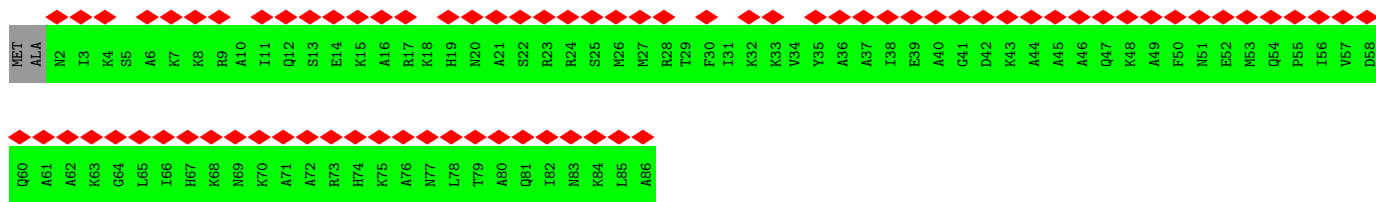
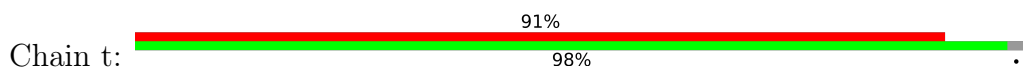
• Molecule 51: 30S ribosomal protein S18



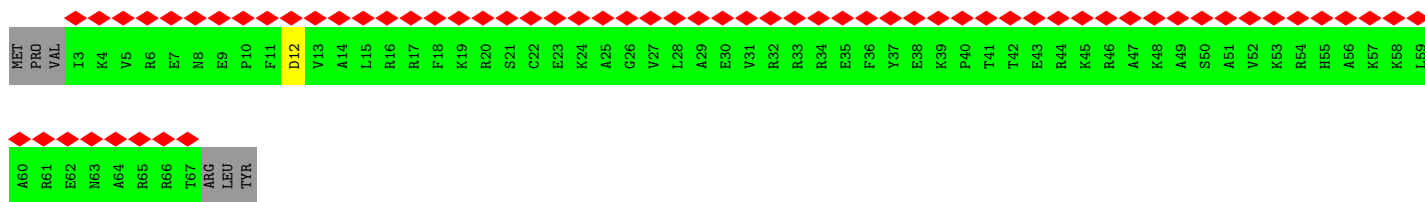
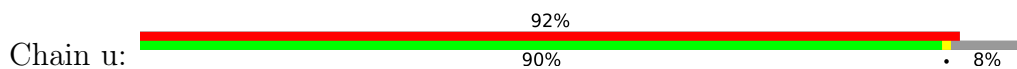
• Molecule 52: 30S ribosomal protein S19



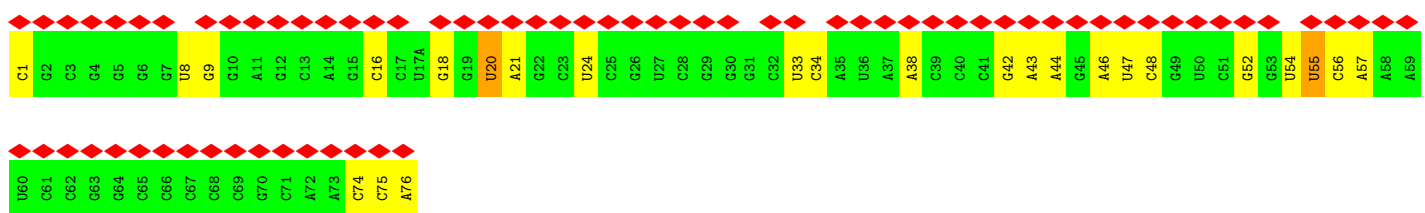
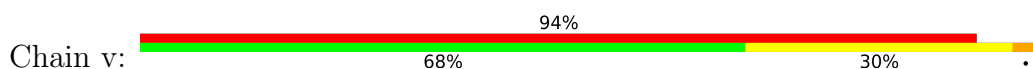
• Molecule 53: 30S ribosomal protein S20



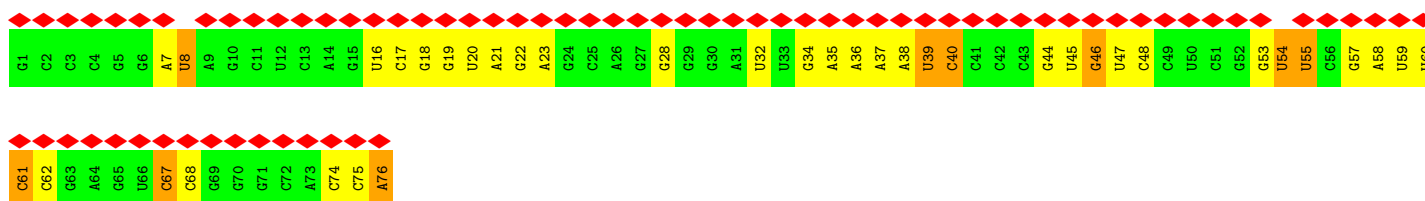
• Molecule 54: 30S ribosomal protein S21



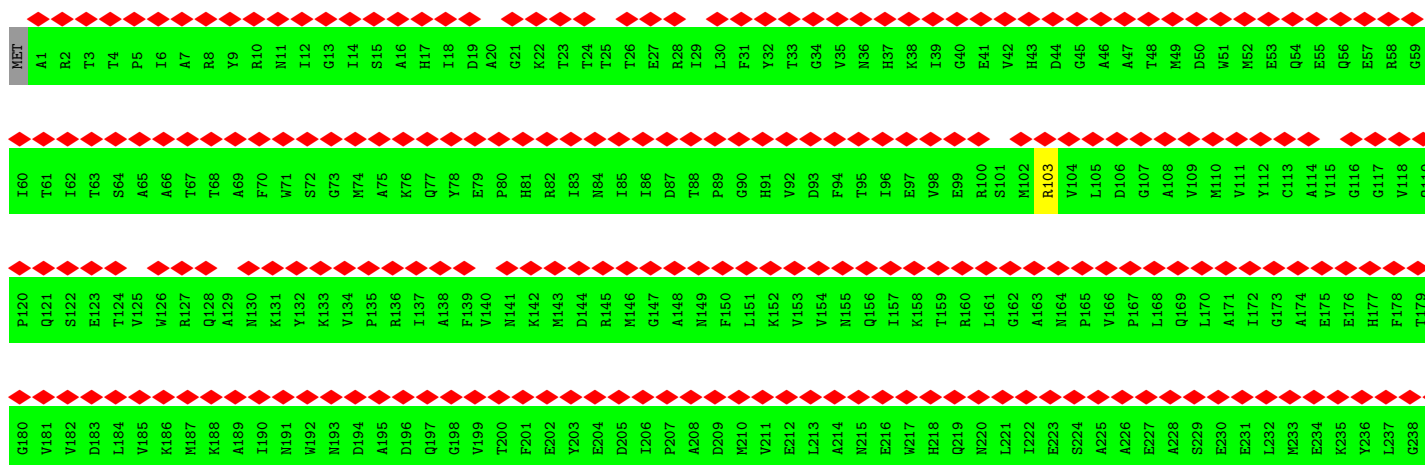
• Molecule 55: P-site tRNA(fMet)



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



• Molecule 57: Elongation factor G



E240	E241	L242	T243	E244	E246	I247	K248	G249	A250	L251	R252	Q253	R254	V255	L256	N257	N258	E259	I260	L262	V263	T264	C265	G266	S267	A268	F269	K270	N271	K272	G273	V274	Q275	A276	M277	L278	D279	A280	V281	I282	D283	Y284	L285	P286	S287	P288	V289	D290	V291	P292	A293	I294	N295	G296	I297	L298	D299		
D300	G301	K302	D303	T304	P305	A306	E307	R308	H309	A310	S311	D312	D313	E314	P315	F316	S317	A318	L319	A320	F321	K322	I323	A324	T325	D326	P327	F328	V329	G330	N331	L332	T333	F334	F335	R336	V337	Y338	S339	G340	N341	V342	N343	S344	G345	D346	T347	V348	L349	N350	S351	V352	K353	A354	A355	R356	I357	R358	F359
G360	R361	I362	V363	K364	M365	H366	A367	N368	K369	R370	E371	S372	I373	K374	E375	V376	R377	A378	G379	D380	I381	A382	A383	A384	I385	G386	L387	K388	D389	V390	T391	T392	G393	D394	T395	L396	C397	D398	P399	D400	A401	P402	I403	I404	L405	E406	R407	M408	E409	F410	P411	E412	P413	V414	I415	S416	A418	V419	
E420	P421	K422	T423	K424	A425	D426	Q427	E428	K429	M430	G431	A433	L434	G435	R436	L437	A438	K439	E440	D441	P442	S443	F444	R445	V446	W447	T448	D449	E450	E451	S452	M453	Q454	T455	I456	I457	A458	G459	M460	G461	E462	L463	H464	L465	D466	I467	I468	E469	D470	R471	M472	K473	R474	E475	F476	N477	V478	E479	
A480	M481	V482	G483	K484	P485	Q486	V487	A488	Y489	R490	E491	T492	I493	R494	Q495	K496	V497	T498	D499	V500	E501	G502	K503	H504	A505	K506	Q507	S508	G509	G510	R511	G512	Q513	Y514	G515	H516	V517	V518	I519	D520	M521	Y522	P523	L524	E525	F526	G527	S528	N529	F530	K531	G532	Y533	E534	F535	I536	N537	D538	I539
K540	G541	G542	V543	I544	P545	G546	E547	Y548	I549	P550	A551	V552	D553	K554	G555	I556	Q557	E558	Q559	L560	K561	A562	G563	P564	L565	A566	G567	Y568	D569	V570	V571	D572	M573	G574	I575	R576	L577	H578	F579	G580	L641	Y642	H643	D644	V645	S646	E647	V648	T649	G650	V651	K652	L653	H654	A655	E656	V657	P658	L659
F600	K601	E602	G603	F604	K605	K606	A607	K608	P609	V610	L611	L612	E613	P614	L615	M616	V618	E619	V620	E621	T622	P623	E624	E625	M626	T627	G628	D629	V630	L631	G632	D633	L634	S635	R636	R637	G638	G639	M640	L641	K642	G643	Q644	E645	S646	E647	V648	T649	G650	V651	K652	L653	H654	A655	E656	V657	P658	L659	
S660	E661	M662	F663	G664	Y665	A666	T667	Q668	L669	R670	S671	L672	T673	K674	G675	R676	S678	Y679	T680	M681	E682	F683	L684	K685	Y686	D687	E688	A689	P690	S691	N692	V693	A694	Q695	A696	V697	I698	E699	A700	R701	G702	K703																	

• Molecule 58: Dipeptide (FME-PHE)



M101	F102
------	------

• Molecule 59: mRNA



G	U	U	A	A	C	A	A	G	G	U	U	A	U	A	U	A	A	C	A	U	A-2	C-1	U0	A1	U2	G3	U4	U5	U6	G7	U8	U	A	U	U	U	A	C
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	-----	-----	----	----	----	----	----	----	----	----	----	---	---	---	---	---	---	---

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9108	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	12.254	Depositor
Minimum map value	-7.636	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 3TD, MIA, 4SU, 5MC, UR3, 4OC, G7M, H2U, FME, 2MA, OMU, 1MG, PSU, OMC, 5MU, AM2, PO4, OMG, GDP, 2MG, 6MZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.39	0/450	0.52	0/599
2	1	0.38	0/416	0.46	0/554
3	2	0.41	0/380	0.53	0/498
4	3	0.47	0/513	0.62	0/676
5	4	0.39	0/303	0.53	0/397
6	5	0.25	0/646	0.50	0/898
7	6	0.45	0/531	0.58	0/709
8	A	0.82	2/69266 (0.0%)	1.00	75/108055 (0.1%)
9	B	0.71	1/2873 (0.0%)	0.90	0/4478
10	C	0.46	0/2121	0.54	0/2852
11	D	0.44	0/1586	0.53	0/2134
12	E	0.43	0/1571	0.53	0/2113
13	F	0.36	0/1434	0.51	0/1926
14	G	0.37	0/1343	0.49	0/1816
15	H	0.30	0/1122	0.57	0/1515
16	I	0.25	0/692	0.49	0/960
17	J	0.44	0/1152	0.49	0/1551
18	K	0.40	0/947	0.53	0/1268
19	L	0.41	0/1054	0.57	0/1403
20	M	0.41	0/1093	0.51	0/1460
21	N	0.43	0/973	0.55	0/1301
22	O	0.40	0/902	0.48	0/1209
23	P	0.44	0/929	0.53	0/1242
24	Q	0.55	0/960	0.52	0/1278
25	R	0.45	0/829	0.58	0/1107
26	S	0.41	0/864	0.56	0/1156
27	T	0.40	0/744	0.54	0/994
28	U	0.43	0/787	0.58	0/1051
29	V	0.42	0/766	0.48	0/1025
30	W	0.44	0/582	0.50	0/769
31	X	0.43	0/635	0.49	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Y	0.34	0/510	0.58	0/677
33	Z	0.38	0/453	0.53	0/605
34	a	0.69	1/36725 (0.0%)	0.97	30/57285 (0.1%)
35	b	0.32	0/1735	0.52	1/2338 (0.0%)
36	c	0.36	0/1651	0.50	0/2225
37	d	0.35	0/1665	0.51	0/2227
38	e	0.37	0/1154	0.52	0/1554
39	f	0.36	0/835	0.49	0/1128
40	g	0.30	0/1195	0.47	0/1602
41	h	0.41	0/989	0.56	0/1326
42	i	0.36	0/1034	0.54	0/1375
43	j	0.34	0/796	0.57	0/1077
44	k	0.37	0/885	0.52	0/1195
45	l	0.40	0/969	0.56	1/1300 (0.1%)
46	m	0.29	0/892	0.49	0/1193
47	n	0.30	0/811	0.44	0/1081
48	o	0.36	0/722	0.49	0/964
49	p	0.38	0/659	0.52	0/884
50	q	0.37	0/657	0.53	0/881
51	r	0.34	0/544	0.50	0/731
52	s	0.33	0/675	0.53	0/908
53	t	0.32	0/671	0.45	0/888
54	u	0.34	0/512	0.54	0/683
55	v	0.65	1/1745 (0.1%)	0.99	5/2716 (0.2%)
56	w	0.61	2/1650 (0.1%)	1.02	6/2569 (0.2%)
57	x	0.37	0/5546	0.55	1/7504 (0.0%)
58	y	0.46	0/11	2.19	0/13
59	z	1.26	2/255 (0.8%)	1.72	7/394 (1.8%)
All	All	0.67	9/164410 (0.0%)	0.88	126/245165 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	1	C	OP3-P	-10.88	1.48	1.61
9	B	1	U	OP3-P	-10.79	1.48	1.61
59	z	1	A	O3'-P	-10.73	1.48	1.61
8	A	1	G	OP3-P	-10.72	1.48	1.61
56	w	34	G	O3'-P	-9.32	1.50	1.61
8	A	2029	G	C3'-O3'	5.63	1.50	1.42
34	a	1494	G	O3'-P	-5.59	1.54	1.61
56	w	76	A	C3'-O3'	5.45	1.49	1.42
59	z	2	U	O3'-P	-5.09	1.55	1.61

