



## Full wwPDB EM Validation Report ⓘ

Nov 30, 2022 – 05:08 am GMT

PDB ID : 7P7Q  
EMDB ID : EMD-13241  
Title : E. faecalis 70S ribosome bound by PoxA-EQ2, high-resolution combined volume  
Authors : Crowe-McAuliffe, C.; Wilson, D.N.  
Deposited on : 2021-07-20  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

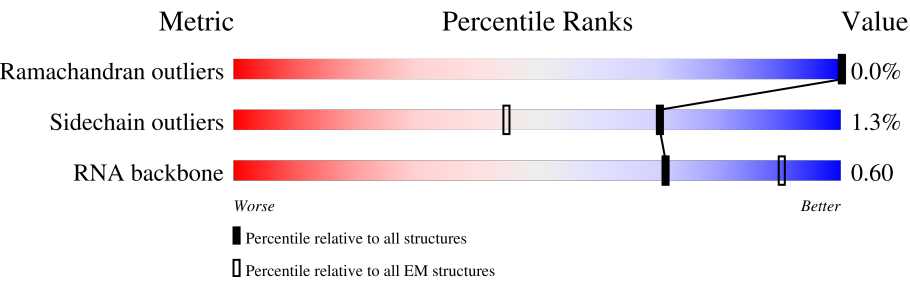
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 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	586	<div><div>87%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>90%</div><div>9%</div></div>
2	1	62	<div><div>47%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>94%</div><div>5%</div></div>
3	2	59	<div><div>22%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>97%</div><div>.</div></div>
4	3	89	<div><div>90%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>90%</div><div>10%</div></div>
5	4	59	<div><div>15%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>90%</div><div>10%</div></div>
6	5	49	<div><div>18%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>96%</div><div>..</div></div>
7	6	44	<div><div>5%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>100%</div><div></div></div>
8	7	66	<div><div>.</div><div><div></div><div></div><div></div><div></div><div></div></div><div>95%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
9	8	38	18% 97% .
10	A	2910	15% 66% 29% 5%
11	B	116	47% 59% 36% ..
12	D	77	73% 70% 27% ..
13	F	229	99% 97% ..
14	G	275	11% 100%
15	H	209	11% 98% ..
16	I	207	26% 99% .
17	J	179	99% 98% ..
18	K	178	92% 96% ..
19	M	147	18% 99% .
20	N	122	14% 100%
21	O	146	29% 98% .
22	P	144	17% 93% 7%
23	Q	127	15% 97% ..
24	R	118	69% 100%
25	S	115	19% 99% .
26	T	119	13% 98% ..
27	U	102	26% 99% .
28	V	115	10% 93% ..
29	W	96	28% 93% 5%
30	X	103	60% 98% .
31	Y	95	7% 77% 22%
32	Z	62	35% 98% .
33	a	1558	60% 67% 28% ..

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Mol	Chain	Length	Quality of chain
34	b	19	
35	c	261	
36	d	218	
37	e	203	
38	f	166	
39	g	100	
40	h	156	
41	i	132	
42	j	130	
43	k	102	
44	l	129	
45	m	137	
46	n	121	
47	o	61	
48	p	89	
49	q	91	
50	r	88	
51	s	79	
52	t	92	
53	u	83	

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 151202 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 ARE-ABC-F family resistance factor PoxTA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	534	Total	C	N	O	S	0	0
			4347	2789	720	823	15		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			491	307	91	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			428	266	80	81	1		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	80	Total	C	N	O	S	0	0
			647	409	110	126	2		

- Molecule 5 is a protein called 50S ribosomal protein L32-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	53	Total	C	N	O	S	0	0
			406	248	84	69	5		

- Molecule 6 is a protein called 50S ribosomal protein L33 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	48	Total	C	N	O	S	0	0
			410	247	84	75	4		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	44	Total	C	N	O	S	0	0
			374	227	91	54	2		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	64	Total	C	N	O	S	0	0
			522	320	122	78	2		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	38	Total	C	N	O	S	0	0
			305	188	66	45	6		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2901	Total	C	N	O	P	0	0
			62272	27798	11451	20122	2901		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	114	Total	C	N	O	P	0	0
			2439	1088	439	798	114		

- Molecule 12 is a RNA chain called fMet-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	76	Total	C	N	O	P	0	0
			1624	724	295	529	76		

- Molecule 13 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	226	Total	C	N	O	S	0	0
			1693	1073	287	327	6		

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	274	Total	C	N	O	S	0	0
			2106	1305	414	380	7		

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	206	Total	C	N	O	S	0	0
			1572	990	291	287	4		

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	205	Total	C	N	O	S	0	0
			1572	984	289	297	2		

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	177	Total	C	N	O	S	0	0
			1392	887	239	260	6		

- Molecule 18 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	174	Total	C	N	O	S	0	0
			1335	838	242	251	4		

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	147	Total	C	N	O	S	0	0
			1146	726	207	209	4		

- Molecule 20 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	122	Total	C	N	O	S	0	0
			923	574	176	171	2		

- Molecule 21 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	146	Total	C	N	O	S	0	0
			1096	677	212	206	1		

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	134	Total	C	N	O	S	0	0
			1070	683	209	173	5		

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	125	Total	C	N	O	S	0	0
			997	615	192	187	3		

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	118	Total	C	N	O	S	0	0
			908	561	176	169	2		

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	S	114	Total	C	N	O	0	0
			925	582	185	158		

- Molecule 26 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	118	Total	C	N	O	S	0	0
			950	602	184	160	4		

- Molecule 27 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	101	Total	C	N	O	S	0	0
			779	497	138	142	2		

- Molecule 28 is a protein called 50S ribosomal protein L22.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	111	Total	C	N	O	S	0	0
			841	527	154	158	2		

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	91	Total	C	N	O	S	0	0
			736	469	129	134	4		

- Molecule 30 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	101	Total	C	N	O	S	0	0
			763	486	135	140	2		

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	74	Total	C	N	O		0	0
			559	344	107	108			

- Molecule 32 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	61	Total	C	N	O	S	0	0
			480	299	97	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1521	Total	C	N	O	P	0	0
			32599	14546	5954	10578	1521		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	13	Total	C	N	O	P	0	0
			285	127	57	88	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	222	Total	C	N	O	S	0	0
			1773	1126	312	326	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	205	Total	C	N	O	S	0	0
			1618	1018	304	293	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	200	Total	C	N	O	S	0	0
			1611	1010	301	296	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	163	Total	C	N	O	S	0	0
			1204	759	222	221	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	96	Total	C	N	O	S	0	0
			786	496	135	152	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	153	Total	C	N	O	S	0	0
			1218	759	232	221	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	131	Total	C	N	O	S	0	0
			1041	662	184	193	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	127	Total	C	N	O	S	0	0
			980	610	195	174	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	96	Total	C	N	O	S	0	0
			773	487	142	142	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	116	Total	C	N	O	S	0	0
			854	527	162	161	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	119	IAS	ASN	conflict	UNP Q839E0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	134	Total	C	N	O	S	0	0
			1051	652	211	186	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	114	Total	C	N	O	S	0	0
			902	552	183	166	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	60	Total	C	N	O	S	0	0
			492	310	100	77	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	85	Total	C	N	O	S	0	0
			716	440	146	129	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	87	Total	C	N	O	S	0	0
			692	437	128	125	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	80	Total	C	N	O	S	0	0
			660	414	124	119	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	63	Total	C	N	O	S	0	0
			511	328	95	87	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	82	Total	C	N	O	S	0	0
			663	426	122	113	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	81	Total	C	N	O	S	0	0
			608	371	118	117	2		

- Molecule 54 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
54	0	1	Total	C	N	O	P	0
			62	20	10	26	6	
54	0	1	Total	C	N	O	P	0
			62	20	10	26	6	

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	0	2	Total	Mg	0
			2	2	
55	7	1	Total	Mg	0
			1	1	
55	A	143	Total	Mg	0
			143	143	
55	B	1	Total	Mg	0
			1	1	
55	G	1	Total	Mg	0
			1	1	
55	Q	1	Total	Mg	0
			1	1	
55	a	46	Total	Mg	0
			46	46	
55	n	1	Total	Mg	0
			1	1	

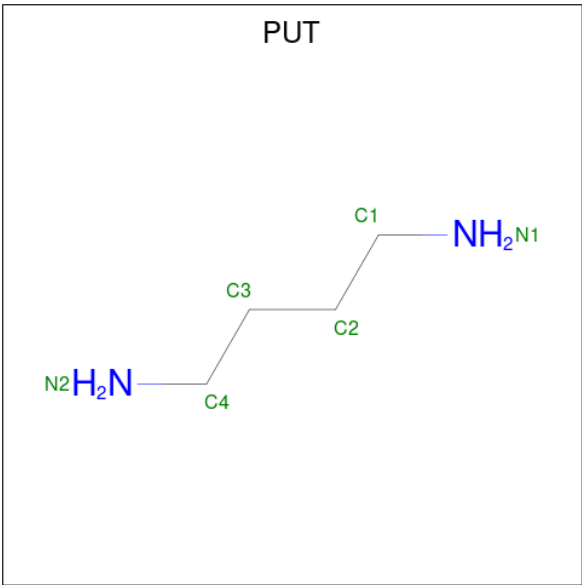
- Molecule 56 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
56	4	1	Total 1	K 1	0
56	7	2	Total 2	K 2	0
56	A	104	Total 104	K 104	0
56	B	3	Total 3	K 3	0
56	G	3	Total 3	K 3	0
56	P	1	Total 1	K 1	0
56	a	37	Total 37	K 37	0
56	g	1	Total 1	K 1	0
56	o	1	Total 1	K 1	0

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

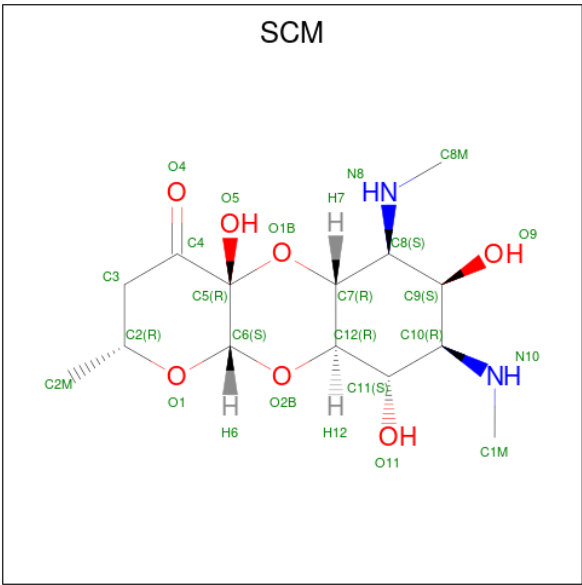
Mol	Chain	Residues	Atoms		AltConf
57	4	1	Total 1	Zn 1	0
57	5	1	Total 1	Zn 1	0
57	8	1	Total 1	Zn 1	0
57	o	1	Total 1	Zn 1	0

- Molecule 58 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
58	A	1	Total	C	N	0
			6	4	2	
58	a	1	Total	C	N	0
			12	8	4	
58	a	1	Total	C	N	0
			12	8	4	

- Molecule 59 is SPECTINOMYCIN (three-letter code: SCM) (formula: C<sub>14</sub>H<sub>24</sub>N<sub>2</sub>O<sub>7</sub>).



- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	0	2	Total 2	O 2	0
60	1	2	Total 2	O 2	0
60	2	1	Total 1	O 1	0
60	4	4	Total 4	O 4	0
60	5	3	Total 3	O 3	0
60	6	14	Total 14	O 14	0
60	7	23	Total 23	O 23	0
60	8	4	Total 4	O 4	0
60	A	2538	Total 2538	O 2538	0
60	B	6	Total 6	O 6	0
60	D	3	Total 3	O 3	0
60	F	6	Total 6	O 6	0
60	G	56	Total 56	O 56	0
60	H	28	Total 28	O 28	0
60	I	34	Total 34	O 34	0
60	K	1	Total 1	O 1	0
60	M	5	Total 5	O 5	0
60	N	9	Total 9	O 9	0
60	O	24	Total 24	O 24	0
60	P	17	Total 17	O 17	0
60	Q	18	Total 18	O 18	0

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Mol	Chain	Residues	Atoms		AltConf
60	S	16	Total 16	O 16	0
60	T	18	Total 18	O 18	0
60	U	6	Total 6	O 6	0
60	V	18	Total 18	O 18	0
60	W	5	Total 5	O 5	0
60	X	2	Total 2	O 2	0
60	Y	12	Total 12	O 12	0
60	Z	4	Total 4	O 4	0
60	a	677	Total 677	O 677	0
60	b	2	Total 2	O 2	0
60	c	2	Total 2	O 2	0
60	d	3	Total 3	O 3	0
60	e	4	Total 4	O 4	0
60	f	3	Total 3	O 3	0
60	g	1	Total 1	O 1	0
60	i	3	Total 3	O 3	0
60	k	3	Total 3	O 3	0
60	l	3	Total 3	O 3	0
60	m	3	Total 3	O 3	0
60	n	2	Total 2	O 2	0
60	o	2	Total 2	O 2	0

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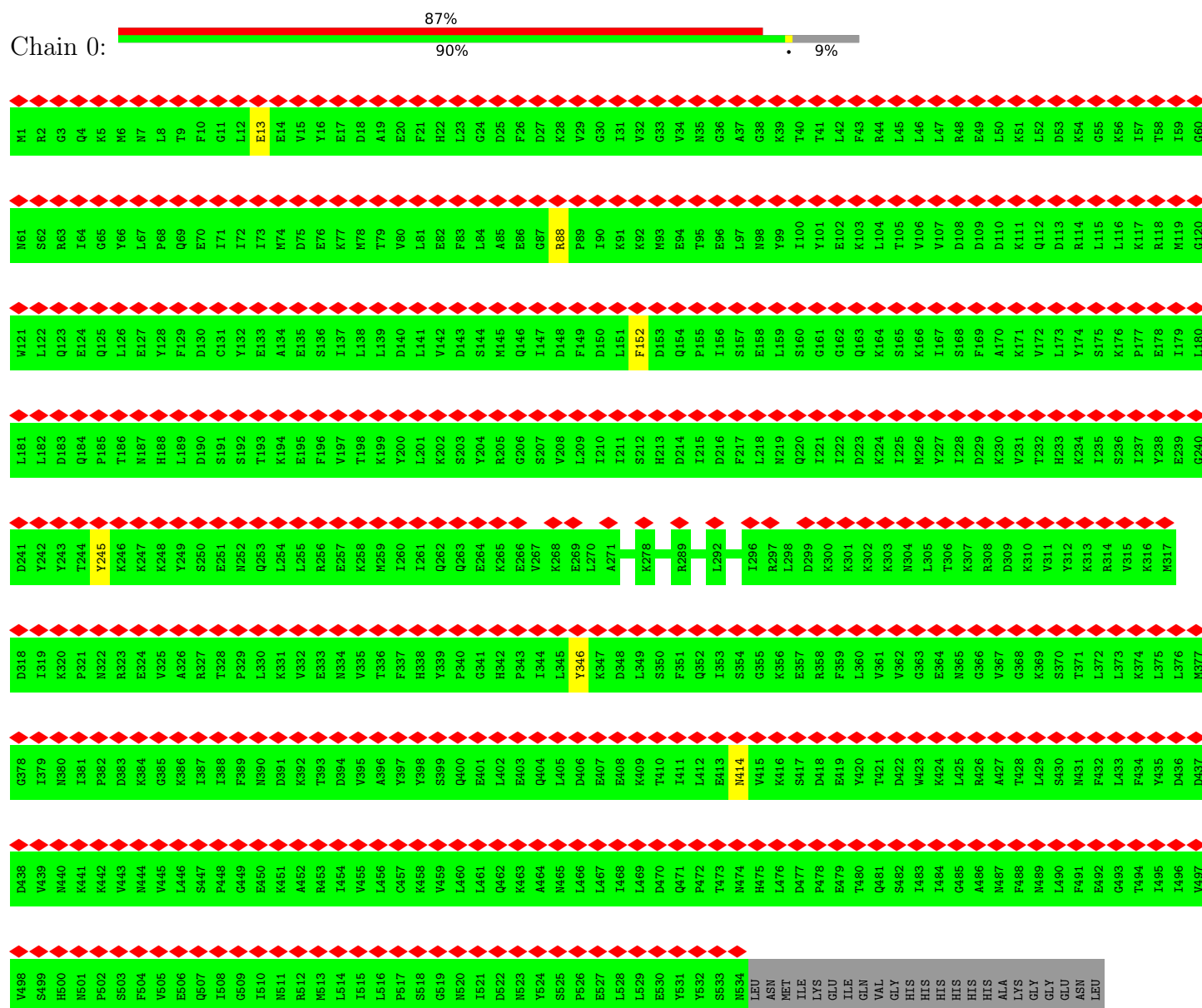
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Mol	Chain	Residues	Atoms		AltConf
60	q	4	Total 4	O 4	0
60	r	2	Total 2	O 2	0
60	s	2	Total 2	O 2	0
60	t	5	Total 5	O 5	0
60	u	1	Total 1	O 1	0