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2103	C	N1-C2-O2	10.08	124.95	118.90
59	z	0	U	O5'-P-OP1	9.74	122.39	110.70
56	w	40	C	C2'-C3'-O3'	8.95	129.18	109.50
8	A	2103	C	N3-C2-O2	-8.93	115.65	121.90
8	A	2103	C	C2-N1-C1'	8.18	127.79	118.80
57	x	402	PRO	N-CA-C	-7.95	91.44	112.10
8	A	2129	C	N1-C2-O2	7.88	123.63	118.90
8	A	2129	C	C2-N1-C1'	7.88	127.46	118.80
34	a	979	C	C2-N1-C1'	7.85	127.43	118.80
8	A	1914	C	C2'-C3'-O3'	7.68	126.41	109.50
8	A	1313	U	C2-N1-C1'	7.68	126.91	117.70
55	v	74	C	C2-N1-C1'	7.43	126.97	118.80
8	A	2474	U	N3-C2-O2	-7.37	117.04	122.20
55	v	74	C	N1-C2-O2	7.36	123.32	118.90
56	w	67	C	C2-N1-C1'	7.35	126.89	118.80
8	A	2342	C	N3-C2-O2	-7.15	116.90	121.90
59	z	7	G	C3'-C2'-C1'	-7.13	95.80	101.50
8	A	2103	C	C6-N1-C2	-7.08	117.47	120.30
8	A	1582	C	N3-C2-O2	-7.06	116.96	121.90
56	w	67	C	C6-N1-C1'	-6.90	112.52	120.80
8	A	2474	U	N1-C2-O2	6.86	127.61	122.80
59	z	3	G	C2'-C3'-O3'	-6.68	94.80	109.50
8	A	170	U	C2-N1-C1'	6.67	125.70	117.70
8	A	915	C	C2-N1-C1'	6.54	126.00	118.80
59	z	6	U	C4'-C3'-O3'	6.54	126.08	113.00
8	A	1771	C	C6-N1-C2	-6.46	117.71	120.30
8	A	2474	U	C2-N1-C1'	6.44	125.42	117.70
59	z	5	U	C1'-C2'-O2'	-6.44	91.29	110.60
8	A	1313	U	N3-C2-O2	-6.37	117.74	122.20
56	w	40	C	C5'-C4'-C3'	-6.35	105.84	116.00
56	w	67	C	N1-C2-O2	6.27	122.66	118.90
8	A	1926	U	O4'-C1'-N1	6.23	113.19	108.20
8	A	958	U	N1-C2-O2	6.20	127.14	122.80
8	A	2656	U	C2-N1-C1'	6.13	125.06	117.70
8	A	1157	G	N9-C4-C5	-6.13	102.95	105.40
34	a	811	C	C2-N1-C1'	6.13	125.54	118.80
8	A	1990	C	N3-C2-O2	-6.12	117.62	121.90
34	a	467	U	C2-N1-C1'	6.03	124.94	117.70
34	a	979	C	C6-N1-C1'	-6.02	113.57	120.80
8	A	2129	C	C6-N1-C1'	-5.97	113.64	120.80
8	A	1179	G	C4-N9-C1'	5.93	134.21	126.50
34	a	1168	U	C2-N1-C1'	5.92	124.80	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2129	C	N3-C2-O2	-5.88	117.78	121.90
8	A	883	G	P-O3'-C3'	5.88	126.75	119.70
34	a	1325	C	C2-N1-C1'	5.87	125.25	118.80
34	a	1493	A	C1'-C2'-O2'	-5.87	93.00	110.60
8	A	2723	C	C6-N1-C2	-5.86	117.95	120.30
34	a	1158	C	N1-C2-O2	5.85	122.41	118.90
8	A	1791	A	N1-C2-N3	5.83	132.22	129.30
8	A	2730	C	N3-C2-O2	-5.83	117.82	121.90
8	A	1918	A	C1'-C2'-O2'	-5.82	93.13	110.60
34	a	1420	U	C2-N1-C1'	5.82	124.68	117.70
34	a	979	C	N1-C2-O2	5.79	122.37	118.90
8	A	1170	C	C2-N1-C1'	5.78	125.16	118.80
8	A	2071	A	C6-C5-N7	-5.76	128.27	132.30
55	v	74	C	N3-C2-O2	-5.76	117.87	121.90
34	a	481	G	C4-N9-C1'	5.74	133.97	126.50
8	A	1314	C	C2-N1-C1'	5.73	125.10	118.80
8	A	1080	A	N1-C6-N6	5.71	122.03	118.60
8	A	2006	C	C2-N1-C1'	5.68	125.04	118.80
8	A	1577	C	N3-C2-O2	-5.66	117.94	121.90
34	a	481	G	C6-C5-N7	-5.64	127.02	130.40
8	A	1533	C	N3-C2-O2	-5.63	117.96	121.90
8	A	2071	A	N7-C8-N9	5.63	116.61	113.80
59	z	7	G	C4'-C3'-C2'	-5.62	96.98	102.60
8	A	1945	G	C8-N9-C1'	-5.61	119.70	127.00
8	A	1157	G	C8-N9-C1'	-5.57	119.75	127.00
35	b	9	LEU	CA-CB-CG	5.57	128.10	115.30
34	a	1158	C	N3-C2-O2	-5.56	118.01	121.90
34	a	1418	A	C8-N9-C4	-5.55	103.58	105.80
8	A	2071	A	C4-N9-C1'	5.55	136.28	126.30
34	a	467	U	N1-C2-O2	5.54	126.68	122.80
8	A	765	C	C2-N1-C1'	5.54	124.89	118.80
8	A	1945	G	C4-N9-C1'	5.52	133.68	126.50
34	a	481	G	C4-C5-N7	5.51	113.00	110.80
8	A	958	U	N3-C2-O2	-5.48	118.36	122.20
59	z	5	U	C2'-C3'-O3'	5.42	122.38	113.70
8	A	1582	C	C6-N1-C2	-5.41	118.14	120.30
8	A	1945	G	N3-C4-N9	5.41	129.24	126.00
8	A	528	A	C2-N3-C4	-5.39	107.90	110.60
8	A	1224	U	O4'-C1'-N1	-5.39	103.89	108.20
8	A	2128	G	C4-N9-C1'	5.38	133.49	126.50
8	A	1080	A	N9-C4-C5	-5.37	103.65	105.80
8	A	2540	C	N3-C2-O2	-5.37	118.14	121.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2090	A	C5-C6-N1	5.35	120.38	117.70
34	a	438	U	O4'-C1'-N1	5.33	112.47	108.20
8	A	2380	C	N3-C2-O2	-5.33	118.17	121.90
8	A	2075	U	C5-C4-O4	-5.32	122.71	125.90
56	w	61	C	C2-N1-C1'	5.31	124.64	118.80
34	a	95	C	C2-N1-C1'	5.30	124.63	118.80
34	a	949	A	C6-N1-C2	-5.28	115.43	118.60
34	a	603	U	N3-C2-O2	-5.27	118.51	122.20
8	A	2071	A	C4-C5-C6	5.26	119.63	117.00
8	A	1080	A	C5-C6-N6	-5.25	119.50	123.70
8	A	481	G	O4'-C1'-N9	5.25	112.40	108.20
8	A	1170	C	N1-C2-O2	5.25	122.05	118.90
34	a	1418	A	OP1-P-OP2	-5.20	111.80	119.60
8	A	1822	C	N3-C2-O2	-5.18	118.27	121.90
8	A	1313	U	N1-C2-O2	5.16	126.41	122.80
8	A	915	C	C6-N1-C1'	-5.15	114.62	120.80
8	A	2090	A	C6-N1-C2	-5.15	115.51	118.60
8	A	2794	C	C2-N1-C1'	5.15	124.47	118.80
34	a	811	C	C6-N1-C1'	-5.14	114.63	120.80
34	a	1158	C	C2-N1-C1'	5.14	124.45	118.80
34	a	575	G	N3-C4-C5	5.13	131.17	128.60
34	a	481	G	C8-N9-C1'	-5.11	120.36	127.00
8	A	1313	U	C6-N1-C1'	-5.11	114.05	121.20
45	l	102	ASP	CB-CG-OD1	5.11	122.90	118.30
8	A	1870	C	C2-N1-C1'	5.10	124.41	118.80
55	v	74	C	C6-N1-C1'	-5.10	114.69	120.80
8	A	433	C	N3-C2-O2	-5.09	118.33	121.90
8	A	2029	G	C2'-C3'-O3'	5.09	121.85	113.70
8	A	2103	C	C6-N1-C1'	-5.09	114.70	120.80
34	a	779	C	C2-N1-C1'	5.08	124.39	118.80
8	A	242	G	P-O3'-C3'	5.07	125.79	119.70
8	A	1870	C	N3-C2-O2	-5.07	118.35	121.90
34	a	404	G	N3-C4-N9	-5.07	122.96	126.00
34	a	761	G	N3-C4-N9	5.06	129.04	126.00
34	a	267	C	C2-N1-C1'	5.06	124.37	118.80
8	A	1071	G	C4-N9-C1'	5.06	133.08	126.50
8	A	515	A	N1-C2-N3	5.05	131.82	129.30
8	A	1577	C	N1-C2-O2	5.04	121.92	118.90
34	a	476	U	C2-N1-C1'	5.02	123.72	117.70
8	A	760	G	C6-C5-N7	-5.01	127.39	130.40
55	v	74	C	C6-N1-C2	-5.01	118.30	120.30
8	A	2901	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

There are no planarity outliers.

## 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	
1	0	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
2	1	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
3	2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
4	3	62/65 (95%)	51 (82%)	11 (18%)	0	100	100
5	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
6	5	129/165 (78%)	98 (76%)	31 (24%)	0	100	100
7	6	64/70 (91%)	53 (83%)	11 (17%)	0	100	100
10	C	269/273 (98%)	229 (85%)	39 (14%)	1 (0%)	34	71
11	D	207/209 (99%)	172 (83%)	35 (17%)	0	100	100
12	E	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
13	F	175/179 (98%)	143 (82%)	32 (18%)	0	100	100
14	G	174/177 (98%)	154 (88%)	20 (12%)	0	100	100
15	H	147/149 (99%)	117 (80%)	30 (20%)	0	100	100
16	I	139/142 (98%)	103 (74%)	36 (26%)	0	100	100
17	J	140/142 (99%)	128 (91%)	12 (9%)	0	100	100
18	K	120/123 (98%)	98 (82%)	22 (18%)	0	100	100
19	L	141/144 (98%)	113 (80%)	28 (20%)	0	100	100
20	M	134/136 (98%)	114 (85%)	20 (15%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	N	118/127 (93%)	106 (90%)	12 (10%)	0	100	100
22	O	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
23	P	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
24	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
25	R	101/103 (98%)	86 (85%)	13 (13%)	2 (2%)	7	40
26	S	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
27	T	91/100 (91%)	79 (87%)	12 (13%)	0	100	100
28	U	100/104 (96%)	85 (85%)	13 (13%)	2 (2%)	7	40
29	V	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
30	W	73/85 (86%)	60 (82%)	13 (18%)	0	100	100
31	X	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
32	Y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	9	44
33	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
35	b	216/240 (90%)	186 (86%)	30 (14%)	0	100	100
36	c	204/233 (88%)	185 (91%)	19 (9%)	0	100	100
37	d	203/206 (98%)	167 (82%)	36 (18%)	0	100	100
38	e	155/167 (93%)	134 (86%)	21 (14%)	0	100	100
39	f	98/135 (73%)	84 (86%)	14 (14%)	0	100	100
40	g	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
41	h	127/130 (98%)	113 (89%)	14 (11%)	0	100	100
42	i	125/130 (96%)	104 (83%)	21 (17%)	0	100	100
43	j	96/103 (93%)	75 (78%)	20 (21%)	1 (1%)	15	53
44	k	114/129 (88%)	97 (85%)	17 (15%)	0	100	100
45	l	121/124 (98%)	95 (78%)	26 (22%)	0	100	100
46	m	112/118 (95%)	96 (86%)	16 (14%)	0	100	100
47	n	99/102 (97%)	83 (84%)	16 (16%)	0	100	100
48	o	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
49	p	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	12	48
50	q	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
51	r	63/75 (84%)	52 (82%)	11 (18%)	0	100	100
52	s	80/92 (87%)	64 (80%)	16 (20%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	t	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
54	u	63/71 (89%)	51 (81%)	11 (18%)	1 (2%)	9	44
57	x	701/704 (100%)	625 (89%)	74 (11%)	2 (0%)	41	75
All	All	6551/6924 (95%)	5653 (86%)	887 (14%)	11 (0%)	50	79

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	U	98	ASN
28	U	16	LYS
57	x	402	PRO
25	R	71	LYS
32	Y	19	LEU
49	p	47	GLU
43	j	58	ASN
54	u	12	ASP
57	x	367	ALA
10	C	240	GLY
25	R	51	VAL

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/52 (98%)	51 (100%)	0	100	100
5	4	34/34 (100%)	34 (100%)	0	100	100
7	6	59/62 (95%)	48 (81%)	11 (19%)	1	10
10	C	216/218 (99%)	216 (100%)	0	100	100
11	D	164/164 (100%)	164 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	148 (100%)	0	100	100
14	G	137/138 (99%)	137 (100%)	0	100	100
15	H	114/114 (100%)	114 (100%)	0	100	100
17	J	116/116 (100%)	115 (99%)	1 (1%)	78	88
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	102 (100%)	0	100	100
20	M	109/109 (100%)	108 (99%)	1 (1%)	78	88
21	N	100/103 (97%)	99 (99%)	1 (1%)	76	86
22	O	86/87 (99%)	86 (100%)	0	100	100
23	P	99/100 (99%)	98 (99%)	1 (1%)	76	86
24	Q	89/90 (99%)	89 (100%)	0	100	100
25	R	84/84 (100%)	83 (99%)	1 (1%)	71	84
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	80 (100%)	0	100	100
28	U	83/85 (98%)	82 (99%)	1 (1%)	71	84
29	V	78/78 (100%)	77 (99%)	1 (1%)	69	82
30	W	57/63 (90%)	57 (100%)	0	100	100
31	X	67/68 (98%)	66 (98%)	1 (2%)	65	80
32	Y	55/55 (100%)	55 (100%)	0	100	100
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	179 (99%)	1 (1%)	86	92
36	c	170/190 (90%)	170 (100%)	0	100	100
37	d	172/173 (99%)	172 (100%)	0	100	100
38	e	114/126 (90%)	114 (100%)	0	100	100
39	f	87/116 (75%)	87 (100%)	0	100	100
40	g	124/147 (84%)	124 (100%)	0	100	100
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	105/107 (98%)	104 (99%)	1 (1%)	76	86
43	j	86/90 (96%)	86 (100%)	0	100	100
44	k	89/99 (90%)	88 (99%)	1 (1%)	73	85

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	l	103/104 (99%)	103 (100%)	0	100	100
46	m	92/96 (96%)	91 (99%)	1 (1%)	73	85
47	n	79/84 (94%)	79 (100%)	0	100	100
48	o	76/77 (99%)	76 (100%)	0	100	100
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/78 (95%)	74 (100%)	0	100	100
51	r	56/65 (86%)	56 (100%)	0	100	100
52	s	72/79 (91%)	72 (100%)	0	100	100
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	46 (100%)	0	100	100
57	x	577/578 (100%)	569 (99%)	8 (1%)	67	81
58	y	1/1 (100%)	1 (100%)	0	100	100
All	All	5204/5408 (96%)	5173 (99%)	31 (1%)	86	92

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	6	48	GLN
7	6	49	ARG
7	6	51	VAL
7	6	53	THR
7	6	56	ARG
7	6	57	VAL
7	6	59	ARG
7	6	60	PHE
7	6	62	LYS
7	6	63	ARG
7	6	65	ASN
17	J	52	ASP
20	M	6	ARG
21	N	2	ARG
23	P	88	ARG
25	R	51	VAL
28	U	6	ARG
29	V	21	ARG
31	X	76	LYS
35	b	73	ARG
42	i	11	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
44	k	36	ARG
46	m	69	ARG
57	x	103	ARG
57	x	294	ILE
57	x	295	ASN
57	x	336	ARG
57	x	471	ARG
57	x	593	LYS
57	x	601	LYS
57	x	697	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	5	ASN
1	0	37	HIS
1	0	41	HIS
2	1	45	HIS
4	3	30	HIS
10	C	89	ASN
10	C	127	ASN
10	C	225	ASN
10	C	238	ASN
11	D	173	GLN
11	D	185	ASN
12	E	163	ASN
14	G	115	GLN
15	H	66	ASN
15	H	135	HIS
17	J	80	HIS
17	J	136	GLN
18	K	3	GLN
18	K	90	ASN
18	K	93	GLN
19	L	4	ASN
21	N	3	HIS
21	N	11	ASN
21	N	23	ASN
22	O	38	GLN
23	P	11	GLN
24	Q	36	GLN
25	R	43	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	S	7	HIS
27	T	48	GLN
27	T	59	ASN
27	T	70	HIS
28	U	68	ASN
33	Z	33	HIS
35	b	17	HIS
35	b	167	HIS
36	c	2	GLN
37	d	35	GLN
37	d	39	GLN
37	d	73	ASN
37	d	88	ASN
37	d	135	GLN
38	e	42	ASN
38	e	121	ASN
39	f	52	ASN
40	g	96	ASN
40	g	147	ASN
41	h	17	GLN
43	j	56	HIS
44	k	21	HIS
45	l	76	HIS
47	n	60	GLN
48	o	34	GLN
48	o	37	HIS
49	p	26	ASN
49	p	79	ASN
50	q	44	HIS
50	q	46	HIS
51	r	51	GLN
52	s	13	HIS
52	s	42	ASN
52	s	55	GLN
52	s	56	HIS
53	t	12	GLN
53	t	19	HIS
53	t	47	GLN
53	t	51	ASN
57	x	36	ASN
57	x	121	GLN
57	x	258	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
57	x	271	ASN
57	x	427	GLN
57	x	454	GLN
57	x	464	HIS
57	x	516	HIS
57	x	559	GLN
57	x	583	HIS
57	x	626	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	347 (22%)	0
55	v	76/77 (98%)	21 (27%)	0
56	w	74/76 (97%)	35 (47%)	0
59	z	10/33 (30%)	8 (80%)	0
8	A	2898/2903 (99%)	717 (24%)	56 (1%)
9	B	119/120 (99%)	23 (19%)	3 (2%)
All	All	4713/4751 (99%)	1151 (24%)	59 (1%)

All (1151) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	12	U
8	A	15	G
8	A	27	G
8	A	35	G
8	A	43	G
8	A	44	A
8	A	46	G
8	A	62	U
8	A	63	A
8	A	71	A
8	A	74	A
8	A	75	G
8	A	84	A
8	A	93	G
8	A	96	C
8	A	101	A
8	A	102	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	103	A
8	A	104	A
8	A	118	A
8	A	120	U
8	A	131	A
8	A	140	C
8	A	141	G
8	A	142	A
8	A	149	A
8	A	160	A
8	A	163	C
8	A	170	U
8	A	175	G
8	A	196	A
8	A	199	A
8	A	200	U
8	A	204	A
8	A	205	G
8	A	215	G
8	A	216	A
8	A	221	A
8	A	222	A
8	A	226	A
8	A	228	C
8	A	229	C
8	A	230	G
8	A	232	G
8	A	233	A
8	A	239	C
8	A	241	A
8	A	242	G
8	A	243	U
8	A	244	A
8	A	245	G
8	A	248	G
8	A	255	A
8	A	264	C
8	A	266	G
8	A	272	A
8	A	275	C
8	A	276	U
8	A	278	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	279	A
8	A	288	U
8	A	291	G
8	A	294	A
8	A	296	U
8	A	302	C
8	A	311	A
8	A	322	A
8	A	323	C
8	A	330	A
8	A	332	A
8	A	345	A
8	A	346	A
8	A	359	G
8	A	361	G
8	A	367	G
8	A	368	A
8	A	370	G
8	A	371	A
8	A	372	G
8	A	373	U
8	A	386	G
8	A	396	G
8	A	401	A
8	A	404	A
8	A	405	U
8	A	406	G
8	A	411	G
8	A	435	C
8	A	451	U
8	A	455	C
8	A	457	A
8	A	458	G
8	A	459	U
8	A	464	U
8	A	478	A
8	A	479	A
8	A	480	A
8	A	481	G
8	A	482	A
8	A	490	C
8	A	491	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	494	G
8	A	496	G
8	A	504	A
8	A	505	A
8	A	507	A
8	A	508	A
8	A	509	C
8	A	518	G
8	A	527	C
8	A	529	A
8	A	531	C
8	A	532	A
8	A	544	C
8	A	545	U
8	A	546	U
8	A	548	G
8	A	549	G
8	A	556	A
8	A	563	A
8	A	572	A
8	A	573	U
8	A	575	A
8	A	603	A
8	A	613	A
8	A	614	A
8	A	615	U
8	A	622	G
8	A	627	A
8	A	637	A
8	A	643	A
8	A	645	C
8	A	646	U
8	A	647	G
8	A	654	A
8	A	655	A
8	A	669	G
8	A	674	G
8	A	682	G
8	A	686	U
8	A	695	G
8	A	704	G
8	A	712	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	714	U
8	A	716	A
8	A	717	C
8	A	730	A
8	A	745	1MG
8	A	747	5MC
8	A	757	G
8	A	760	G
8	A	764	A
8	A	765	C
8	A	775	G
8	A	776	G
8	A	782	A
8	A	783	A
8	A	784	G
8	A	785	G
8	A	800	A
8	A	803	U
8	A	805	G
8	A	806	C
8	A	811	U
8	A	812	C
8	A	819	A
8	A	827	U
8	A	828	U
8	A	831	G
8	A	846	U
8	A	847	U
8	A	856	G
8	A	857	G
8	A	859	G
8	A	882	G
8	A	883	G
8	A	884	U
8	A	885	C
8	A	887	A
8	A	889	C
8	A	890	C
8	A	891	G
8	A	893	C
8	A	894	U
8	A	895	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	896	A
8	A	897	C
8	A	899	A
8	A	901	C
8	A	902	C
8	A	903	C
8	A	904	G
8	A	907	G
8	A	910	A
8	A	915	C
8	A	917	A
8	A	927	A
8	A	931	U
8	A	934	U
8	A	941	A
8	A	946	C
8	A	953	G
8	A	957	C
8	A	958	U
8	A	959	A
8	A	961	C
8	A	973	A
8	A	974	G
8	A	980	A
8	A	983	A
8	A	990	A
8	A	995	C
8	A	996	A
8	A	1002	G
8	A	1003	G
8	A	1005	C
8	A	1009	A
8	A	1012	U
8	A	1013	C
8	A	1026	G
8	A	1033	U
8	A	1041	G
8	A	1045	C
8	A	1046	A
8	A	1047	G
8	A	1048	A
8	A	1052	C