### 3 Residue-property plots

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

- Molecule 1: ARE-ABC-F family resistance factor PoxA



TYR PHE GLN GLY VAL ALA ASP TYR LYS ASP HIS ASP GLY ASP TYR LYS ASP HIS ASP TLE ASP TYR LYS ASP ASP ASP ASP GLY

• Molecule 2: 50S ribosomal protein L29

Chain 1: 47% 94% 5%

MET K2 V3 K4 E5 I6 R7 E8 L9 T10 T11 A12 E13 M14 L15 D16 K17 E18 K19 Q20 L25 R29 Q35 Q36 L37 E38 R42 E45 R58 E59 Q60 ALA ASN

• Molecule 3: 50S ribosomal protein L30

Chain 2: 22% 97% 1%

MET A2 E3 L4 K5 R10 Q17 T36 K37 E41 M48 D55 V56 E57 E58 VAL

• Molecule 4: 50S ribosomal protein L31 type B

Chain 3: 90% 90% 10%

M1 K2 Q3 D4 I5 H6 P7 N8 Y9 Q10 P11 V12 V13 F14 M15 D16 S17 T18 T19 G20 F21 K22 F23 L24 S25 G26 S27 T28 K29 G30 S31 S32 E33 T34 V35 E36 W37 E38 D39 G40 M41 T42 Y43 P44 L45 L46 R47 V48 E49 V50 T51 S52 D53 S54 H55 P56 F57 Y58 T59 G60 R61 Q62 K63 F64 T65 Q66 A67 D68 G69 R70 V71 D72 R73 F74 N75 K76 K77 Y78 G79 L80 LYS ASP GLU ASN ALA ASN PRO ASP ALA

• Molecule 5: 50S ribosomal protein L32-3

Chain 4: 15% 90% 10%

MET A2 T24 K25 Q26 E35 R36 D50 G51 K52 D53 V54 MET SER LYS GLU ALA

• Molecule 6: 50S ribosomal protein L33 3

Chain 5: 18% 96% 2%

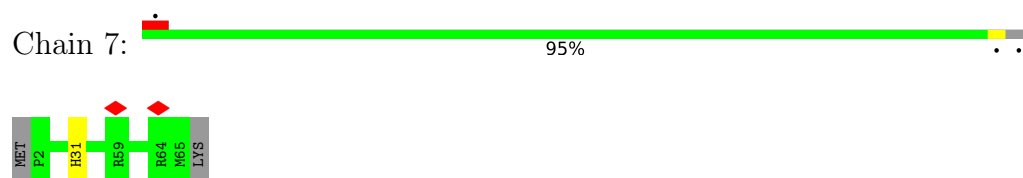
M1 E14 R24 D28 R29 L30 E31 K32 R38 T48 LYS