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1055	G
8	A	1056	G
8	A	1057	A
8	A	1058	U
8	A	1059	G
8	A	1060	U
8	A	1061	U
8	A	1062	G
8	A	1063	G
8	A	1066	U
8	A	1067	A
8	A	1068	G
8	A	1069	A
8	A	1070	A
8	A	1071	G
8	A	1072	C
8	A	1073	A
8	A	1074	G
8	A	1075	C
8	A	1077	A
8	A	1078	U
8	A	1079	C
8	A	1080	A
8	A	1081	U
8	A	1082	U
8	A	1083	U
8	A	1084	A
8	A	1085	A
8	A	1086	A
8	A	1087	G
8	A	1088	A
8	A	1089	A
8	A	1091	G
8	A	1092	C
8	A	1093	G
8	A	1094	U
8	A	1095	A
8	A	1096	A
8	A	1097	U
8	A	1098	A
8	A	1100	C
8	A	1101	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1102	C
8	A	1103	A
8	A	1105	U
8	A	1109	C
8	A	1111	A
8	A	1112	G
8	A	1115	G
8	A	1122	G
8	A	1130	U
8	A	1131	G
8	A	1132	U
8	A	1133	A
8	A	1135	C
8	A	1139	G
8	A	1142	A
8	A	1143	A
8	A	1151	A
8	A	1154	G
8	A	1155	A
8	A	1174	U
8	A	1175	A
8	A	1176	U
8	A	1179	G
8	A	1180	U
8	A	1181	U
8	A	1204	A
8	A	1210	G
8	A	1211	C
8	A	1212	G
8	A	1225	G
8	A	1227	G
8	A	1234	U
8	A	1247	A
8	A	1250	G
8	A	1252	G
8	A	1253	A
8	A	1256	G
8	A	1263	U
8	A	1264	A
8	A	1265	A
8	A	1271	G
8	A	1272	A

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1273	U
8	A	1275	A
8	A	1284	A
8	A	1300	G
8	A	1301	A
8	A	1302	A
8	A	1306	C
8	A	1313	U
8	A	1314	C
8	A	1321	A
8	A	1330	C
8	A	1340	U
8	A	1341	G
8	A	1352	U
8	A	1365	A
8	A	1368	G
8	A	1373	A
8	A	1374	G
8	A	1376	C
8	A	1378	A
8	A	1379	U
8	A	1383	A
8	A	1395	A
8	A	1407	G
8	A	1409	U
8	A	1410	G
8	A	1413	A
8	A	1415	U
8	A	1416	G
8	A	1420	A
8	A	1421	G
8	A	1425	G
8	A	1428	C
8	A	1429	G
8	A	1434	A
8	A	1452	G
8	A	1455	G
8	A	1458	U
8	A	1459	G
8	A	1460	U
8	A	1461	C
8	A	1473	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1475	G
8	A	1478	G
8	A	1482	G
8	A	1490	A
8	A	1491	G
8	A	1493	C
8	A	1494	A
8	A	1497	U
8	A	1503	A
8	A	1504	A
8	A	1508	A
8	A	1515	A
8	A	1522	A
8	A	1524	G
8	A	1534	U
8	A	1536	C
8	A	1537	G
8	A	1538	G
8	A	1558	C
8	A	1566	A
8	A	1567	G
8	A	1569	A
8	A	1578	U
8	A	1584	U
8	A	1585	C
8	A	1598	A
8	A	1608	A
8	A	1610	A
8	A	1616	A
8	A	1622	G
8	A	1634	A
8	A	1635	A
8	A	1646	C
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1651	G
8	A	1654	A
8	A	1664	A
8	A	1665	A
8	A	1672	A
8	A	1674	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1694	C
8	A	1695	G
8	A	1698	A
8	A	1699	G
8	A	1713	A
8	A	1715	G
8	A	1716	U
8	A	1729	U
8	A	1730	C
8	A	1731	G
8	A	1738	G
8	A	1746	A
8	A	1756	G
8	A	1757	A
8	A	1758	U
8	A	1764	C
8	A	1773	A
8	A	1779	U
8	A	1781	U
8	A	1785	A
8	A	1791	A
8	A	1800	C
8	A	1801	A
8	A	1802	A
8	A	1808	A
8	A	1809	A
8	A	1814	G
8	A	1815	A
8	A	1816	C
8	A	1829	A
8	A	1833	C
8	A	1835	2MG
8	A	1838	C
8	A	1857	G
8	A	1862	G
8	A	1866	A
8	A	1869	G
8	A	1871	A
8	A	1873	G
8	A	1884	G
8	A	1889	A
8	A	1890	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1901	A
8	A	1906	G
8	A	1908	C
8	A	1910	G
8	A	1912	A
8	A	1913	A
8	A	1914	C
8	A	1916	A
8	A	1917	PSU
8	A	1918	A
8	A	1919	A
8	A	1922	G
8	A	1924	C
8	A	1925	C
8	A	1926	U
8	A	1927	A
8	A	1929	G
8	A	1930	G
8	A	1937	A
8	A	1938	A
8	A	1939	5MU
8	A	1942	C
8	A	1955	U
8	A	1964	G
8	A	1965	C
8	A	1967	C
8	A	1970	A
8	A	1971	U
8	A	1972	G
8	A	1976	U
8	A	1977	A
8	A	1982	U
8	A	1991	U
8	A	1992	G
8	A	1993	U
8	A	1997	C
8	A	2020	A
8	A	2022	U
8	A	2023	C
8	A	2032	G
8	A	2033	A
8	A	2034	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2036	C
8	A	2043	C
8	A	2046	G
8	A	2052	A
8	A	2055	C
8	A	2056	G
8	A	2060	A
8	A	2061	G
8	A	2062	A
8	A	2069	G7M
8	A	2076	U
8	A	2089	C
8	A	2092	U
8	A	2093	G
8	A	2101	A
8	A	2102	G
8	A	2103	C
8	A	2104	C
8	A	2107	G
8	A	2110	G
8	A	2111	U
8	A	2112	G
8	A	2114	A
8	A	2115	G
8	A	2116	G
8	A	2118	U
8	A	2119	A
8	A	2120	G
8	A	2123	G
8	A	2124	G
8	A	2125	G
8	A	2126	A
8	A	2127	G
8	A	2128	G
8	A	2129	C
8	A	2130	U
8	A	2131	U
8	A	2132	U
8	A	2133	G
8	A	2134	A
8	A	2135	A
8	A	2136	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2138	G
8	A	2139	U
8	A	2143	C
8	A	2146	C
8	A	2147	A
8	A	2148	G
8	A	2150	C
8	A	2151	U
8	A	2153	C
8	A	2154	A
8	A	2155	U
8	A	2157	G
8	A	2159	G
8	A	2161	C
8	A	2162	G
8	A	2163	A
8	A	2164	C
8	A	2166	U
8	A	2169	A
8	A	2170	A
8	A	2171	A
8	A	2172	U
8	A	2173	A
8	A	2175	C
8	A	2180	U
8	A	2181	U
8	A	2182	U
8	A	2183	A
8	A	2186	G
8	A	2187	U
8	A	2188	U
8	A	2190	G
8	A	2193	G
8	A	2194	U
8	A	2198	A
8	A	2203	U
8	A	2204	G
8	A	2212	A
8	A	2213	U
8	A	2225	A
8	A	2226	C
8	A	2238	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2239	G
8	A	2243	U
8	A	2266	A
8	A	2267	A
8	A	2273	A
8	A	2279	G
8	A	2280	G
8	A	2283	C
8	A	2287	A
8	A	2288	A
8	A	2304	G
8	A	2305	U
8	A	2307	G
8	A	2309	A
8	A	2320	U
8	A	2321	U
8	A	2322	A
8	A	2325	G
8	A	2327	A
8	A	2333	A
8	A	2335	A
8	A	2347	C
8	A	2350	C
8	A	2357	G
8	A	2358	A
8	A	2361	G
8	A	2382	G
8	A	2383	G
8	A	2384	U
8	A	2385	C
8	A	2388	A
8	A	2392	A
8	A	2402	U
8	A	2403	C
8	A	2406	A
8	A	2410	G
8	A	2423	U
8	A	2425	A
8	A	2429	G
8	A	2430	A
8	A	2432	A
8	A	2434	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2435	A
8	A	2438	U
8	A	2441	U
8	A	2445	2MG
8	A	2447	G
8	A	2448	A
8	A	2449	U
8	A	2450	A
8	A	2469	A
8	A	2475	C
8	A	2476	A
8	A	2478	A
8	A	2480	C
8	A	2484	G
8	A	2487	G
8	A	2491	U
8	A	2498	OMC
8	A	2501	C
8	A	2502	G
8	A	2504	PSU
8	A	2506	U
8	A	2518	A
8	A	2520	C
8	A	2529	G
8	A	2535	G
8	A	2547	A
8	A	2548	U
8	A	2553	G
8	A	2554	U
8	A	2556	C
8	A	2566	A
8	A	2567	G
8	A	2572	A
8	A	2573	C
8	A	2576	G
8	A	2585	U
8	A	2602	A
8	A	2603	G
8	A	2609	U
8	A	2613	U
8	A	2615	U
8	A	2621	G

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2623	G
8	A	2629	U
8	A	2630	G
8	A	2634	A
8	A	2646	C
8	A	2647	U
8	A	2654	A
8	A	2655	G
8	A	2656	U
8	A	2660	A
8	A	2663	G
8	A	2673	G
8	A	2682	A
8	A	2684	U
8	A	2689	U
8	A	2690	U
8	A	2702	G
8	A	2707	U
8	A	2712	C
8	A	2713	U
8	A	2714	G
8	A	2717	C
8	A	2726	A
8	A	2729	G
8	A	2733	A
8	A	2744	G
8	A	2748	A
8	A	2751	G
8	A	2752	C
8	A	2755	C
8	A	2757	A
8	A	2758	A
8	A	2764	A
8	A	2765	A
8	A	2769	U
8	A	2776	A
8	A	2778	A
8	A	2779	U
8	A	2780	G
8	A	2790	U
8	A	2791	G
8	A	2794	C

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2796	U
8	A	2797	U
8	A	2798	U
8	A	2799	A
8	A	2800	A
8	A	2801	G
8	A	2803	G
8	A	2804	U
8	A	2808	G
8	A	2809	A
8	A	2818	U
8	A	2820	A
8	A	2833	U
8	A	2834	G
8	A	2836	U
8	A	2846	G
8	A	2849	U
8	A	2866	U
8	A	2867	G
8	A	2872	A
8	A	2873	A
8	A	2879	A
8	A	2880	C
8	A	2883	A
8	A	2886	A
8	A	2894	G
8	A	2902	C
9	B	9	G
9	B	14	U
9	B	24	G
9	B	25	U
9	B	32	U
9	B	33	G
9	B	35	C
9	B	37	C
9	B	42	C
9	B	44	G
9	B	45	A
9	B	56	G
9	B	66	A
9	B	67	G
9	B	73	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	B	83	G
9	B	88	C
9	B	89	U
9	B	90	C
9	B	91	C
9	B	108	A
9	B	109	A
9	B	120	U
34	a	2	A
34	a	6	G
34	a	7	A
34	a	9	G
34	a	22	G
34	a	31	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	51	A
34	a	64	G
34	a	70	U
34	a	71	A
34	a	74	A
34	a	76	G
34	a	78	A
34	a	80	A
34	a	81	A
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	89	U
34	a	92	U
34	a	94	G
34	a	96	U
34	a	108	G
34	a	119	A
34	a	121	U
34	a	130	A
34	a	131	A
34	a	141	G
34	a	144	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	154	U
34	a	160	A
34	a	161	A
34	a	166	U
34	a	182	A
34	a	183	C
34	a	184	G
34	a	197	A
34	a	198	G
34	a	205	A
34	a	208	U
34	a	210	C
34	a	211	G
34	a	218	U
34	a	240	G
34	a	245	U
34	a	247	G
34	a	251	G
34	a	262	A
34	a	266	G
34	a	267	C
34	a	281	G
34	a	289	G
34	a	298	A
34	a	299	G
34	a	306	A
34	a	321	A
34	a	328	C
34	a	329	A
34	a	344	A
34	a	346	G
34	a	352	C
34	a	356	A
34	a	363	A
34	a	367	U
34	a	371	A
34	a	372	C
34	a	373	A
34	a	376	G
34	a	377	G
34	a	381	C
34	a	383	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	384	G
34	a	388	G
34	a	397	A
34	a	406	G
34	a	411	A
34	a	413	G
34	a	414	A
34	a	421	U
34	a	423	G
34	a	424	G
34	a	428	G
34	a	429	U
34	a	439	U
34	a	461	A
34	a	462	G
34	a	465	A
34	a	466	A
34	a	467	U
34	a	468	A
34	a	470	C
34	a	479	U
34	a	482	A
34	a	484	G
34	a	496	A
34	a	505	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	512	U
34	a	517	G
34	a	518	C
34	a	521	G
34	a	527	G7M
34	a	530	G
34	a	531	U
34	a	532	A
34	a	546	A
34	a	547	A
34	a	559	A
34	a	562	U
34	a	564	C
34	a	572	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	573	A
34	a	576	C
34	a	577	G
34	a	596	A
34	a	605	U
34	a	607	A
34	a	608	A
34	a	615	G
34	a	629	A
34	a	632	U
34	a	633	G
34	a	650	G
34	a	665	A
34	a	687	A
34	a	691	G
34	a	703	G
34	a	704	A
34	a	723	U
34	a	724	G
34	a	733	G
34	a	734	G
34	a	748	G
34	a	753	A
34	a	755	G
34	a	760	G
34	a	761	G
34	a	773	G
34	a	777	A
34	a	779	C
34	a	781	A
34	a	792	A
34	a	793	U
34	a	794	A
34	a	813	U
34	a	814	A
34	a	815	A
34	a	817	C
34	a	819	A
34	a	821	G
34	a	829	G
34	a	841	C
34	a	842	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	843	U
34	a	844	G
34	a	845	A
34	a	846	G
34	a	849	G
34	a	851	G
34	a	868	C
34	a	885	G
34	a	889	A
34	a	890	G
34	a	902	G
34	a	913	A
34	a	914	A
34	a	922	G
34	a	928	G
34	a	934	C
34	a	935	A
34	a	958	A
34	a	960	U
34	a	966	2MG
34	a	967	5MC
34	a	968	A
34	a	969	A
34	a	970	C
34	a	971	G
34	a	973	G
34	a	975	A
34	a	976	G
34	a	977	A
34	a	981	U
34	a	982	U
34	a	984	C
34	a	990	C
34	a	992	U
34	a	993	G
34	a	994	A
34	a	996	A
34	a	1004	A
34	a	1006	G
34	a	1012	A
34	a	1014	A
34	a	1016	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	1017	U
34	a	1020	G
34	a	1023	U
34	a	1025	U
34	a	1026	G
34	a	1030	U
34	a	1031	C
34	a	1032	G
34	a	1037	C
34	a	1043	G
34	a	1045	C
34	a	1050	G
34	a	1053	G
34	a	1056	U
34	a	1063	C
34	a	1065	U
34	a	1085	U
34	a	1086	U
34	a	1092	A
34	a	1094	G
34	a	1101	A
34	a	1104	G
34	a	1108	G
34	a	1126	U
34	a	1134	G
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1144	G
34	a	1147	C
34	a	1151	A
34	a	1159	U
34	a	1167	A
34	a	1168	U
34	a	1179	A
34	a	1182	G
34	a	1183	U
34	a	1184	G
34	a	1196	A
34	a	1197	A
34	a	1210	C
34	a	1211	U

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	1212	U
34	a	1213	A
34	a	1215	G
34	a	1218	C
34	a	1224	U
34	a	1225	A
34	a	1226	C
34	a	1227	A
34	a	1239	A
34	a	1241	G
34	a	1248	A
34	a	1254	A
34	a	1256	A
34	a	1257	A
34	a	1258	G
34	a	1260	G
34	a	1261	A
34	a	1270	G
34	a	1275	A
34	a	1278	G
34	a	1280	A
34	a	1281	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1294	G
34	a	1297	G
34	a	1298	U
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1305	G
34	a	1306	A
34	a	1307	U
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1322	C
34	a	1325	C
34	a	1331	G
34	a	1332	A
34	a	1338	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	1340	A
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1353	G
34	a	1361	G
34	a	1363	A
34	a	1370	G
34	a	1374	A
34	a	1378	C
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1408	A
34	a	1413	A
34	a	1417	G
34	a	1418	A
34	a	1419	G
34	a	1420	U
34	a	1426	G
34	a	1427	C
34	a	1428	A
34	a	1429	A
34	a	1434	A
34	a	1441	A
34	a	1442	G
34	a	1443	C
34	a	1446	A
34	a	1451	U
34	a	1452	C
34	a	1467	C
34	a	1472	U
34	a	1473	G
34	a	1474	U
34	a	1482	G
34	a	1483	A
34	a	1484	C
34	a	1485	U
34	a	1486	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	1487	G
34	a	1491	G
34	a	1492	A
34	a	1497	G
34	a	1499	A
34	a	1503	A
34	a	1504	G
34	a	1506	U
34	a	1517	G
34	a	1523	G
34	a	1529	G
34	a	1530	G
34	a	1533	C
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1538	C
34	a	1539	C
34	a	1540	U
55	v	9	G
55	v	16	C
55	v	18	G
55	v	20	H2U
55	v	21	A
55	v	24	U
55	v	33	U
55	v	34	C
55	v	38	A
55	v	42	G
55	v	43	A
55	v	44	A
55	v	46	A
55	v	47	U
55	v	48	C
55	v	52	G
55	v	55	PSU
55	v	56	C
55	v	57	A
55	v	75	C
55	v	76	A
56	w	7	A
56	w	8	4SU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
56	w	16	U
56	w	17	C
56	w	18	G
56	w	19	G
56	w	20	U
56	w	21	A
56	w	22	G
56	w	23	A
56	w	28	G
56	w	35	A
56	w	36	A
56	w	38	A
56	w	39	PSU
56	w	40	C
56	w	44	G
56	w	45	U
56	w	46	G7M
56	w	47	U
56	w	48	C
56	w	53	G
56	w	54	5MU
56	w	55	PSU
56	w	57	G
56	w	58	A
56	w	59	U
56	w	60	U
56	w	61	C
56	w	62	C
56	w	67	C
56	w	68	C
56	w	74	C
56	w	75	C
56	w	76	A
59	z	-1	C
59	z	0	U
59	z	2	U
59	z	3	G
59	z	4	U
59	z	5	U
59	z	7	G
59	z	8	U

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	242	G
8	A	310	A
8	A	369	U
8	A	446	G
8	A	458	G
8	A	479	A
8	A	481	G
8	A	503	A
8	A	530	G
8	A	545	U
8	A	555	G
8	A	571	U
8	A	715	A
8	A	774	G
8	A	784	G
8	A	883	G
8	A	894	U
8	A	1024	G
8	A	1062	G
8	A	1082	U
8	A	1090	A
8	A	1093	G
8	A	1182	G
8	A	1224	U
8	A	1300	G
8	A	1331	G
8	A	1451	C
8	A	1473	G
8	A	1490	A
8	A	1647	U
8	A	1663	G
8	A	1715	G
8	A	1730	C
8	A	1907	G
8	A	1912	A
8	A	1917	PSU
8	A	1918	A
8	A	1926	U
8	A	1939	5MU
8	A	2149	U
8	A	2150	C
8	A	2158	A
8	A	2192	U

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
8	A	2287	A
8	A	2319	G
8	A	2324	U
8	A	2428	G
8	A	2449	U
8	A	2468	A
8	A	2505	G
8	A	2655	G
8	A	2706	A
8	A	2728	U
8	A	2756	U
8	A	2796	U
8	A	2808	G
9	B	36	C
9	B	66	A
9	B	89	U

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

46 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	OMG	A	2251	8	18,26,27	1.24	2 (11%)	20,38,41	2.13	6 (30%)
34	UR3	a	1498	34	14,22,23	2.72	4 (28%)	15,32,35	0.79	0
58	FME	y	101	58	8,9,10	0.48	0	7,9,11	1.04	1 (14%)
8	2MA	A	2503	8	17,25,26	3.60	5 (29%)	19,37,40	1.61	3 (15%)
8	PSU	A	2580	8	17,21,22	1.34	3 (17%)	20,30,33	3.26	8 (40%)
34	5MC	a	967	34	15,22,23	3.14	5 (33%)	19,32,35	1.23	2 (10%)
34	2MG	a	1207	34	19,26,27	4.74	7 (36%)	21,38,41	2.09	8 (38%)
56	G7M	w	46	56	20,26,27	3.46	8 (40%)	20,39,42	2.48	5 (25%)
8	OMC	A	2498	8	15,22,23	0.93	0	17,31,34	1.40	2 (11%)
34	PSU	a	516	34	17,21,22	1.51	3 (17%)	20,30,33	3.07	7 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	MA6	a	1518	34	19,26,27	1.04	1 (5%)	18,38,41	2.55	2 (11%)
34	G7M	a	527	34	20,26,27	3.39	8 (40%)	20,39,42	2.29	5 (25%)
56	4SU	w	8	56	14,21,22	3.37	5 (35%)	15,30,33	1.21	2 (13%)
55	H2U	v	20	55	18,21,22	3.03	5 (27%)	21,30,33	2.04	5 (23%)
8	OMU	A	2552	8	14,22,23	3.35	5 (35%)	14,31,34	0.70	0
34	MA6	a	1519	34	19,26,27	1.03	1 (5%)	18,38,41	2.66	2 (11%)
56	5MU	w	54	56	15,22,23	1.17	1 (6%)	16,32,35	2.06	3 (18%)
8	PSU	A	2604	8	17,21,22	1.23	3 (17%)	20,30,33	3.02	7 (35%)
8	3TD	A	1915	8	21,23,23	6.71	9 (42%)	26,35,35	5.02	12 (46%)
55	4SU	v	8	55	14,21,22	3.23	5 (35%)	15,30,33	1.14	2 (13%)
8	2MG	A	1835	8	19,26,27	4.75	8 (42%)	21,38,41	2.26	8 (38%)
34	4OC	a	1402	34	16,23,24	3.18	6 (37%)	17,32,35	1.16	1 (5%)
8	PSU	A	1917	8	17,21,22	3.21	6 (35%)	20,30,33	4.30	12 (60%)
8	PSU	A	746	8	17,21,22	1.25	3 (17%)	20,30,33	3.25	6 (30%)
8	5MC	A	747	8	15,22,23	2.93	5 (33%)	19,32,35	1.31	3 (15%)
8	PSU	A	2504	8	17,21,22	1.22	3 (17%)	20,30,33	3.08	6 (30%)
8	PSU	A	955	8	17,21,22	1.12	2 (11%)	20,30,33	3.21	5 (25%)
8	6MZ	A	1618	8	18,25,26	2.17	4 (22%)	16,36,39	2.03	3 (18%)
8	PSU	A	1911	8	17,21,22	1.11	3 (17%)	20,30,33	3.13	6 (30%)
34	2MG	a	1516	34	19,26,27	4.75	8 (42%)	21,38,41	2.29	7 (33%)
55	5MU	v	54	55	15,22,23	2.82	3 (20%)	16,32,35	2.79	2 (12%)
8	2MG	A	2445	8	19,26,27	1.19	2 (10%)	21,38,41	2.26	7 (33%)
8	1MG	A	745	8	18,26,27	3.48	5 (27%)	19,39,42	1.94	2 (10%)
8	6MZ	A	2030	8	18,25,26	1.28	2 (11%)	16,36,39	2.30	6 (37%)
8	G7M	A	2069	8	20,26,27	3.34	8 (40%)	20,39,42	2.42	5 (25%)
55	PSU	v	55	55	17,21,22	1.09	2 (11%)	20,30,33	3.17	5 (25%)
34	2MG	a	966	34	19,26,27	4.76	7 (36%)	21,38,41	2.15	8 (38%)
34	5MC	a	1407	34	15,22,23	3.07	5 (33%)	19,32,35	1.41	3 (15%)
56	PSU	w	55	56	17,21,22	1.55	3 (17%)	20,30,33	3.19	7 (35%)
8	PSU	A	2457	8	17,21,22	1.69	3 (17%)	20,30,33	3.11	6 (30%)
56	PSU	w	32	56	17,21,22	2.56	4 (23%)	20,30,33	4.14	11 (55%)
56	MIA	w	37	56	24,31,32	3.90	9 (37%)	26,44,47	3.57	14 (53%)
8	PSU	A	2605	8	17,21,22	1.17	3 (17%)	20,30,33	3.03	6 (30%)
56	PSU	w	39	56	17,21,22	3.05	5 (29%)	20,30,33	4.39	14 (70%)
8	5MC	A	1962	8	15,22,23	2.99	5 (33%)	19,32,35	1.60	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	5MU	A	1939	8	15,22,23	2.85	3 (20%)	16,32,35	2.83	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
8	OMG	A	2251	8	-	2/5/27/28	0/3/3/3
34	UR3	a	1498	34	-	0/5/25/26	0/2/2/2
58	FME	y	101	58	-	4/7/9/11	-
8	2MA	A	2503	8	-	2/3/25/26	0/3/3/3
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
34	5MC	a	967	34	-	2/5/25/26	0/2/2/2
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
56	G7M	w	46	56	-	2/3/25/26	0/3/3/3
8	OMC	A	2498	8	-	1/7/27/28	0/2/2/2
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	3/7/29/30	0/3/3/3
34	G7M	a	527	34	-	2/3/25/26	0/3/3/3
56	4SU	w	8	56	-	0/5/25/26	0/2/2/2
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
8	OMU	A	2552	8	-	1/7/27/28	0/2/2/2
34	MA6	a	1519	34	-	3/7/29/30	0/3/3/3
56	5MU	w	54	56	-	1/5/25/26	0/2/2/2
8	PSU	A	2604	8	-	1/7/25/26	0/2/2/2
8	3TD	A	1915	8	-	4/10/26/26	0/2/2/2
55	4SU	v	8	55	-	1/5/25/26	0/2/2/2
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
34	4OC	a	1402	34	-	3/9/29/30	0/2/2/2
8	PSU	A	1917	8	-	5/7/25/26	0/2/2/2
8	PSU	A	746	8	-	4/7/25/26	0/2/2/2
8	5MC	A	747	8	-	0/5/25/26	0/2/2/2
8	PSU	A	2504	8	-	2/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	2/5/27/28	0/3/3/3
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
55	5MU	v	54	55	-	0/5/25/26	0/2/2/2

Continued on next page...



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
8	1MG	A	745	8	-	2/3/25/26	0/3/3/3
8	6MZ	A	2030	8	-	5/5/27/28	0/3/3/3
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
55	PSU	v	55	55	-	3/7/25/26	0/2/2/2
34	2MG	a	966	34	-	2/5/27/28	0/3/3/3
34	5MC	a	1407	34	-	0/5/25/26	0/2/2/2
56	PSU	w	55	56	-	2/7/25/26	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
56	PSU	w	32	56	-	3/7/25/26	0/2/2/2
56	MIA	w	37	56	-	6/11/33/34	0/3/3/3
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	5/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	2/5/25/26	0/2/2/2
8	5MU	A	1939	8	-	2/5/25/26	0/2/2/2

All (197) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C2'-C1'	-21.88	1.28	1.54
34	a	1516	2MG	C2-N2	15.74	1.47	1.34
34	a	1207	2MG	C2-N2	15.51	1.47	1.34
8	A	1835	2MG	C2-N2	15.49	1.47	1.34
34	a	966	2MG	C2-N2	15.35	1.47	1.34
56	w	37	MIA	C2-S10	-15.05	1.62	1.75
8	A	1915	3TD	O4'-C1'	13.48	1.64	1.44
56	w	39	PSU	C5-C1'	-9.56	1.44	1.52
55	v	20	H2U	C2-N1	9.24	1.48	1.35
55	v	54	5MU	C4-C5	8.94	1.60	1.41
8	A	1915	3TD	C5-C1'	-8.84	1.44	1.52
8	A	1939	5MU	C4-C5	8.82	1.60	1.41
34	a	966	2MG	C4-N3	8.80	1.49	1.35
56	w	46	G7M	C4-N3	8.75	1.49	1.35
8	A	1835	2MG	C4-N3	8.70	1.49	1.35
34	a	1207	2MG	C4-N3	8.69	1.49	1.35
34	a	527	G7M	C4-N3	8.69	1.49	1.35
56	w	32	PSU	C5-C1'	-8.62	1.44	1.52
8	A	745	1MG	C4-N3	8.48	1.49	1.35
8	A	2069	G7M	C4-N3	8.33	1.48	1.35
34	a	1516	2MG	C4-N3	8.14	1.48	1.35

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2503	2MA	C4-N3	8.04	1.48	1.35
56	w	8	4SU	C5-C4	7.67	1.47	1.38
8	A	1917	PSU	C5-C1'	-7.56	1.45	1.52
8	A	1618	6MZ	C6-N6	7.47	1.47	1.35
8	A	1962	5MC	C4-N3	7.41	1.45	1.35
34	a	1407	5MC	C4-N3	7.34	1.45	1.35
34	a	1402	4OC	C6-N1	7.34	1.44	1.35
56	w	37	MIA	C13-C14	7.24	1.53	1.32
8	A	2503	2MA	C6-C5	7.23	1.52	1.41
34	a	967	5MC	C4-N3	7.22	1.45	1.35
55	v	8	4SU	C5-C4	7.18	1.46	1.38
8	A	1915	3TD	O4'-C4'	-7.06	1.29	1.45
8	A	1917	PSU	C2'-C1'	-7.02	1.45	1.54
34	a	1498	UR3	C6-N1	6.99	1.44	1.35
8	A	747	5MC	C4-N3	6.94	1.45	1.35
34	a	966	2MG	C6-C5	6.92	1.53	1.41
34	a	527	G7M	C6-C5	6.91	1.53	1.41
8	A	2503	2MA	C2-N3	6.91	1.46	1.34
8	A	2069	G7M	C6-C5	6.89	1.53	1.41
8	A	745	1MG	C2-N3	6.88	1.44	1.34
8	A	2552	OMU	C4-N3	6.86	1.45	1.33
56	w	46	G7M	C6-C5	6.83	1.53	1.41
8	A	1915	3TD	C6-C5	6.81	1.48	1.38
8	A	2552	OMU	C6-N1	6.75	1.44	1.35
34	a	1516	2MG	C6-C5	6.69	1.52	1.41
8	A	745	1MG	C2-N2	6.63	1.47	1.33
8	A	1835	2MG	C6-C5	6.51	1.52	1.41
8	A	1915	3TD	O3'-C3'	-6.48	1.27	1.43
34	a	1207	2MG	C6-C5	6.43	1.52	1.41
55	v	20	H2U	C2-N3	6.34	1.49	1.38
56	w	46	G7M	C6-N1	6.12	1.43	1.33
8	A	745	1MG	C6-C5	6.10	1.51	1.41
56	w	39	PSU	C2'-C1'	-6.09	1.47	1.54
8	A	2552	OMU	C2-N3	5.91	1.49	1.38
8	A	2503	2MA	C2-N1	5.73	1.44	1.34
34	a	966	2MG	C6-N1	5.73	1.43	1.33
34	a	527	G7M	C6-N1	5.72	1.43	1.33
8	A	2069	G7M	C6-N1	5.62	1.42	1.33
34	a	1207	2MG	C6-N1	5.61	1.42	1.33
34	a	1516	2MG	C6-N1	5.60	1.42	1.33
56	w	37	MIA	C2'-C1'	-5.56	1.45	1.53
8	A	1939	5MU	C4-N3	-5.53	1.23	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1407	5MC	C2-N3	5.50	1.49	1.38
8	A	1835	2MG	C6-N1	5.44	1.42	1.33
34	a	967	5MC	C2-N3	5.39	1.48	1.38
56	w	8	4SU	C6-N1	5.36	1.42	1.35
8	A	1962	5MC	C2-N3	5.34	1.48	1.38
34	a	1402	4OC	C4-N3	5.33	1.44	1.34
55	v	54	5MU	C4-N3	-5.30	1.23	1.33
34	a	527	G7M	C2-N2	5.29	1.44	1.33
56	w	46	G7M	C2-N2	5.25	1.44	1.33
56	w	46	G7M	C2-N1	5.17	1.44	1.35
8	A	747	5MC	C2-N3	5.08	1.48	1.38
8	A	2069	G7M	C2-N2	5.08	1.44	1.33
34	a	1402	4OC	C2-N3	5.04	1.48	1.38
34	a	1498	UR3	C6-C5	4.99	1.49	1.38
55	v	20	H2U	C4-N3	4.98	1.46	1.37
55	v	8	4SU	C4-S4	-4.98	1.58	1.67
34	a	967	5MC	C5-C4	4.96	1.49	1.41
55	v	8	4SU	C6-N1	4.95	1.41	1.35
34	a	967	5MC	C4-N4	4.93	1.46	1.34
8	A	2457	PSU	C5-C1'	-4.90	1.48	1.52
56	w	8	4SU	C6-C5	4.89	1.48	1.38
34	a	1407	5MC	C4-N4	4.84	1.46	1.34
56	w	8	4SU	C2-N3	4.83	1.47	1.38
8	A	747	5MC	C4-N4	4.83	1.46	1.34
8	A	1962	5MC	C4-N4	4.83	1.46	1.34
8	A	2069	G7M	C2-N1	4.77	1.43	1.35
56	w	8	4SU	C4-S4	-4.75	1.58	1.67
8	A	1915	3TD	C2-N1	4.75	1.47	1.38
34	a	1402	4OC	C6-C5	4.71	1.48	1.38
34	a	527	G7M	C2-N1	4.71	1.43	1.35
55	v	8	4SU	C2-N3	4.68	1.47	1.38
55	v	8	4SU	C6-C5	4.56	1.48	1.38
8	A	2552	OMU	C6-C5	4.47	1.47	1.38
34	a	1498	UR3	C4-N3	4.33	1.44	1.38
8	A	1915	3TD	C6-N1	4.26	1.43	1.34
8	A	747	5MC	C5-C4	4.19	1.47	1.41
56	w	55	PSU	C5-C1'	-4.18	1.48	1.52
34	a	1407	5MC	C5-C4	4.13	1.47	1.41
8	A	1917	PSU	C2-N1	-3.99	1.30	1.38
34	a	1402	4OC	C4-N4	3.89	1.44	1.36
34	a	516	PSU	C5-C1'	-3.87	1.49	1.52
8	A	2251	OMG	C6-C5	3.86	1.48	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1402	4OC	C5-C4	3.83	1.48	1.39
8	A	2503	2MA	C6-N1	3.82	1.42	1.35
8	A	1962	5MC	C5-C4	3.70	1.47	1.41
34	a	1207	2MG	C2-N3	3.70	1.45	1.34
34	a	966	2MG	C2-N3	3.69	1.45	1.34
34	a	1516	2MG	C2-N3	3.68	1.45	1.34
34	a	967	5MC	C6-C5	3.65	1.50	1.40
8	A	1835	2MG	C2-N3	3.63	1.45	1.34
8	A	1917	PSU	C2-N3	-3.63	1.31	1.38
8	A	2030	6MZ	O3'-C3'	3.56	1.51	1.43
34	a	1407	5MC	C6-C5	3.56	1.49	1.40
8	A	2445	2MG	C6-C5	3.56	1.47	1.41
8	A	1917	PSU	C6-C5	-3.47	1.33	1.38
56	w	54	5MU	C4-C5	3.33	1.48	1.41
8	A	1962	5MC	C6-C5	3.26	1.49	1.40
8	A	1915	3TD	C4-C5	3.26	1.48	1.41
8	A	747	5MC	C6-C5	3.25	1.49	1.40
34	a	516	PSU	C4-C5	3.15	1.48	1.41
56	w	37	MIA	C4-N3	-3.14	1.30	1.35
8	A	1835	2MG	O6-C6	-3.10	1.16	1.24
34	a	1516	2MG	C2-N1	3.08	1.44	1.34
55	v	55	PSU	C4-N3	3.07	1.38	1.33
8	A	2580	PSU	O4'-C1'	-3.05	1.40	1.44
34	a	1207	2MG	C2-N1	3.04	1.43	1.34
34	a	966	2MG	C2-N1	3.03	1.43	1.34
56	w	55	PSU	C4-C5	2.99	1.47	1.41
8	A	1618	6MZ	C5-C4	-2.95	1.33	1.40
8	A	746	PSU	C4-N3	2.94	1.38	1.33
8	A	2457	PSU	O4'-C1'	-2.92	1.40	1.44
8	A	1835	2MG	C2-N1	2.91	1.43	1.34
34	a	1516	2MG	O6-C6	-2.88	1.17	1.24
34	a	1207	2MG	O6-C6	-2.87	1.17	1.24
34	a	966	2MG	O6-C6	-2.86	1.17	1.24
8	A	2604	PSU	C5-C1'	-2.85	1.49	1.52
56	w	32	PSU	C2-N1	-2.85	1.32	1.38
8	A	2504	PSU	C4-N3	2.83	1.38	1.33
8	A	2457	PSU	C4-N3	2.76	1.37	1.33
34	a	1518	MA6	C5-C4	-2.74	1.33	1.40
8	A	2580	PSU	C5-C1'	-2.73	1.49	1.52
56	w	37	MIA	C2'-C3'	-2.72	1.45	1.53
8	A	745	1MG	C6-N1	2.69	1.42	1.38
8	A	955	PSU	C4-N3	2.65	1.37	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	46	G7M	C2-N3	2.65	1.47	1.34
34	a	1519	MA6	C5-C4	-2.64	1.34	1.40
34	a	527	G7M	C2-N3	2.63	1.47	1.34
8	A	1618	6MZ	C2-N3	2.62	1.36	1.32
8	A	2605	PSU	C4-N3	2.61	1.37	1.33
8	A	2069	G7M	C5-C4	-2.61	1.36	1.39
8	A	746	PSU	C5-C1'	-2.60	1.50	1.52
8	A	1939	5MU	O4-C4	-2.59	1.18	1.24
8	A	1911	PSU	C4-N3	2.58	1.37	1.33
56	w	39	PSU	C2-N1	-2.57	1.33	1.38
8	A	2604	PSU	C4-N3	2.54	1.37	1.33
56	w	46	G7M	O6-C6	-2.52	1.18	1.24
8	A	2580	PSU	C4-N3	2.51	1.37	1.33
34	a	527	G7M	O6-C6	-2.50	1.18	1.24
8	A	2552	OMU	O4-C4	-2.50	1.18	1.24
34	a	1498	UR3	O4-C4	-2.48	1.18	1.24
8	A	2069	G7M	C2-N3	2.46	1.46	1.34
8	A	2069	G7M	O6-C6	-2.46	1.18	1.24
56	w	39	PSU	O4'-C1'	-2.44	1.41	1.44
56	w	37	MIA	C3'-C4'	-2.44	1.46	1.53
56	w	39	PSU	C3'-C4'	-2.44	1.46	1.53
34	a	527	G7M	C5-C4	-2.41	1.36	1.39
55	v	54	5MU	O4-C4	-2.40	1.18	1.24
8	A	1618	6MZ	C6-N1	-2.40	1.30	1.34
8	A	2504	PSU	O4'-C1'	-2.38	1.41	1.44
55	v	20	H2U	O4-C4	-2.35	1.18	1.23
56	w	46	G7M	C5-C4	-2.34	1.36	1.39
8	A	2604	PSU	O4'-C1'	-2.32	1.41	1.44
56	w	37	MIA	O5'-C5'	-2.29	1.39	1.44
8	A	2605	PSU	O4'-C1'	-2.29	1.41	1.44
55	v	20	H2U	O2-C2	-2.26	1.18	1.23
8	A	2504	PSU	C5-C1'	-2.23	1.50	1.52
8	A	2251	OMG	C5-C4	2.18	1.46	1.40
8	A	955	PSU	O4'-C1'	-2.17	1.41	1.44
8	A	1835	2MG	C5-C4	-2.14	1.35	1.40
8	A	2445	2MG	C5-C4	2.14	1.46	1.40
8	A	2030	6MZ	C5-C4	2.14	1.46	1.40
8	A	2605	PSU	C5-C1'	-2.13	1.50	1.52
8	A	1911	PSU	C5-C1'	-2.13	1.50	1.52
56	w	55	PSU	C2-N3	-2.13	1.34	1.38
34	a	516	PSU	C2-N3	-2.12	1.34	1.38
8	A	746	PSU	O4'-C1'	-2.12	1.41	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	32	PSU	O5'-C5'	-2.12	1.39	1.44
56	w	32	PSU	O4'-C1'	-2.11	1.41	1.44
8	A	1917	PSU	C6-N1	-2.11	1.30	1.34
56	w	37	MIA	O4'-C4'	-2.11	1.40	1.45
34	a	1516	2MG	C5-C4	-2.07	1.35	1.40
56	w	37	MIA	C2-N3	-2.06	1.30	1.34
55	v	55	PSU	O4'-C1'	-2.05	1.41	1.44
8	A	1911	PSU	O4'-C1'	-2.02	1.41	1.44