• Molecule 7: 50S ribosomal protein L34

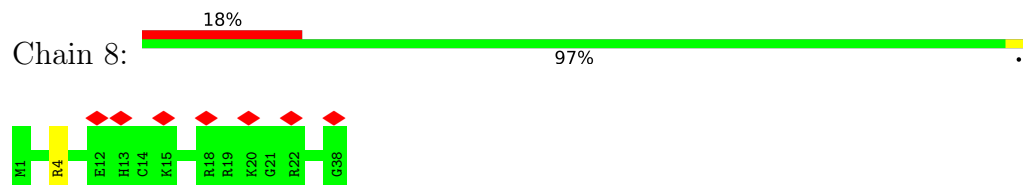
Chain 6: 5% 100%

M1 A44

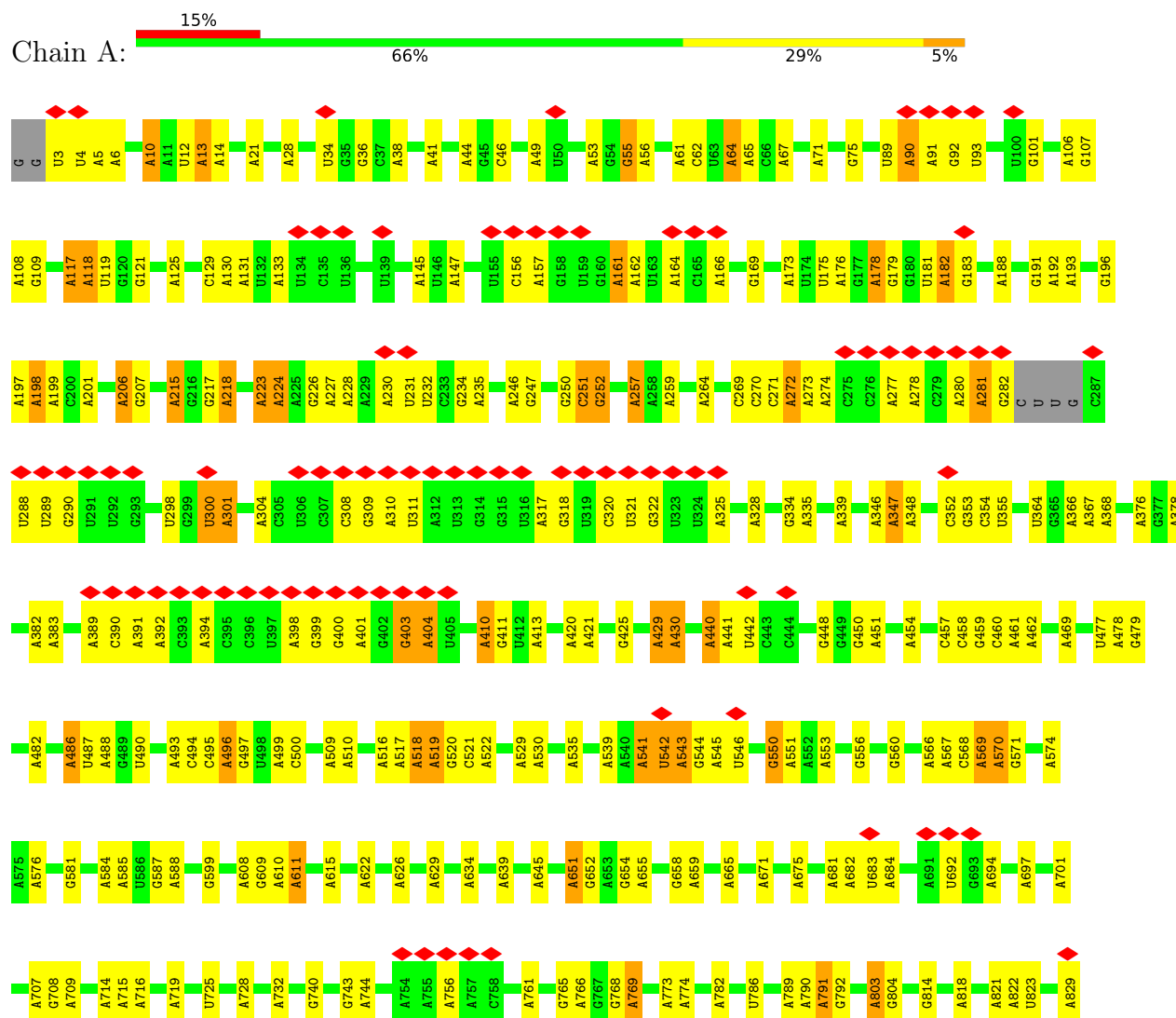
- Molecule 8: 50S ribosomal protein L35

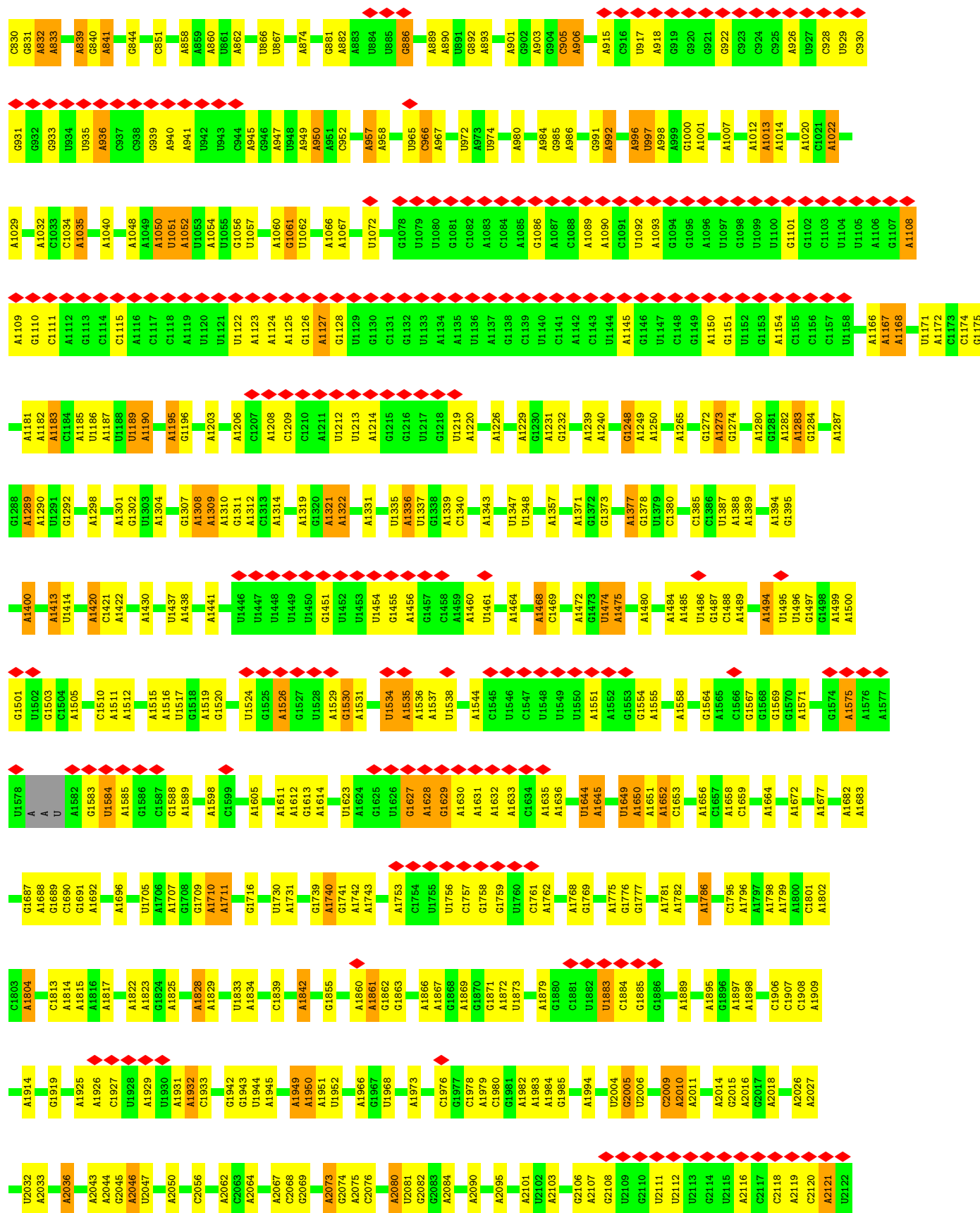


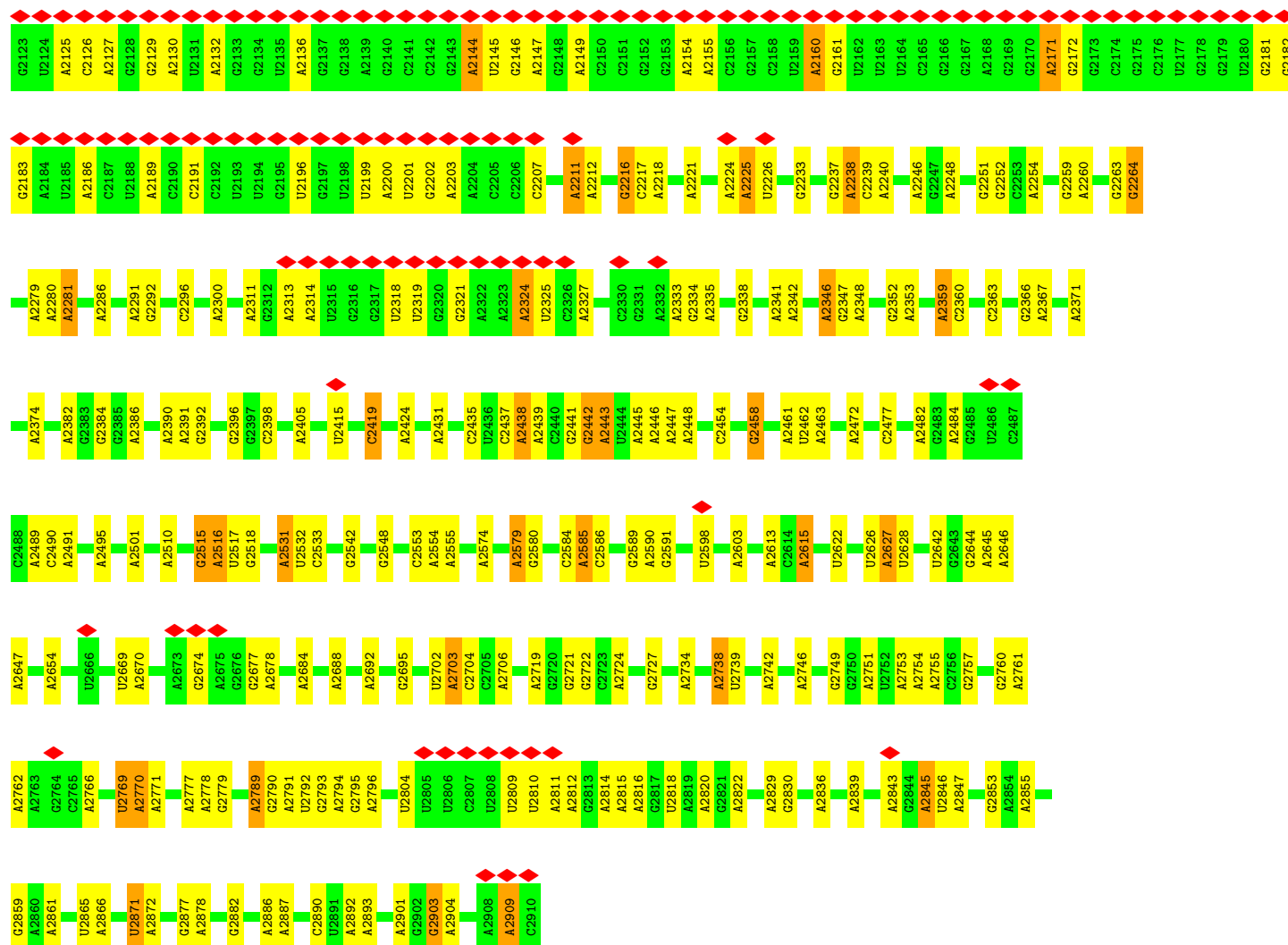
- Molecule 9: 50S ribosomal protein L36



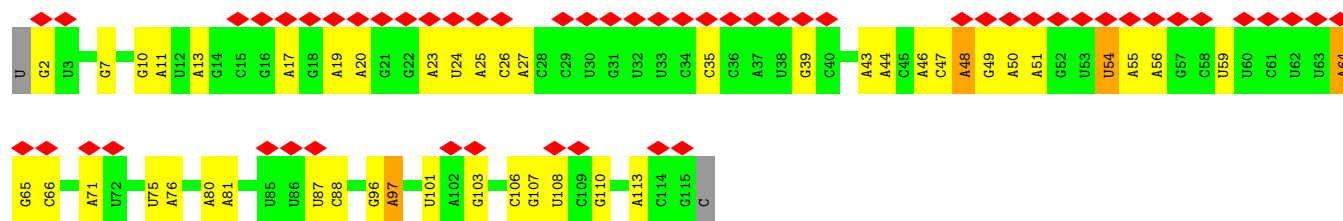
- Molecule 10: 23S rRNA



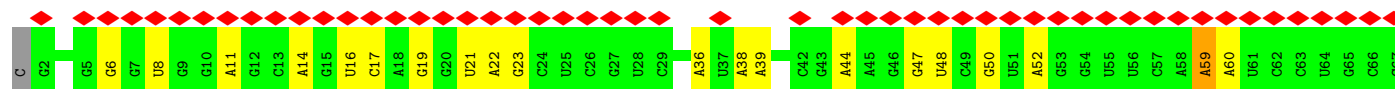
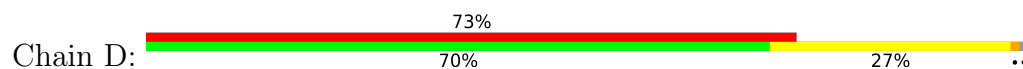