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1915	3TD	C5-C1'-C2'	-12.76	92.56	115.32
8	A	1915	3TD	O9-P-O5'	-12.58	73.25	106.73
8	A	746	PSU	N1-C2-N3	-11.07	119.63	128.43
8	A	955	PSU	N1-C2-N3	-11.00	119.69	128.43
55	v	55	PSU	N1-C2-N3	-10.72	119.91	128.43
8	A	1911	PSU	N1-C2-N3	-10.69	119.94	128.43
8	A	1917	PSU	C5-C1'-C2'	-10.63	96.36	115.32
8	A	2580	PSU	N1-C2-N3	-10.61	119.99	128.43
8	A	1915	3TD	O9-P-OP1	-10.59	67.16	107.64
8	A	2457	PSU	N1-C2-N3	-10.47	120.11	128.43
8	A	2504	PSU	N1-C2-N3	-10.32	120.22	128.43
8	A	2605	PSU	N1-C2-N3	-10.18	120.33	128.43
8	A	2604	PSU	N1-C2-N3	-9.98	120.50	128.43
34	a	1519	MA6	N1-C6-N6	-9.71	106.83	117.06
56	w	39	PSU	C5-C1'-C2'	-9.61	98.18	115.32
8	A	1939	5MU	C5-C6-N1	-9.14	112.35	122.19
34	a	1518	MA6	N1-C6-N6	-8.97	107.61	117.06
56	w	32	PSU	C4-N3-C2	8.49	122.31	115.14
56	w	55	PSU	N1-C2-N3	-8.34	121.80	128.43
55	v	54	5MU	C5-C6-N1	-8.29	113.26	122.19
8	A	1917	PSU	N1-C2-N3	-8.24	121.88	128.43
56	w	37	MIA	C12-C13-C14	-8.14	111.30	127.14
34	a	516	PSU	N1-C2-N3	-8.03	122.05	128.43
56	w	46	G7M	C1'-N9-C4	-7.96	112.65	126.64
56	w	32	PSU	N1-C2-N3	-7.79	122.24	128.43
56	w	39	PSU	C5-C4-N3	-7.69	115.45	125.36
8	A	2069	G7M	C1'-N9-C4	-7.57	113.34	126.64
56	w	32	PSU	C5-C4-N3	-7.44	115.78	125.36
8	A	1915	3TD	OP1-P-O5'	7.18	125.84	106.73
55	v	54	5MU	C4-N3-C2	7.15	121.18	115.14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	39	PSU	C4-N3-C2	7.11	121.15	115.14
55	v	20	H2U	C4-N3-C2	-7.05	119.94	125.79
56	w	32	PSU	C4'-O4'-C1'	-6.92	100.89	109.42
56	w	55	PSU	C4-N3-C2	6.90	120.96	115.14
8	A	745	1MG	C1'-N9-C4	-6.85	114.61	126.64
56	w	54	5MU	C4-N3-C2	6.45	120.59	115.14
56	w	32	PSU	C5-C1'-C2'	-6.35	103.99	115.32
8	A	955	PSU	C4-N3-C2	6.32	120.47	115.14
34	a	516	PSU	C4-N3-C2	6.31	120.47	115.14
34	a	527	G7M	C1'-N9-C4	-6.29	115.59	126.64
8	A	1917	PSU	C4-N3-C2	6.17	120.35	115.14
8	A	2030	6MZ	C2-N1-C6	6.16	121.87	116.59
8	A	1939	5MU	C4-N3-C2	6.16	120.34	115.14
55	v	55	PSU	C4-N3-C2	5.97	120.18	115.14
56	w	37	MIA	C11-S10-C2	-5.90	97.86	102.27
56	w	37	MIA	O3'-C3'-C2'	-5.85	92.88	111.82
8	A	2504	PSU	C4-N3-C2	5.81	120.05	115.14
8	A	1915	3TD	C3'-C2'-C1'	5.77	108.58	101.93
8	A	1915	3TD	O4'-C1'-C5	5.70	118.76	109.93
56	w	39	PSU	N1-C2-N3	-5.68	123.92	128.43
56	w	37	MIA	C5-C6-N1	-5.64	116.13	120.81
8	A	2580	PSU	C4-N3-C2	5.64	119.90	115.14
8	A	746	PSU	C4-N3-C2	5.61	119.88	115.14
8	A	1618	6MZ	C9-N6-C6	-5.59	118.06	122.87
56	w	39	PSU	C4'-O4'-C1'	-5.48	102.67	109.42
56	w	37	MIA	O2'-C2'-C3'	-5.41	94.31	111.82
34	a	1518	MA6	N3-C2-N1	-5.36	120.30	128.68
8	A	2605	PSU	C4-N3-C2	5.34	119.65	115.14
34	a	527	G7M	N3-C2-N1	-5.26	120.20	127.22
8	A	1917	PSU	O2'-C2'-C1'	-5.24	99.47	111.94
8	A	1911	PSU	C4-N3-C2	5.23	119.56	115.14
8	A	2251	OMG	C2-N3-C4	5.17	121.26	115.36
56	w	39	PSU	O4'-C1'-C2'	-5.15	96.32	104.66
56	w	55	PSU	C5-C4-N3	-5.11	118.78	125.36
34	a	1519	MA6	N3-C2-N1	-5.10	120.70	128.68
56	w	46	G7M	N3-C2-N1	-5.10	120.42	127.22
8	A	1915	3TD	C5-C6-N1	-5.08	118.20	124.44
8	A	2457	PSU	C4-N3-C2	5.04	119.39	115.14
8	A	2604	PSU	C4-N3-C2	5.03	119.39	115.14
56	w	39	PSU	O4'-C1'-C5	5.01	117.69	109.93
8	A	2069	G7M	N3-C2-N1	-5.00	120.55	127.22
8	A	1835	2MG	C1'-N9-C4	-4.99	117.87	126.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1917	PSU	C3'-C2'-C1'	4.90	107.58	101.93
34	a	516	PSU	C5-C4-N3	-4.88	119.07	125.36
56	w	37	MIA	O4'-C1'-C2'	-4.86	99.83	106.93
8	A	1618	6MZ	N3-C2-N1	-4.83	121.13	128.68
8	A	2445	2MG	C2-N3-C4	4.82	120.75	115.28
8	A	1915	3TD	C5-C4-N3	4.69	122.45	118.66
34	a	1516	2MG	C1'-N9-C4	-4.69	118.40	126.64
56	w	32	PSU	C2'-C3'-C4'	-4.67	93.56	102.64
8	A	2445	2MG	CM2-N2-C2	-4.65	117.98	123.59
34	a	1516	2MG	CM2-N2-C2	-4.63	118.01	123.59
56	w	37	MIA	C3'-C2'-C1'	4.53	107.79	100.98
56	w	39	PSU	C5-C6-N1	-4.51	118.89	124.44
34	a	966	2MG	CM2-N2-C2	-4.49	118.18	123.59
8	A	2457	PSU	C5-C4-N3	-4.46	119.61	125.36
55	v	55	PSU	C5-C4-N3	-4.46	119.61	125.36
34	a	966	2MG	C2-N3-C4	4.45	120.33	115.28
34	a	1207	2MG	C2-N3-C4	4.43	120.30	115.28
8	A	2504	PSU	C5-C4-N3	-4.42	119.66	125.36
34	a	527	G7M	C2-N3-C4	4.42	120.41	115.36
8	A	1835	2MG	C2-N3-C4	4.42	120.30	115.28
8	A	1917	PSU	C5-C4-N3	-4.41	119.68	125.36
56	w	37	MIA	C15-C14-C13	-4.40	109.94	122.65
8	A	2503	2MA	C2-N3-C4	4.39	119.09	115.52
8	A	955	PSU	C5-C4-N3	-4.35	119.76	125.36
8	A	2580	PSU	C5-C4-N3	-4.32	119.80	125.36
56	w	55	PSU	C5-C1'-C2'	-4.23	107.78	115.32
8	A	2604	PSU	C5-C4-N3	-4.20	119.94	125.36
8	A	746	PSU	C5-C4-N3	-4.15	120.01	125.36
8	A	2498	OMC	C2-N3-C4	4.11	120.51	116.34
34	a	1516	2MG	C2-N3-C4	4.10	119.94	115.28
8	A	1917	PSU	C4-C5-C1'	4.07	128.80	121.12
8	A	1835	2MG	N3-C2-N1	-4.03	119.86	126.23
8	A	2605	PSU	C5-C4-N3	-3.98	120.23	125.36
8	A	2445	2MG	C5-C6-N1	-3.95	118.02	123.43
34	a	1516	2MG	N2-C2-N1	3.94	120.75	116.96
8	A	1917	PSU	O4'-C1'-C2'	-3.92	98.31	104.66
34	a	516	PSU	C6-N1-C2	3.91	121.81	115.36
8	A	2030	6MZ	C9-N6-C6	-3.90	119.52	122.87
34	a	1207	2MG	N3-C2-N1	-3.86	120.13	126.23
8	A	746	PSU	C5-C1'-C2'	-3.85	108.44	115.32
56	w	55	PSU	C6-N1-C2	3.81	121.65	115.36
8	A	2251	OMG	C5-C6-N1	-3.81	118.22	123.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	516	PSU	C5-C6-N1	-3.81	119.76	124.44
34	a	1407	5MC	C2-N3-C4	3.81	120.61	116.02
8	A	2069	G7M	C2-N3-C4	3.79	119.69	115.36
8	A	1915	3TD	O9-P-OP2	-3.78	95.88	110.68
56	w	37	MIA	C4-C5-N7	-3.77	105.47	109.40
8	A	1911	PSU	C5-C4-N3	-3.76	120.52	125.36
8	A	2251	OMG	C6-N1-C2	3.75	121.89	115.93
56	w	37	MIA	C2'-C3'-C4'	-3.73	95.39	102.64
8	A	2457	PSU	C5-C6-N1	-3.73	119.86	124.44
56	w	55	PSU	C5-C6-N1	-3.70	119.89	124.44
8	A	2445	2MG	C6-N1-C2	3.67	121.76	115.18
34	a	1516	2MG	N3-C2-N1	-3.64	120.47	126.23
8	A	745	1MG	C2-N3-C4	3.64	119.51	115.36
56	w	46	G7M	C2-N3-C4	3.60	119.47	115.36
34	a	966	2MG	N3-C2-N1	-3.59	120.56	126.23
8	A	2445	2MG	C6-C5-C4	-3.55	117.41	120.80
34	a	1207	2MG	CM2-N2-C2	-3.55	119.31	123.59
8	A	2604	PSU	C5-C6-N1	-3.52	120.11	124.44
8	A	2251	OMG	C6-C5-C4	-3.52	117.44	120.80
8	A	1962	5MC	C2-N3-C4	3.51	120.25	116.02
56	w	54	5MU	C3'-C2'-C1'	3.50	106.25	100.98
56	w	39	PSU	C3'-C2'-C1'	-3.50	97.90	101.93
34	a	966	2MG	N2-C2-N1	3.44	120.27	116.96
34	a	967	5MC	C2-N3-C4	3.42	120.14	116.02
8	A	1915	3TD	O2'-C2'-C1'	-3.41	103.83	111.94
8	A	1835	2MG	N2-C2-N3	3.40	120.23	116.96
34	a	1207	2MG	N2-C2-N1	3.39	120.21	116.96
56	w	37	MIA	O2'-C2'-C1'	-3.38	98.39	110.85
8	A	1962	5MC	N4-C4-N3	3.37	121.80	117.03
34	a	1402	4OC	CM4-N4-C4	-3.37	120.07	122.97
8	A	1835	2MG	CM2-N2-C2	-3.37	119.53	123.59
34	a	1207	2MG	C1'-N9-C4	-3.36	120.73	126.64
8	A	1962	5MC	CM5-C5-C4	-3.33	118.35	121.72
8	A	1911	PSU	C5-C1'-C2'	-3.33	109.38	115.32
8	A	2503	2MA	C5-C6-N1	-3.32	119.58	123.06
8	A	2605	PSU	C5-C6-N1	-3.24	120.46	124.44
8	A	2457	PSU	C6-N1-C2	3.23	120.69	115.36
8	A	746	PSU	C6-N1-C2	3.19	120.63	115.36
8	A	1917	PSU	C6-N1-C2	3.19	120.61	115.36
8	A	1917	PSU	O4'-C1'-C5	3.17	114.84	109.93
8	A	2030	6MZ	C4-C5-N7	-3.16	106.10	109.40
8	A	1911	PSU	C5-C6-N1	-3.16	120.55	124.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	746	PSU	C5-C6-N1	-3.15	120.57	124.44
8	A	1911	PSU	C6-N1-C2	3.14	120.54	115.36
56	w	37	MIA	C16-C14-C13	-3.14	113.58	122.65
56	w	39	PSU	O4'-C4'-C3'	-3.12	98.94	105.11
8	A	1915	3TD	C6-N1-C2	3.11	120.49	115.36
8	A	2580	PSU	O4'-C1'-C5	-3.10	105.12	109.93
34	a	966	2MG	C1'-N9-C4	-3.09	121.21	126.64
55	v	20	H2U	N3-C2-N1	3.09	119.92	116.65
8	A	2251	OMG	N3-C2-N1	-3.08	123.12	127.22
8	A	1835	2MG	N2-C2-N1	3.07	119.91	116.96
55	v	55	PSU	C6-N1-C2	3.03	120.36	115.36
8	A	2604	PSU	C6-N1-C2	3.01	120.33	115.36
8	A	747	5MC	C2-N3-C4	2.96	119.59	116.02
8	A	2605	PSU	C6-N1-C2	2.96	120.23	115.36
56	w	8	4SU	C5-C4-N3	-2.94	119.89	123.83
34	a	1407	5MC	N4-C4-N3	2.94	121.19	117.03
55	v	20	H2U	C5-C4-N3	2.94	119.95	116.65
55	v	55	PSU	C5-C6-N1	-2.93	120.84	124.44
8	A	2030	6MZ	N3-C2-N1	-2.92	124.11	128.68
56	w	32	PSU	C5-C6-N1	-2.90	120.87	124.44
8	A	955	PSU	C6-N1-C2	2.89	120.12	115.36
34	a	516	PSU	C3'-C2'-C1'	2.88	105.25	101.93
8	A	1917	PSU	C4'-O4'-C1'	2.88	112.98	109.42
56	w	8	4SU	C2-N3-C4	2.86	119.29	115.15
8	A	2580	PSU	C6-N1-C2	2.84	120.05	115.36
34	a	1516	2MG	C5-C6-N1	-2.83	119.56	123.43
8	A	2251	OMG	C4-C5-N7	-2.81	106.47	109.40
34	a	1207	2MG	N2-C2-N3	2.80	119.65	116.96
8	A	2580	PSU	C5-C1'-C2'	2.77	120.25	115.32
8	A	2504	PSU	C5-C1'-C2'	-2.74	110.43	115.32
55	v	8	4SU	C5-C4-N3	-2.72	120.19	123.83
8	A	747	5MC	N4-C4-N3	2.71	120.87	117.03
56	w	32	PSU	C4-C5-C1'	2.71	126.22	121.12
8	A	2069	G7M	C5-C6-N1	-2.68	119.76	123.43
55	v	20	H2U	C5-C6-N1	2.68	120.44	111.61
58	y	101	FME	O-C-CA	-2.68	117.77	124.78
56	w	39	PSU	C6-N1-C2	2.67	119.76	115.36
8	A	2580	PSU	C5-C6-N1	-2.66	121.17	124.44
55	v	8	4SU	C2-N3-C4	2.66	119.01	115.15
8	A	2580	PSU	O4'-C1'-C2'	2.64	108.94	104.66
55	v	20	H2U	O2-C2-N1	-2.64	119.79	123.11
56	w	54	5MU	C5-C6-N1	-2.63	119.36	122.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	32	PSU	C6-N1-C2	2.63	119.69	115.36
8	A	2503	2MA	N3-C2-N1	-2.62	120.89	125.72
8	A	1915	3TD	C5'-C4'-C3'	-2.61	105.40	115.18
8	A	2504	PSU	C6-N1-C2	2.61	119.66	115.36
8	A	2604	PSU	C5-C1'-C2'	-2.54	110.78	115.32
34	a	966	2MG	C5-C6-N1	-2.53	119.98	123.43
34	a	1207	2MG	C5-C6-N1	-2.52	119.98	123.43
56	w	32	PSU	O4'-C1'-C2'	2.50	108.70	104.66
34	a	1407	5MC	CM5-C5-C4	-2.50	119.20	121.72
8	A	747	5MC	C5-C6-N1	-2.42	119.58	122.19
56	w	46	G7M	C5-C6-N1	-2.40	120.15	123.43
8	A	2457	PSU	O4'-C1'-C2'	2.40	108.54	104.66
8	A	1835	2MG	C6-N1-C2	2.39	119.45	115.18
8	A	2030	6MZ	C2'-C3'-C4'	-2.39	98.00	102.64
8	A	1962	5MC	C5-C6-N1	-2.37	119.64	122.19
56	w	37	MIA	O4'-C4'-C3'	-2.36	100.45	105.11
34	a	1207	2MG	C6-N1-C2	2.34	119.36	115.18
8	A	2605	PSU	C5-C1'-C2'	-2.31	111.19	115.32
8	A	1917	PSU	O4'-C4'-C3'	-2.31	100.55	105.11
56	w	32	PSU	C5'-C4'-C3'	-2.30	106.54	115.18
34	a	966	2MG	N2-C2-N3	2.30	119.17	116.96
56	w	55	PSU	C3'-C2'-C1'	2.29	104.57	101.93
34	a	1516	2MG	C6-N1-C2	2.28	119.27	115.18
8	A	2445	2MG	C4-C5-N7	-2.28	107.02	109.40
8	A	2504	PSU	C5-C6-N1	-2.28	121.64	124.44
34	a	516	PSU	C5-C1'-C2'	-2.27	111.27	115.32
56	w	39	PSU	O5'-C5'-C4'	2.27	116.70	108.99
8	A	2445	2MG	N2-C2-N1	2.25	119.12	116.96
56	w	39	PSU	C4-C5-C1'	-2.25	116.88	121.12
34	a	527	G7M	C5-C6-N1	-2.25	120.36	123.43
8	A	1835	2MG	C5-C6-N1	-2.23	120.38	123.43
34	a	967	5MC	N4-C4-N3	2.22	120.17	117.03
8	A	2069	G7M	C6-N1-C2	2.20	119.42	115.93
56	w	39	PSU	C2'-C3'-C4'	2.20	106.91	102.64
34	a	966	2MG	C6-N1-C2	2.18	119.07	115.18
8	A	1618	6MZ	C1'-N9-C4	-2.16	122.85	126.64
8	A	2498	OMC	N4-C4-N3	2.13	119.86	116.49
56	w	46	G7M	C6-N1-C2	2.09	119.25	115.93
8	A	955	PSU	C5-C6-N1	-2.03	121.94	124.44
56	w	37	MIA	C2-N1-C6	2.03	120.81	117.19
34	a	527	G7M	C6-N1-C2	2.02	119.14	115.93
8	A	2604	PSU	O4'-C1'-C2'	2.02	107.93	104.66

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2030	6MZ	O4'-C1'-C2'	-2.01	103.99	106.93

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
8	A	745	1MG	O4'-C4'-C5'-O5'
8	A	746	PSU	C2'-C1'-C5-C4
8	A	746	PSU	O4'-C1'-C5-C4
8	A	746	PSU	C2'-C1'-C5-C6
8	A	746	PSU	O4'-C1'-C5-C6
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C6
8	A	1917	PSU	C2'-C1'-C5-C4
8	A	1917	PSU	O4'-C1'-C5-C4
8	A	1917	PSU	C2'-C1'-C5-C6
8	A	1917	PSU	O4'-C1'-C5-C6
8	A	1962	5MC	O4'-C1'-N1-C6
8	A	1962	5MC	C2'-C1'-N1-C6
8	A	2030	6MZ	N1-C6-N6-C9
8	A	2030	6MZ	O4'-C4'-C5'-O5'
8	A	2030	6MZ	C3'-C4'-C5'-O5'
8	A	2251	OMG	C1'-C2'-O2'-CM2
8	A	2504	PSU	C3'-C4'-C5'-O5'
8	A	2504	PSU	O4'-C4'-C5'-O5'
8	A	2552	OMU	C1'-C2'-O2'-CM2
34	a	966	2MG	O4'-C4'-C5'-O5'
34	a	966	2MG	C3'-C4'-C5'-O5'
34	a	967	5MC	O4'-C4'-C5'-O5'
34	a	967	5MC	C3'-C4'-C5'-O5'
34	a	1402	4OC	C1'-C2'-O2'-CM2
34	a	1518	MA6	C5-C6-N6-C9
34	a	1518	MA6	C5-C6-N6-C10
34	a	1519	MA6	C3'-C4'-C5'-O5'
56	w	32	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C6
56	w	37	MIA	C5-C6-N6-C12
56	w	37	MIA	N1-C6-N6-C12
56	w	37	MIA	N1-C2-S10-C11
56	w	37	MIA	N3-C2-S10-C11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
56	w	39	PSU	O4'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C6
56	w	39	PSU	C3'-C4'-C5'-O5'
56	w	39	PSU	C4'-C5'-O5'-P
56	w	55	PSU	C3'-C4'-C5'-O5'
58	y	101	FME	O1-CN-N-CA
58	y	101	FME	N-CA-CB-CG
58	y	101	FME	C-CA-CB-CG
8	A	745	1MG	C3'-C4'-C5'-O5'
8	A	1835	2MG	O4'-C4'-C5'-O5'
8	A	1939	5MU	C3'-C4'-C5'-O5'
8	A	1939	5MU	O4'-C4'-C5'-O5'
8	A	2445	2MG	C3'-C4'-C5'-O5'
8	A	2498	OMC	O4'-C4'-C5'-O5'
8	A	2503	2MA	O4'-C4'-C5'-O5'
34	a	1402	4OC	O4'-C4'-C5'-O5'
56	w	39	PSU	O4'-C4'-C5'-O5'
56	w	55	PSU	O4'-C4'-C5'-O5'
8	A	1915	3TD	O4'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
34	a	1519	MA6	O4'-C4'-C5'-O5'
34	a	1518	MA6	N1-C6-N6-C10
8	A	2030	6MZ	C4'-C5'-O5'-P
8	A	2445	2MG	O4'-C4'-C5'-O5'
8	A	1835	2MG	C3'-C4'-C5'-O5'
34	a	527	G7M	C3'-C4'-C5'-O5'
58	y	101	FME	CB-CG-SD-CE
8	A	2503	2MA	C3'-C4'-C5'-O5'
34	a	1519	MA6	C4'-C5'-O5'-P
34	a	527	G7M	C4'-C5'-O5'-P
56	w	54	5MU	C4'-C5'-O5'-P
8	A	1917	PSU	C3'-C4'-C5'-O5'
55	v	55	PSU	C4'-C5'-O5'-P
8	A	1618	6MZ	C3'-C4'-C5'-O5'
8	A	2251	OMG	C4'-C5'-O5'-P
56	w	46	G7M	C4'-C5'-O5'-P
56	w	46	G7M	C3'-C4'-C5'-O5'
8	A	2604	PSU	O4'-C1'-C5-C4
8	A	1618	6MZ	O4'-C4'-C5'-O5'
56	w	32	PSU	O4'-C4'-C5'-O5'

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	2030	6MZ	C5-C6-N6-C9
55	v	8	4SU	O4'-C4'-C5'-O5'
8	A	2069	G7M	O4'-C4'-C5'-O5'
8	A	1915	3TD	C3'-C4'-C5'-O5'

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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	GDP	x	801	-	24,30,30	1.13	2 (8%)	31,47,47	2.27	10 (32%)
60	AM2	a	2001	-	40,40,40	0.83	1 (2%)	53,60,60	1.73	12 (22%)
61	PO4	x	802	-	4,4,4	1.11	0	6,6,6	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GDP	x	801	-	-	5/12/32/32	0/3/3/3
60	AM2	a	2001	-	-	4/12/84/84	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	x	801	GDP	C6-C5	3.85	1.48	1.41
60	a	2001	AM2	CA6-CA7	-2.62	1.48	1.53
62	x	801	GDP	C5-C4	2.02	1.46	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	x	801	GDP	PA-O3A-PB	-5.36	114.44	132.83
62	x	801	GDP	C2-N3-C4	5.01	121.07	115.36
62	x	801	GDP	C6-C5-C4	-4.61	116.40	120.80
60	a	2001	AM2	OA6-CA6-CA7	-4.20	101.18	109.66
60	a	2001	AM2	CA8-CA7-CA6	-3.87	98.68	110.06
60	a	2001	AM2	CC2-CC3-CC4	-3.81	104.93	111.37
60	a	2001	AM2	OA4-CA1-CA2	3.76	118.62	110.25
62	x	801	GDP	C6-N1-C2	3.73	121.85	115.93
60	a	2001	AM2	CA8-CA7-NA7	-3.52	104.71	111.00
62	x	801	GDP	C5-C6-N1	-3.47	118.68	123.43
60	a	2001	AM2	CA1-OA4-CA5	3.47	118.65	113.06
62	x	801	GDP	N3-C2-N1	-3.22	122.92	127.22
62	x	801	GDP	C4-C5-N7	-3.17	106.10	109.40
60	a	2001	AM2	CB5-CB4-NB4	-2.70	105.33	110.92
60	a	2001	AM2	CA5-CA6-CA7	-2.51	104.77	110.62
62	x	801	GDP	C2'-C3'-C4'	2.48	107.46	102.64
60	a	2001	AM2	CA6-CA7-NA7	-2.32	104.83	111.28
60	a	2001	AM2	CA1-OA1-CC1	-2.32	112.22	117.96
62	x	801	GDP	N2-C2-N1	2.28	120.80	117.25
60	a	2001	AM2	CA6-CA5-CA4	-2.16	105.97	110.93
62	x	801	GDP	O2B-PB-O3A	2.02	111.41	104.64
60	a	2001	AM2	OA8-CB1-CB2	-2.01	102.88	108.10

There are no chirality outliers.

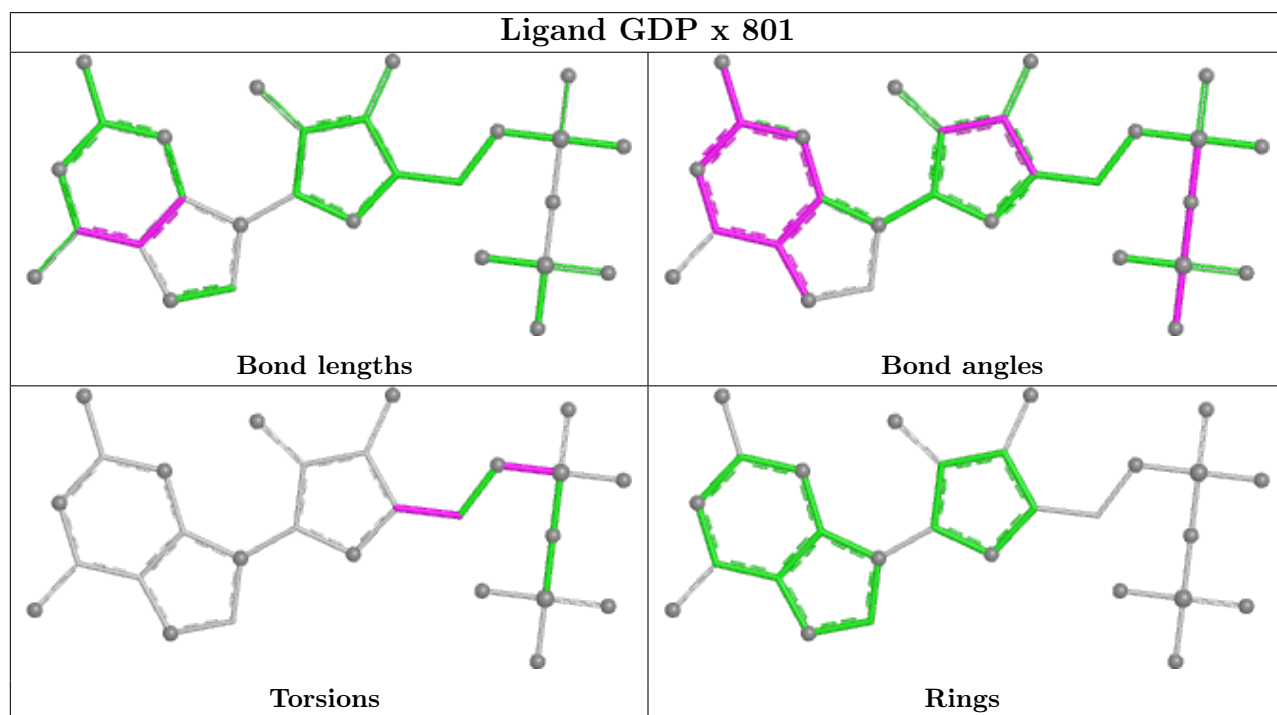
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	x	801	GDP	C5'-O5'-PA-O1A
62	x	801	GDP	C5'-O5'-PA-O2A
60	a	2001	AM2	OB1-CB5-CB6-OB6
62	x	801	GDP	O4'-C4'-C5'-O5'
60	a	2001	AM2	CB4-CB5-CB6-OB6
62	x	801	GDP	C3'-C4'-C5'-O5'
60	a	2001	AM2	CA8-CA7-NA7-CA9
60	a	2001	AM2	OA5-CA8-OA8-CB1
62	x	801	GDP	C5'-O5'-PA-O3A

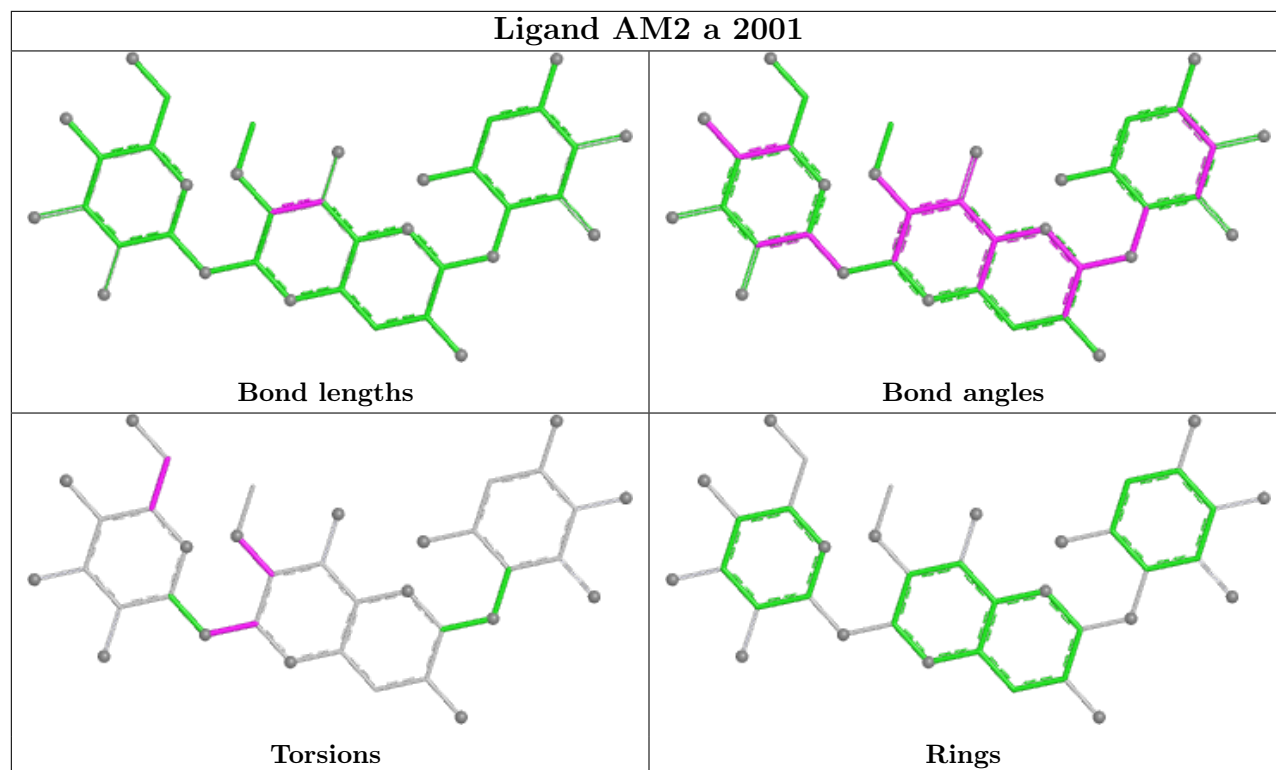
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

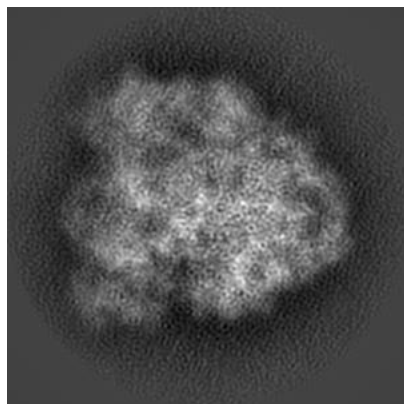
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13462. These allow visual inspection of the internal detail of the map and identification of artifacts.