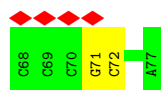


### • Molecule 11: 5S rRNA

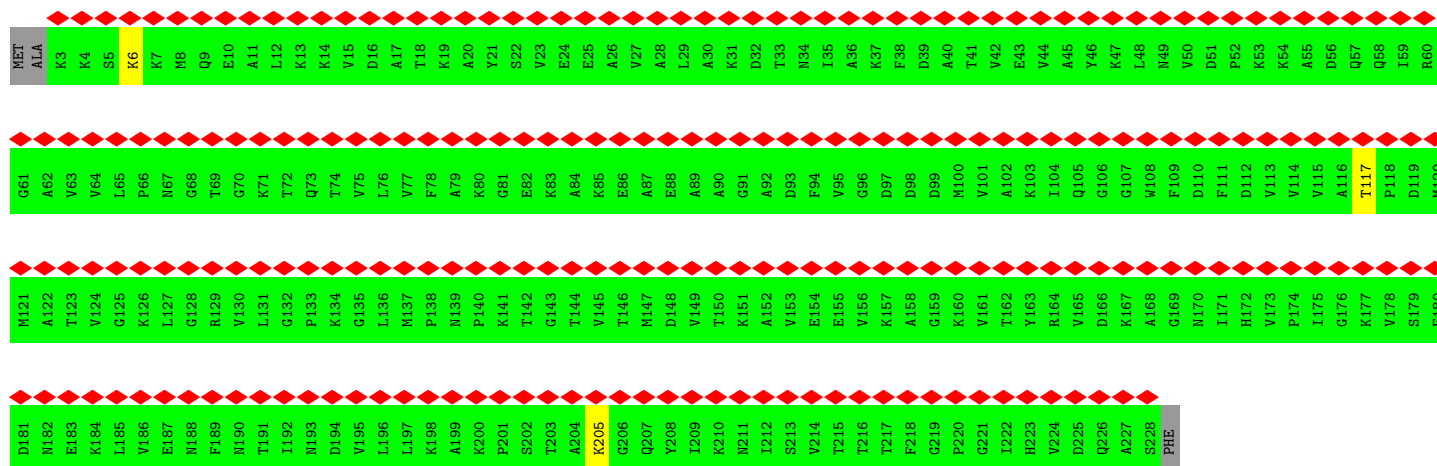


### • Molecule 12: fMet-tRNA





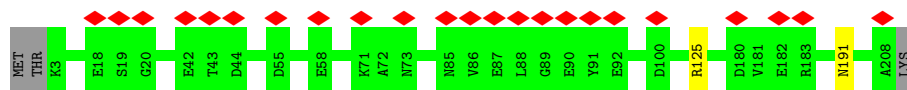
- Molecule 13: 50S ribosomal protein L1



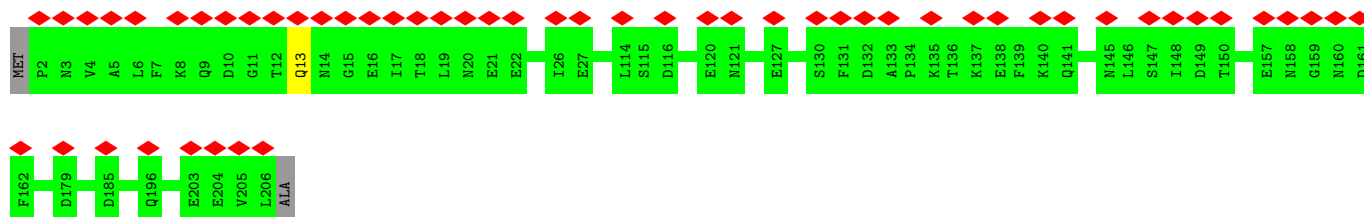
- Molecule 14: 50S ribosomal protein L2



- Molecule 15: 50S ribosomal protein L3

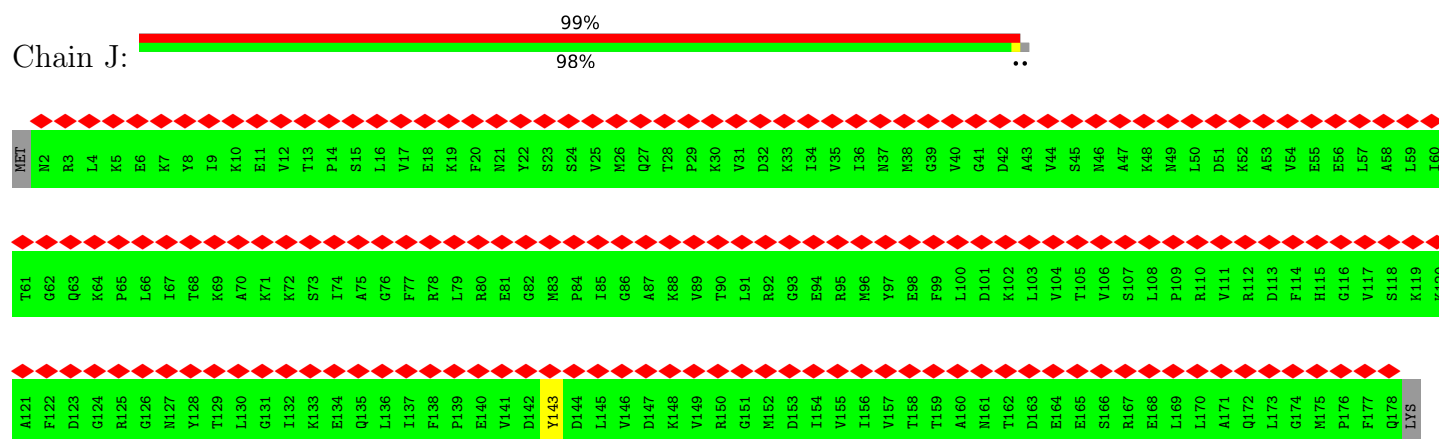


- Molecule 16: 50S ribosomal protein L4

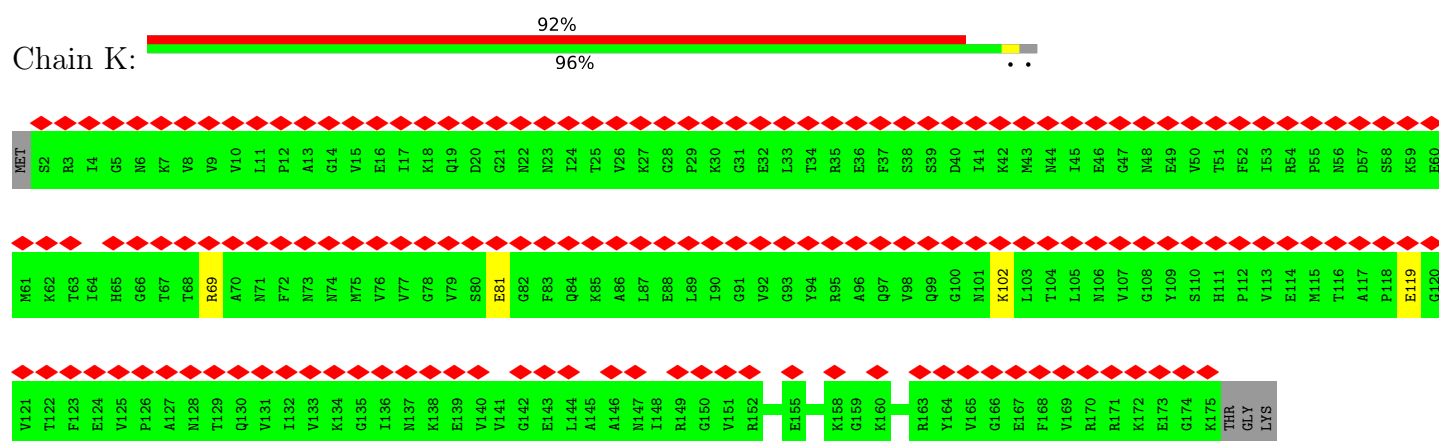


- Molecule 17: 50S ribosomal protein L5

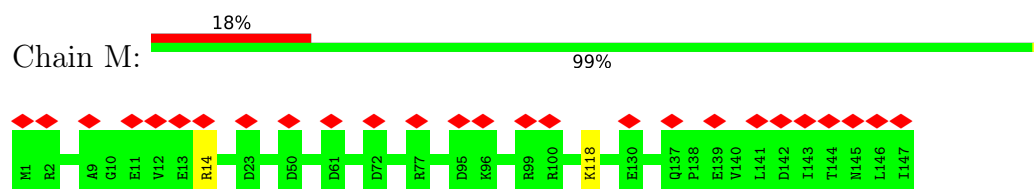




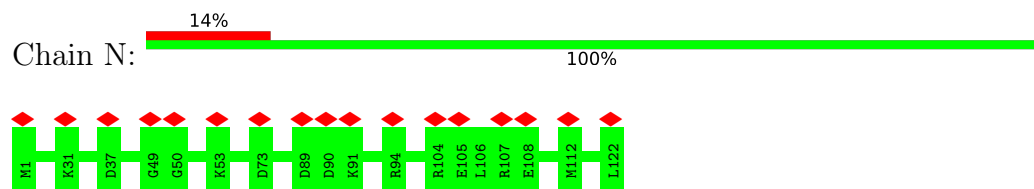
• Molecule 18: 50S ribosomal protein L6



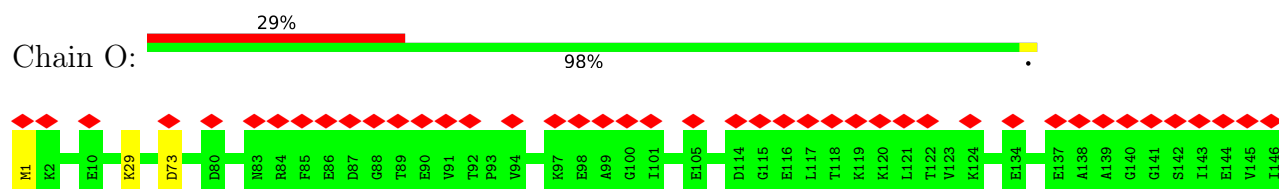
• Molecule 19: 50S ribosomal protein L13