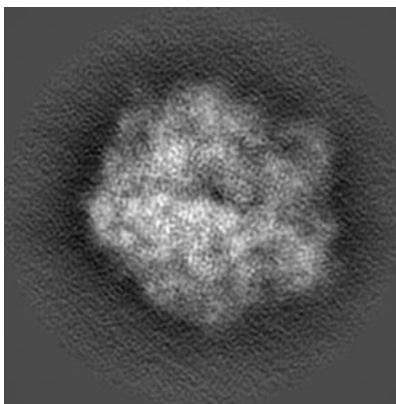
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

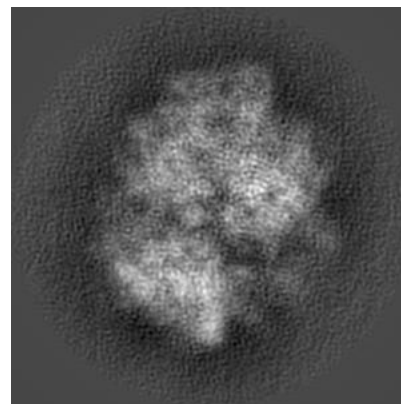
#### 6.1.1 Primary map



X

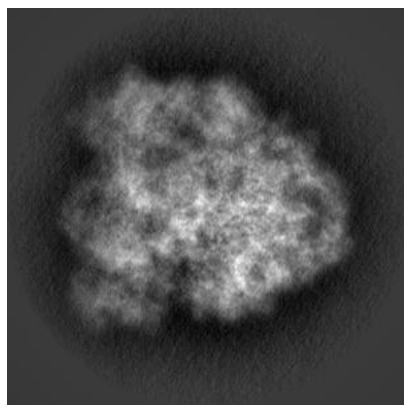


Y

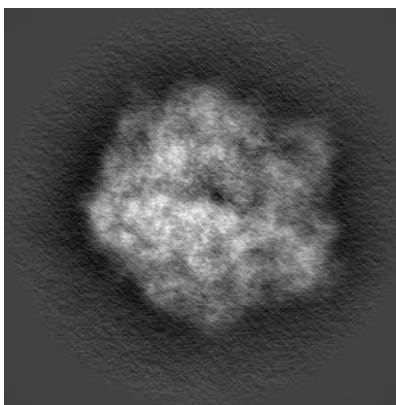


Z

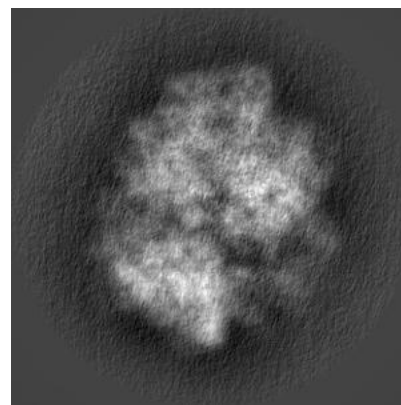
#### 6.1.2 Raw map



X



Y

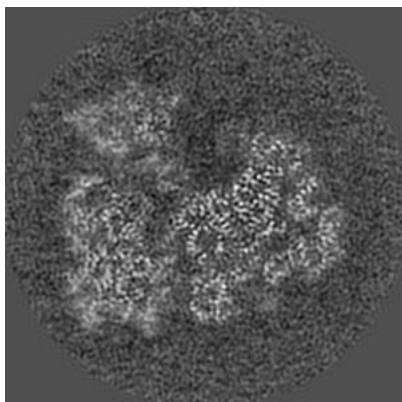


Z

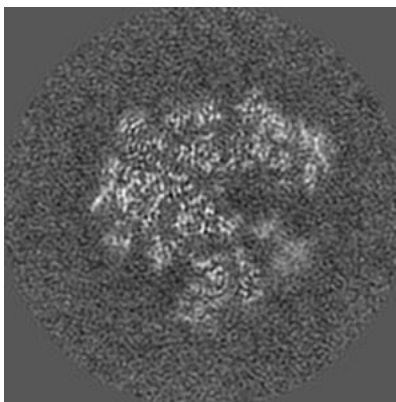
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

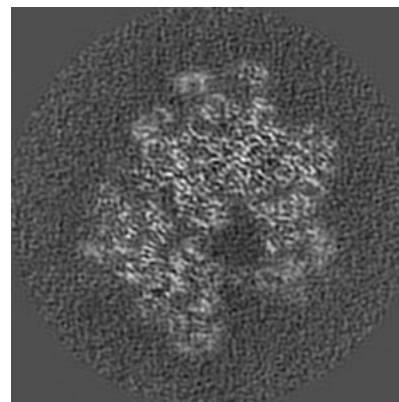
### 6.2.1 Primary map



X Index: 144

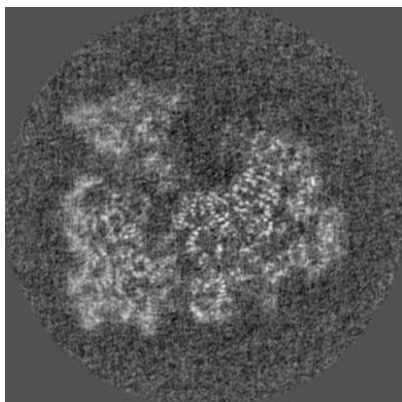


Y Index: 144

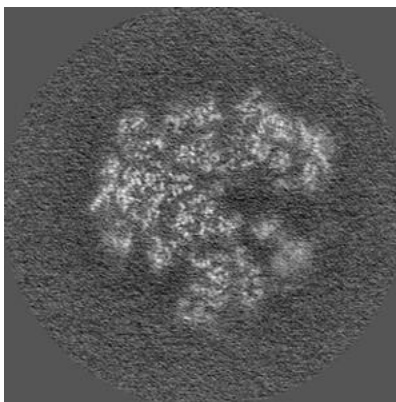


Z Index: 144

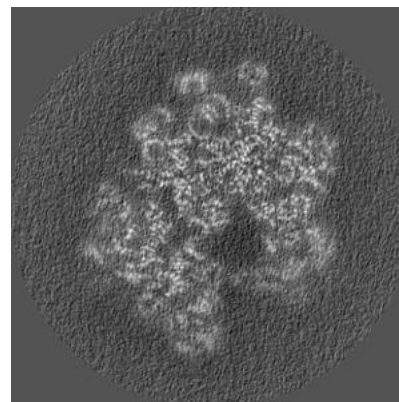
### 6.2.2 Raw map



X Index: 144



Y Index: 144

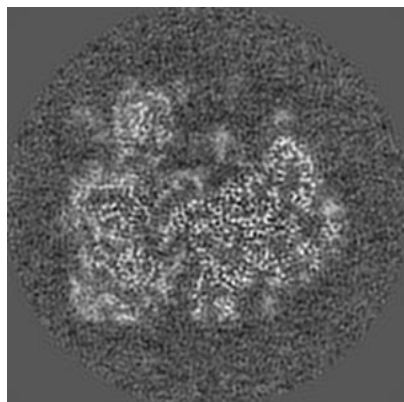


Z Index: 144

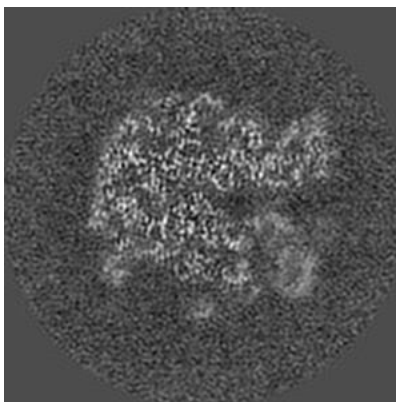
The images above show central slices of the map in three orthogonal directions.

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

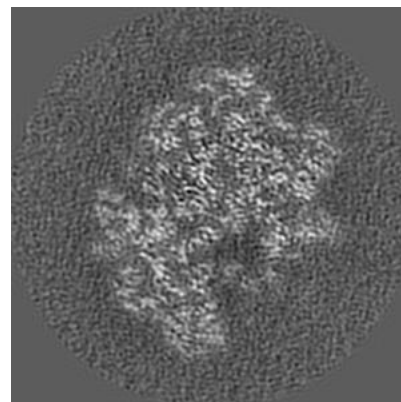
### 6.3.1 Primary map



X Index: 138

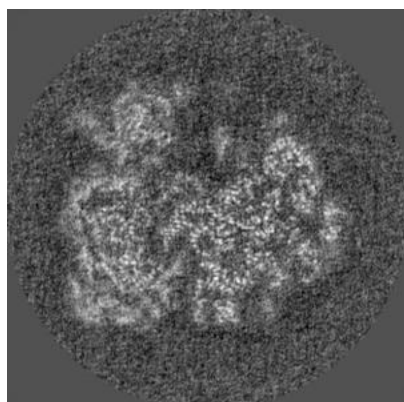


Y Index: 157

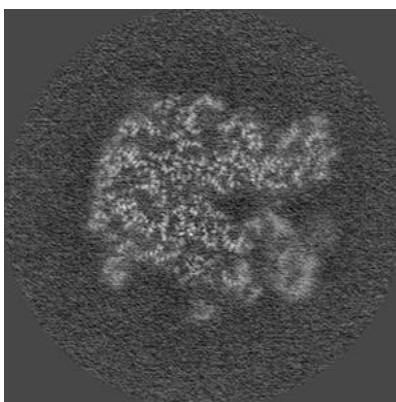


Z Index: 134

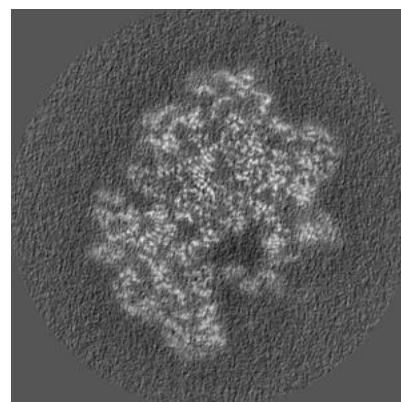
### 6.3.2 Raw map



X Index: 139



Y Index: 157

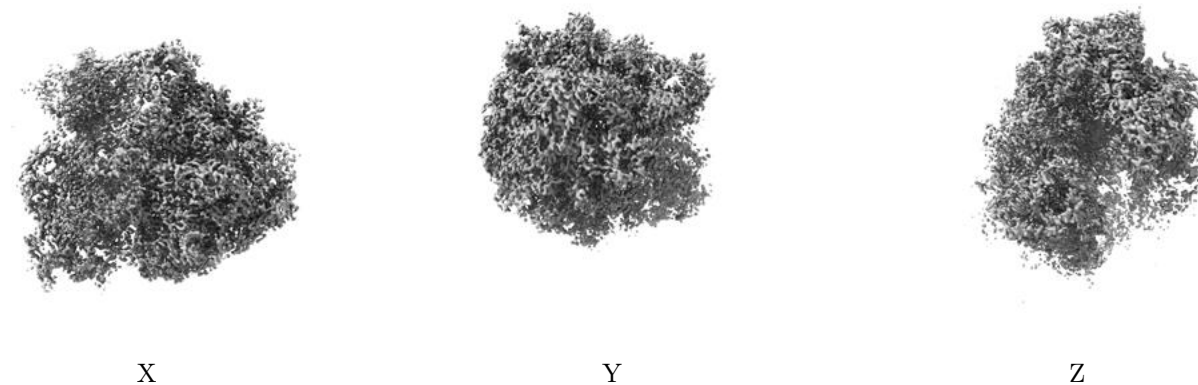


Z Index: 135

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

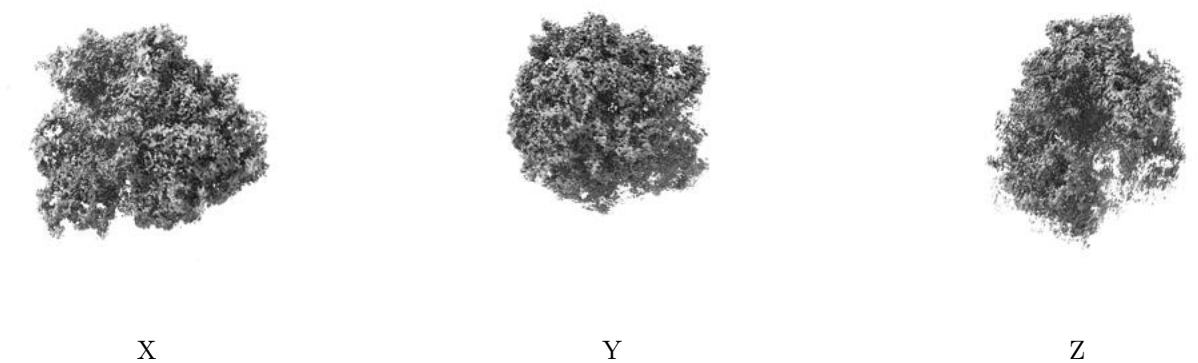
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

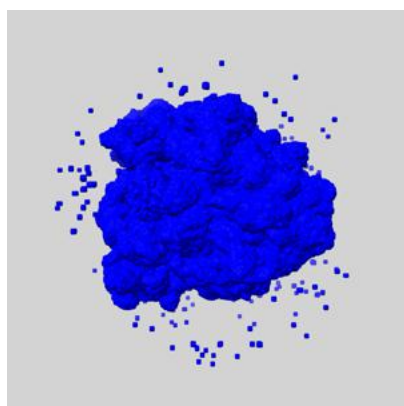
## 6.5 Mask visualisation [i](#)

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

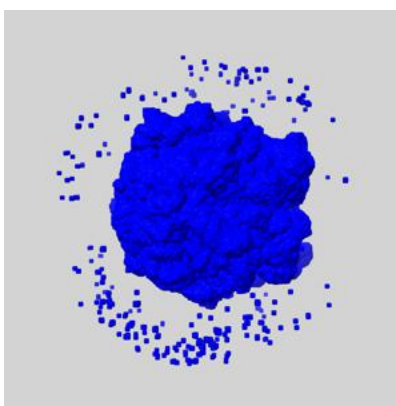
A mask typically either:

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

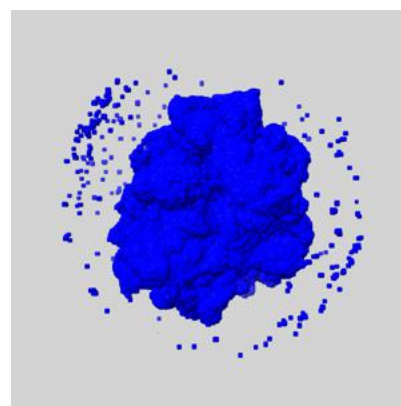
### 6.5.1 emd\_13462\_msk\_1.map [i](#)