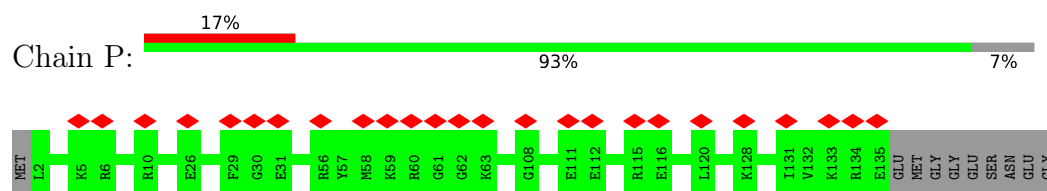
• Molecule 20: 50S ribosomal protein L14



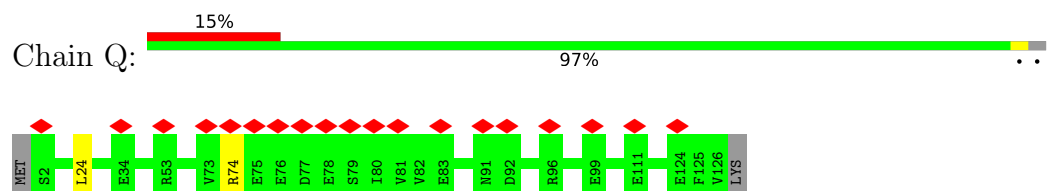
• Molecule 21: 50S ribosomal protein L15



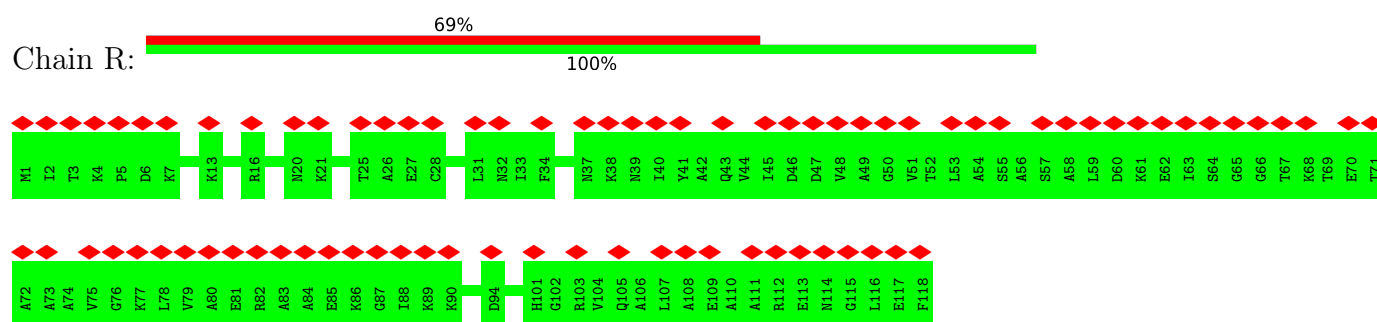
- Molecule 22: 50S ribosomal protein L16



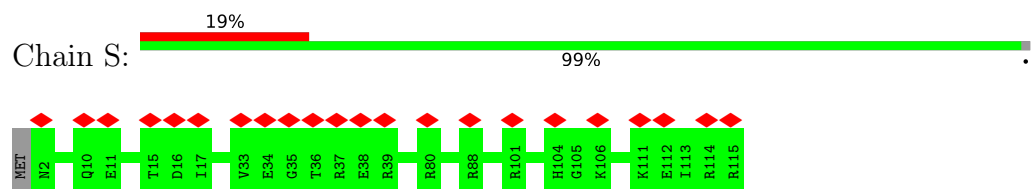
- Molecule 23: 50S ribosomal protein L17



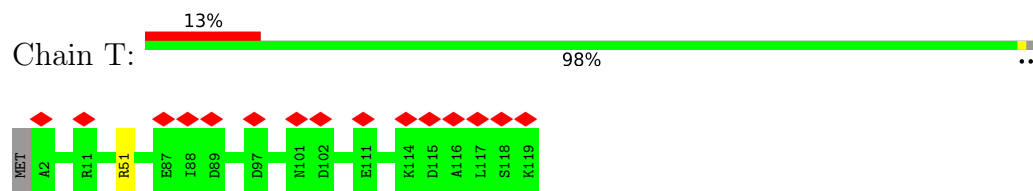
- Molecule 24: 50S ribosomal protein L18



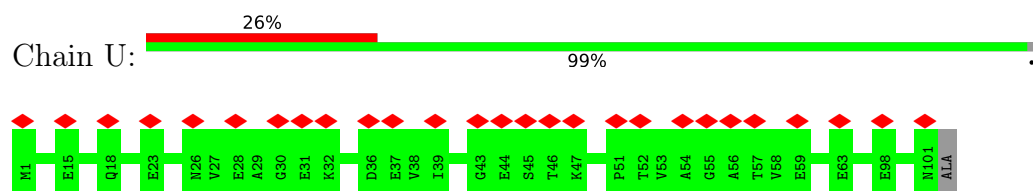
- Molecule 25: 50S ribosomal protein L19



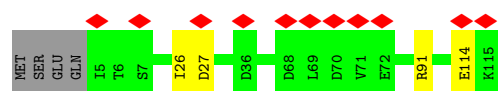
- Molecule 26: 50S ribosomal protein L20



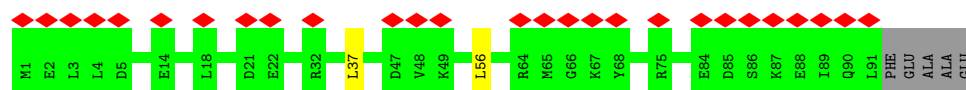
- Molecule 27: 50S ribosomal protein L21



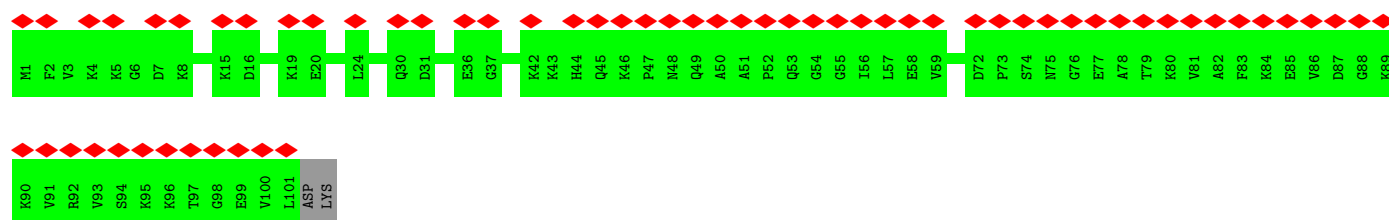
- Molecule 28: 50S ribosomal protein L22



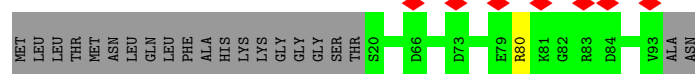
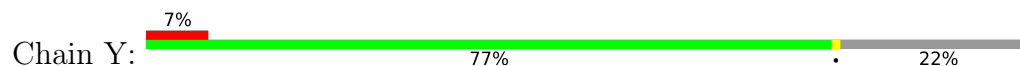
- Molecule 29: 50S ribosomal protein L23



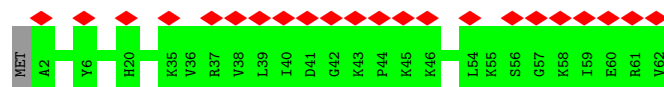
- Molecule 30: 50S ribosomal protein L24



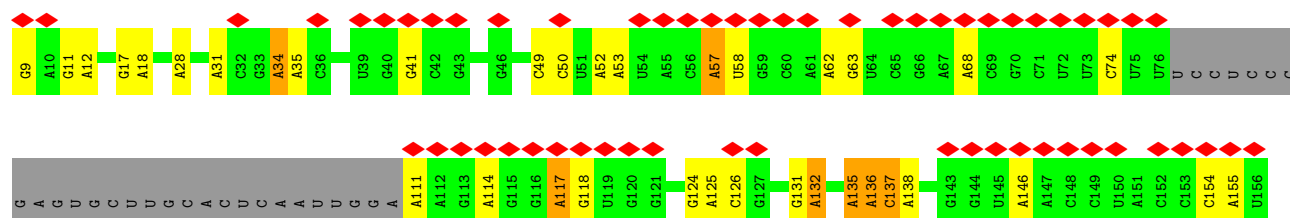
- Molecule 31: 50S ribosomal protein L27