X



Y

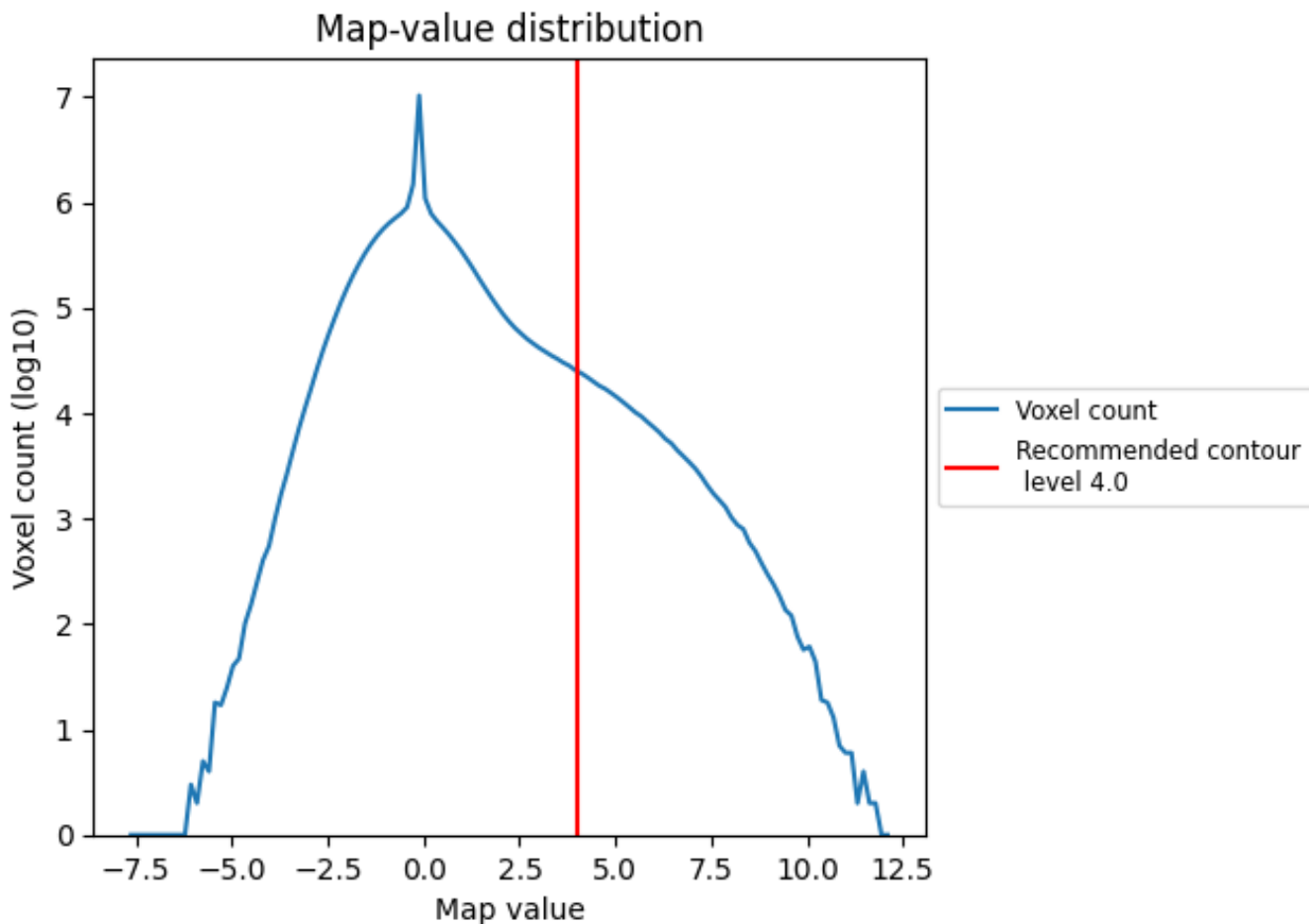


Z

## 7 Map analysis [i](#)

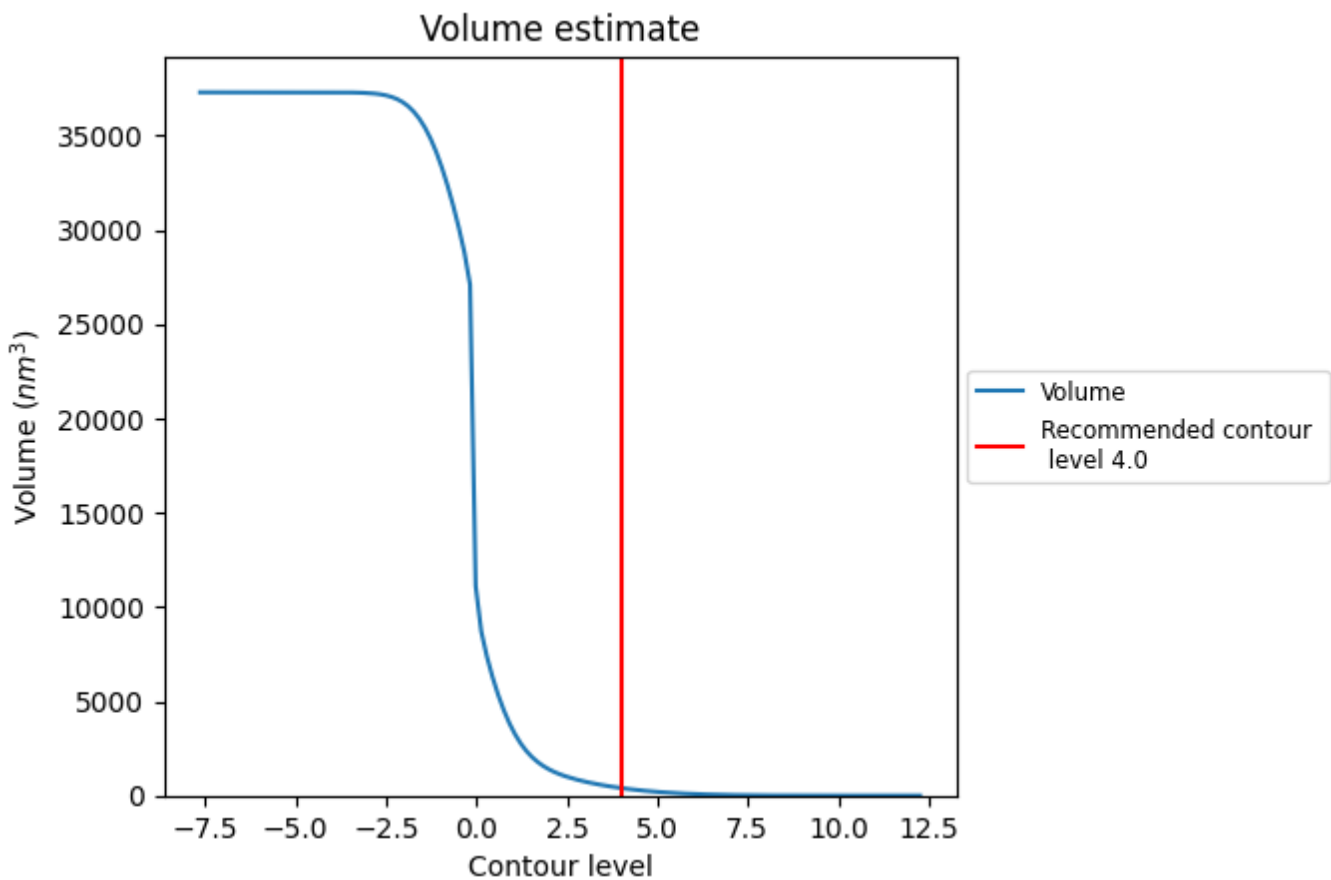
This section contains the results of statistical analysis of the map.

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



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

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

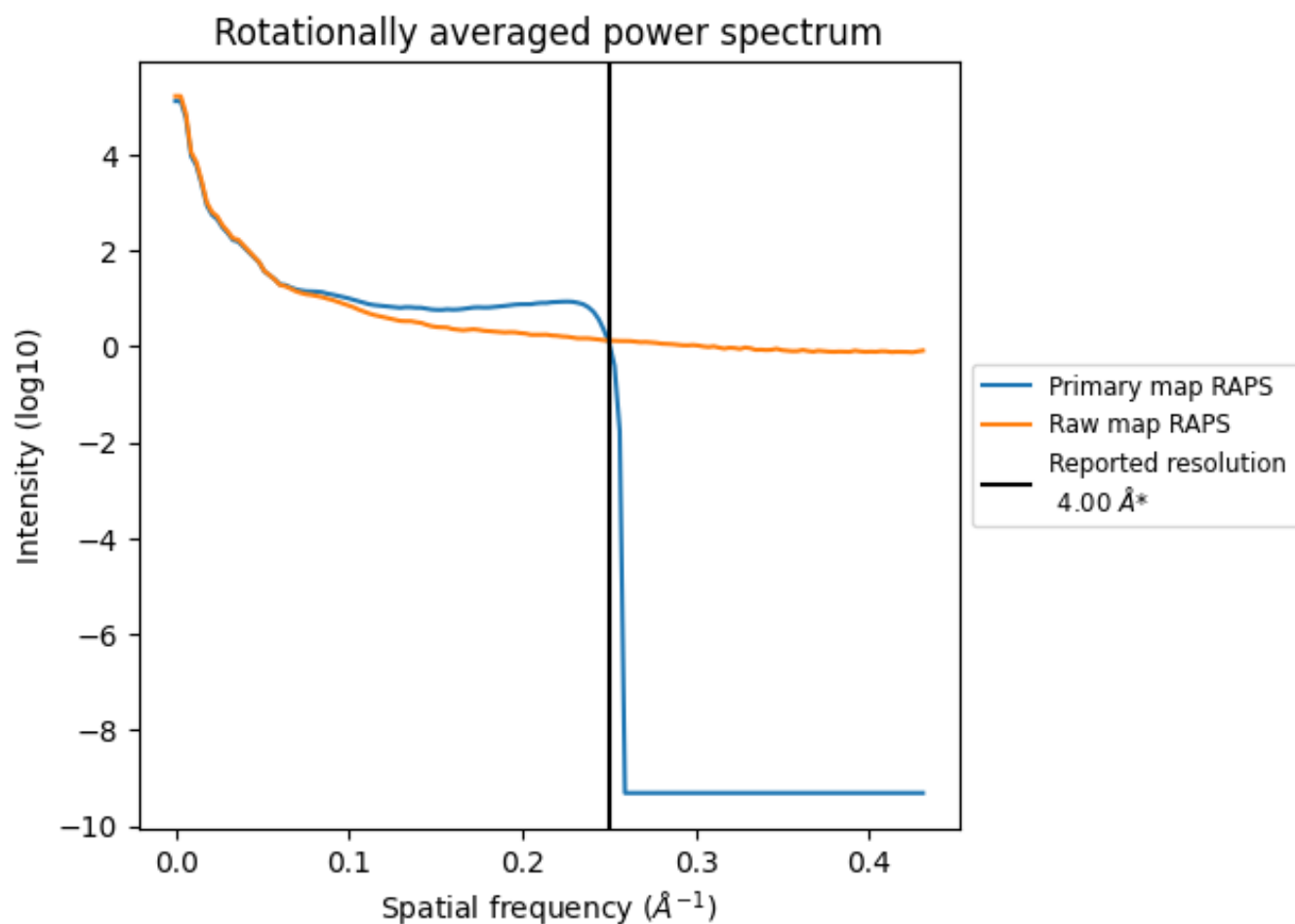


The volume at the recommended contour level is 397  $\text{nm}^3$ ; this corresponds to an approximate mass of 359 kDa.

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



### 7.3 Rotationally averaged power spectrum i

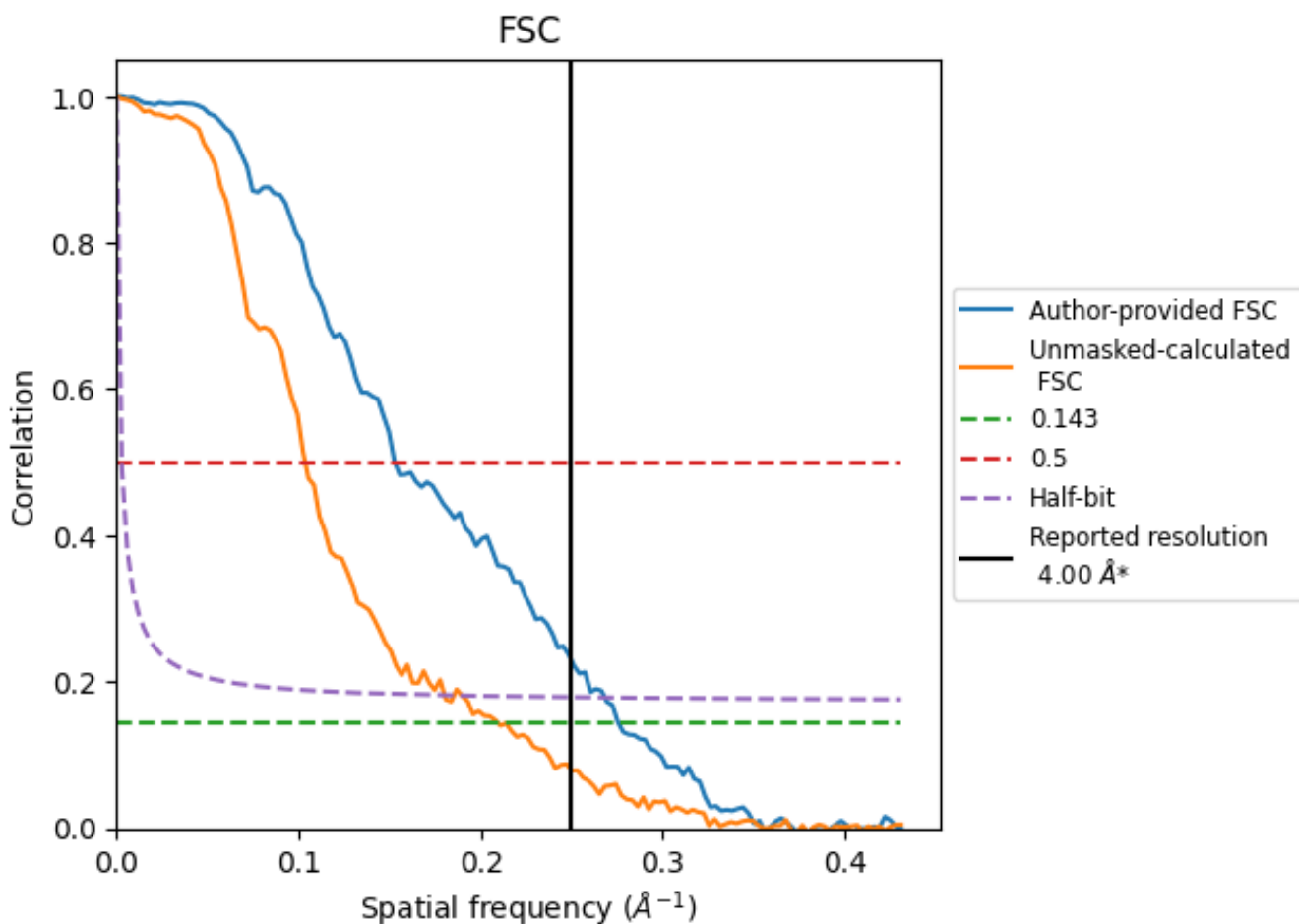


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 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 0.250 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

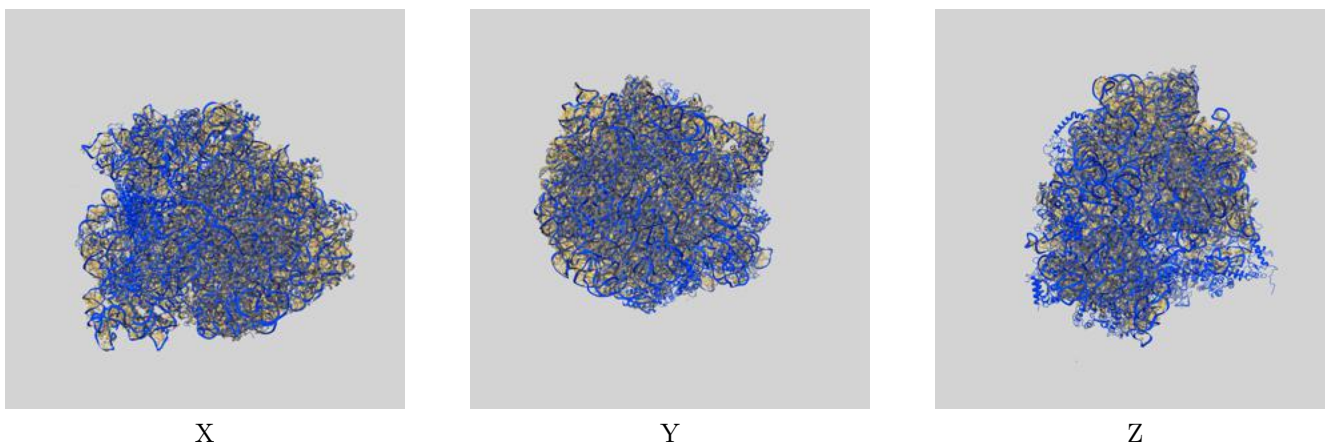
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.63	6.54	3.73
Unmasked-calculated*	4.77	9.64	5.55

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.77 differs from the reported value 4.0 by more than 10 %

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

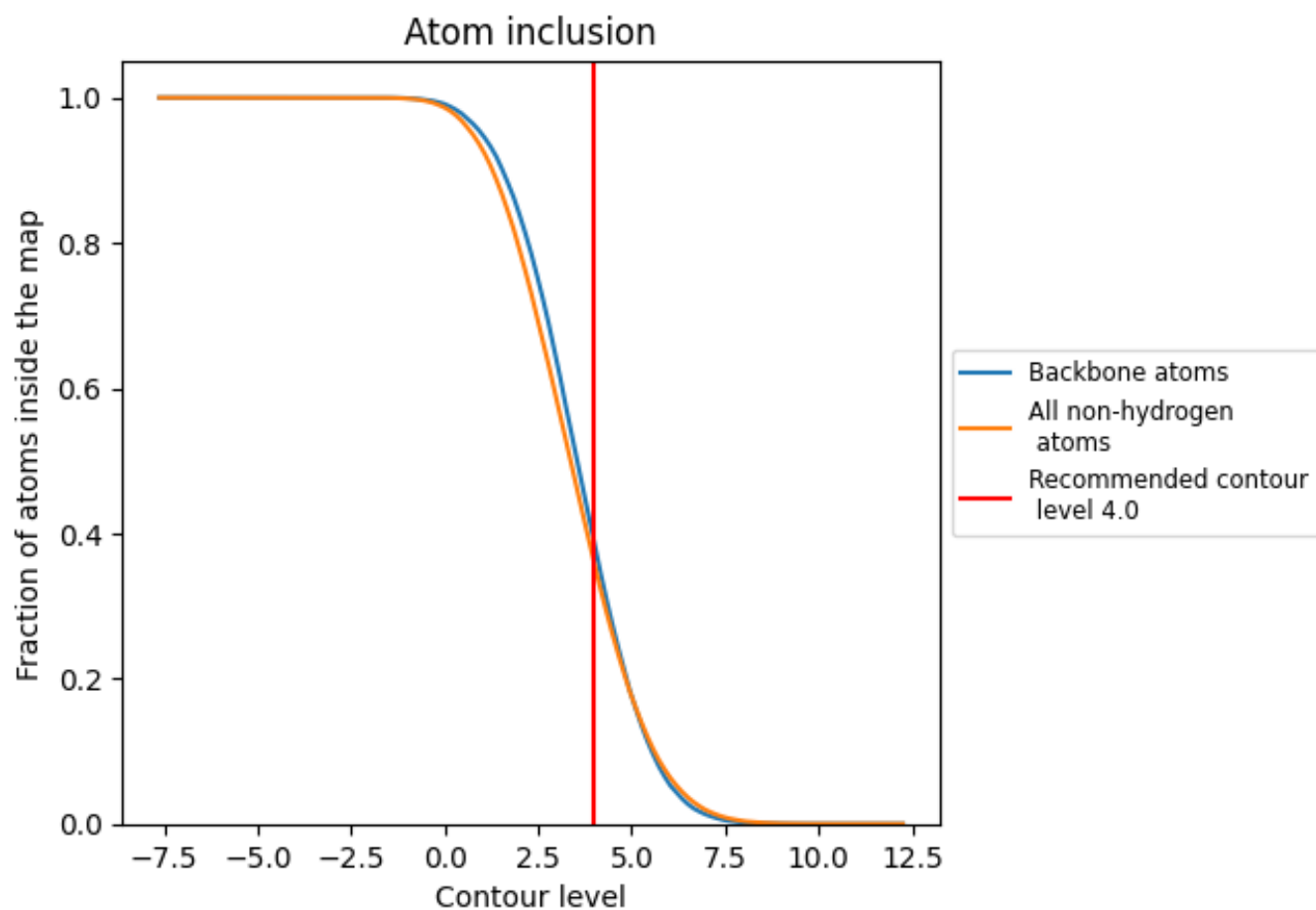
This section contains information regarding the fit between EMDB map EMD-13462 and PDB model 7PJW. Per-residue inclusion information can be found in section 3 on page 17.

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



The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.