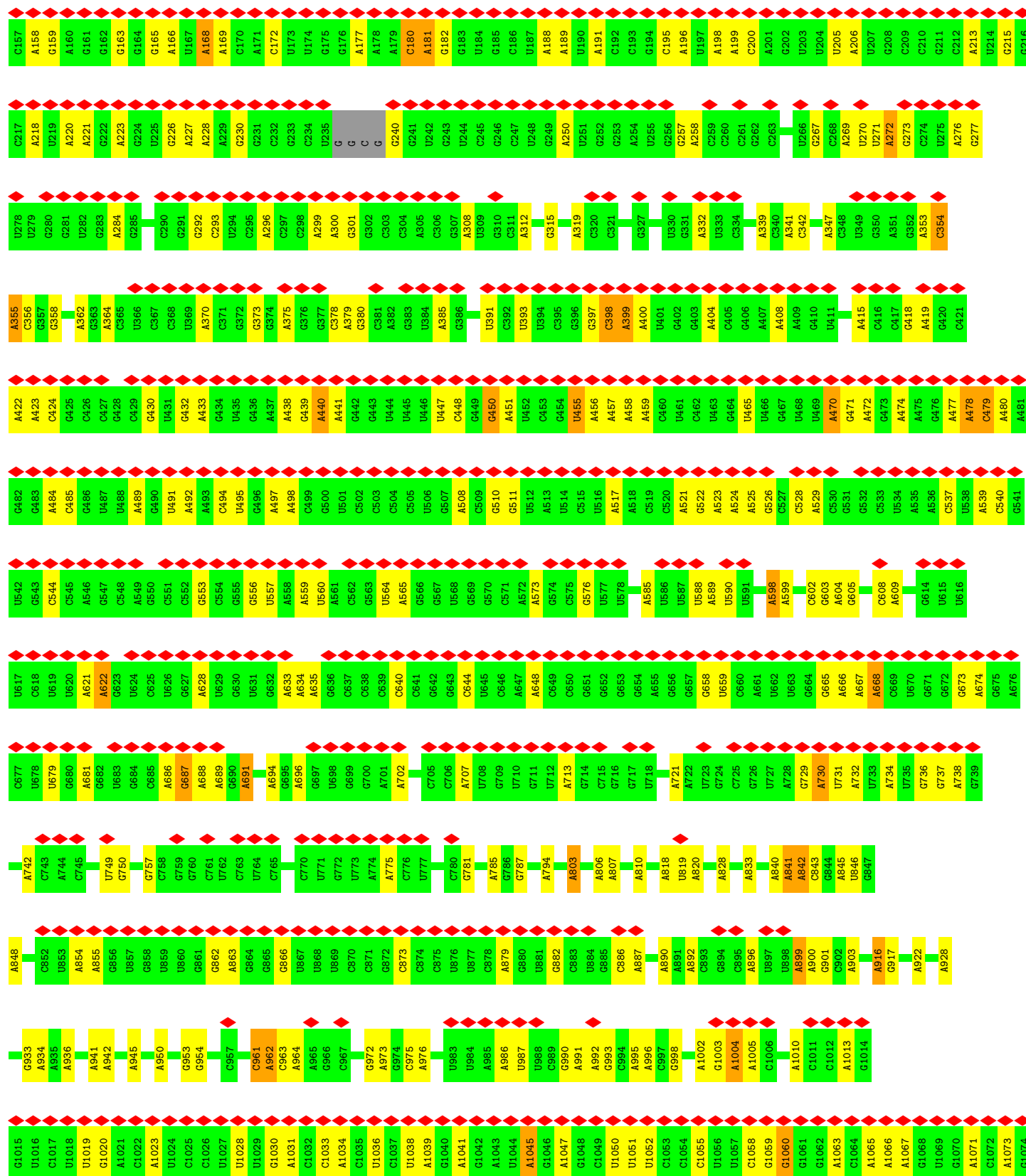


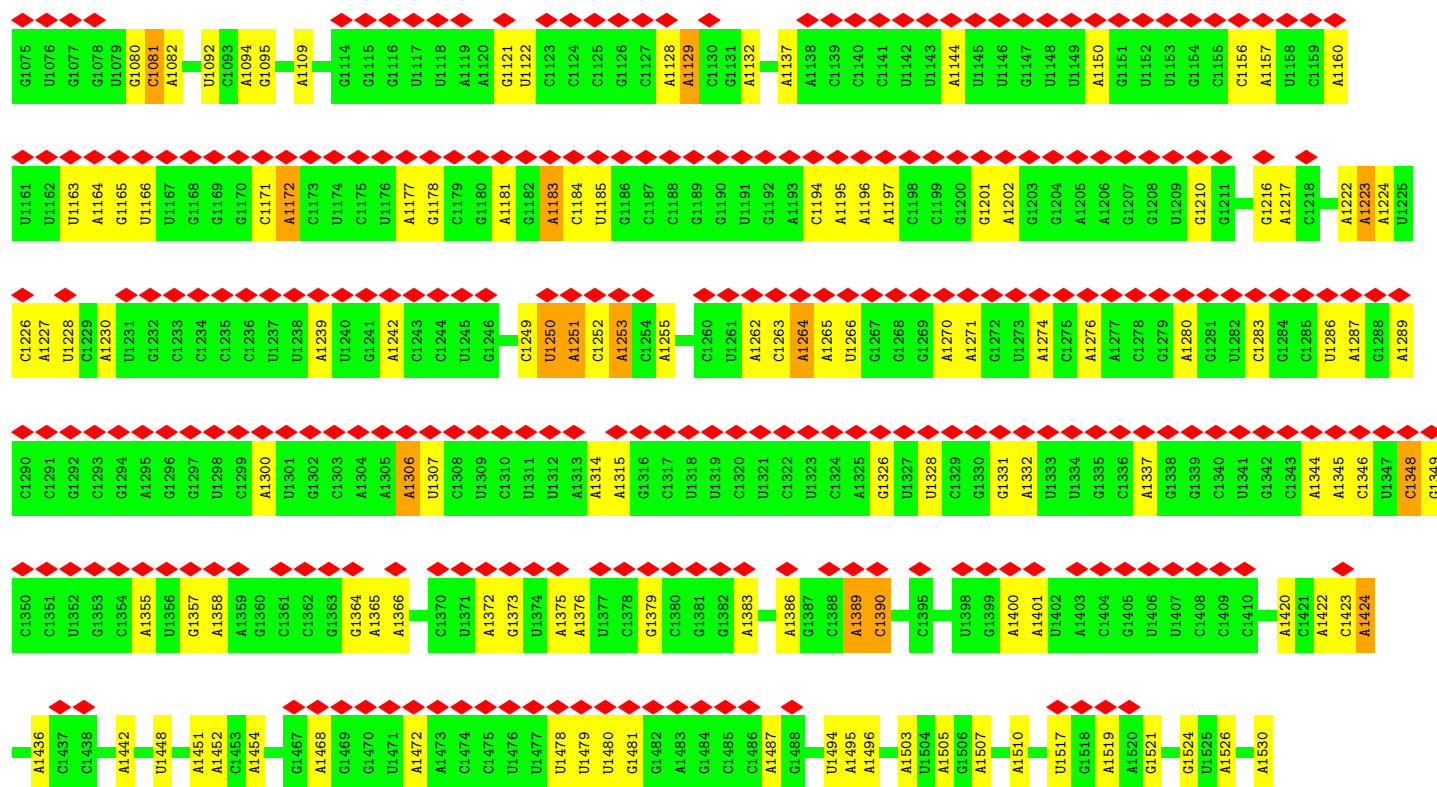
- Molecule 32: 50S ribosomal protein L28



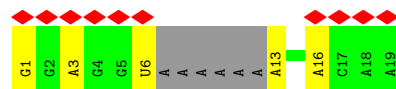
- Molecule 33: 16S rRNA



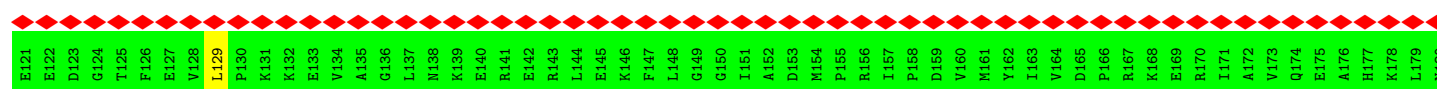
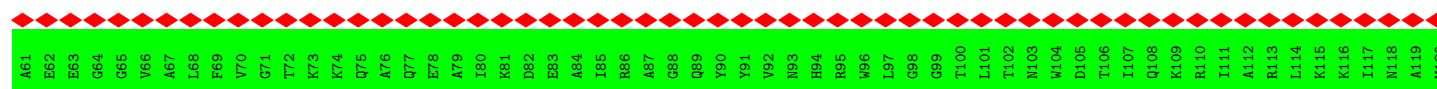
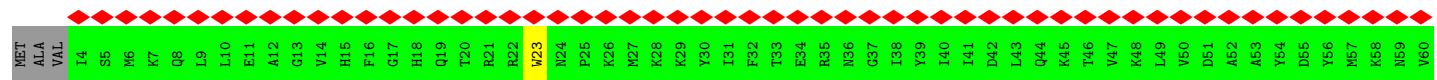
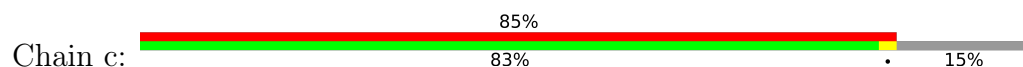


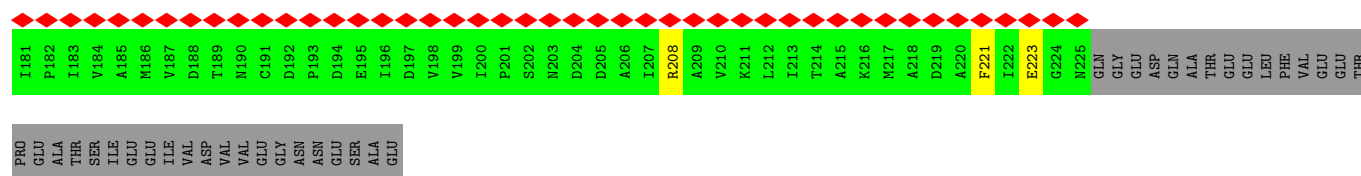


### • Molecule 34: mRNA

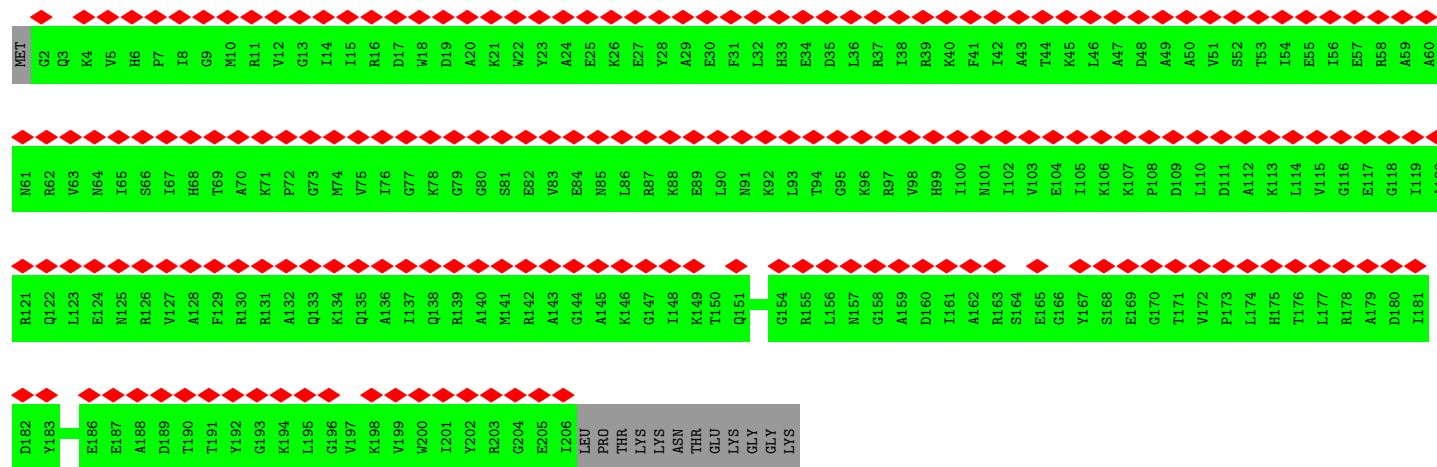
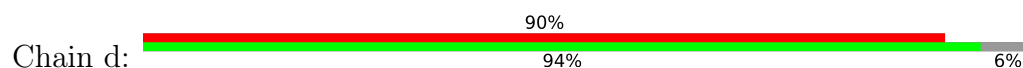


### • Molecule 35: 30S ribosomal protein S2

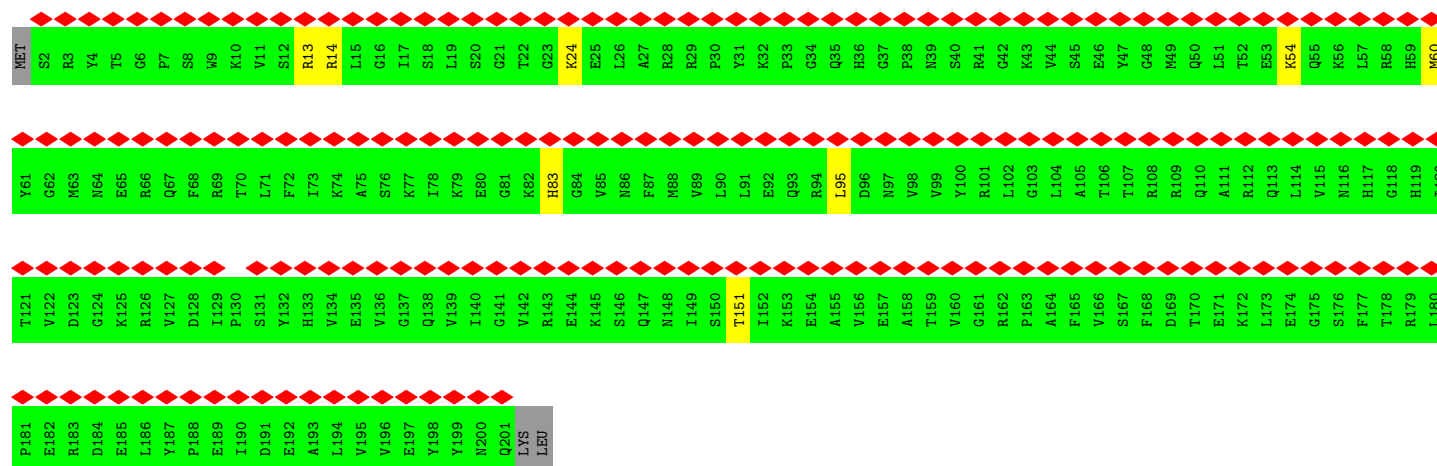




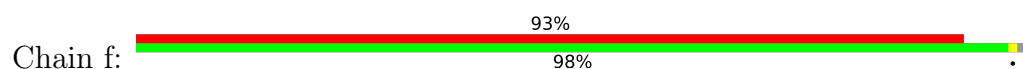
• Molecule 36: 30S ribosomal protein S3



• Molecule 37: 30S ribosomal protein S4

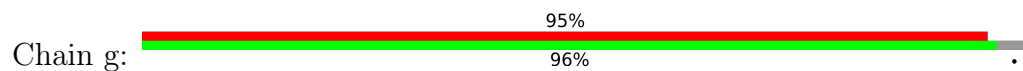


• Molecule 38: 30S ribosomal protein S5

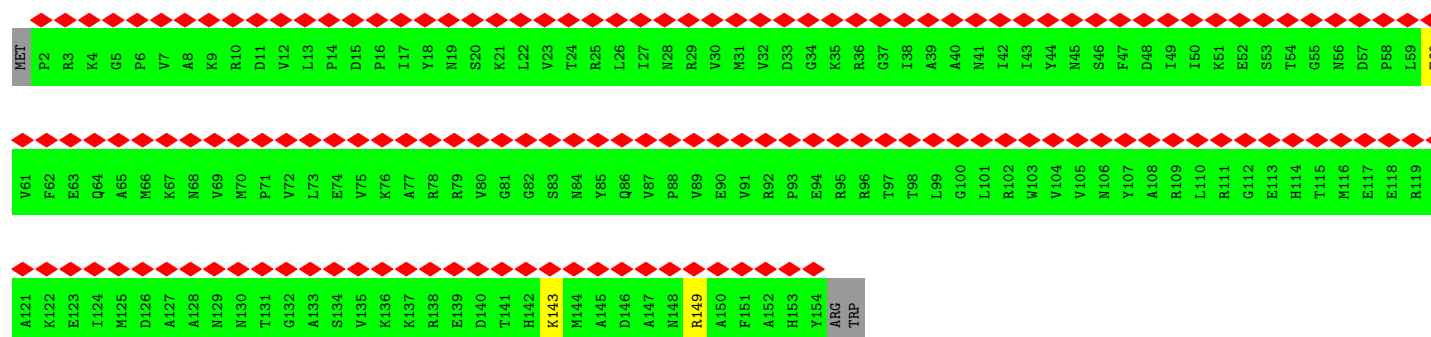




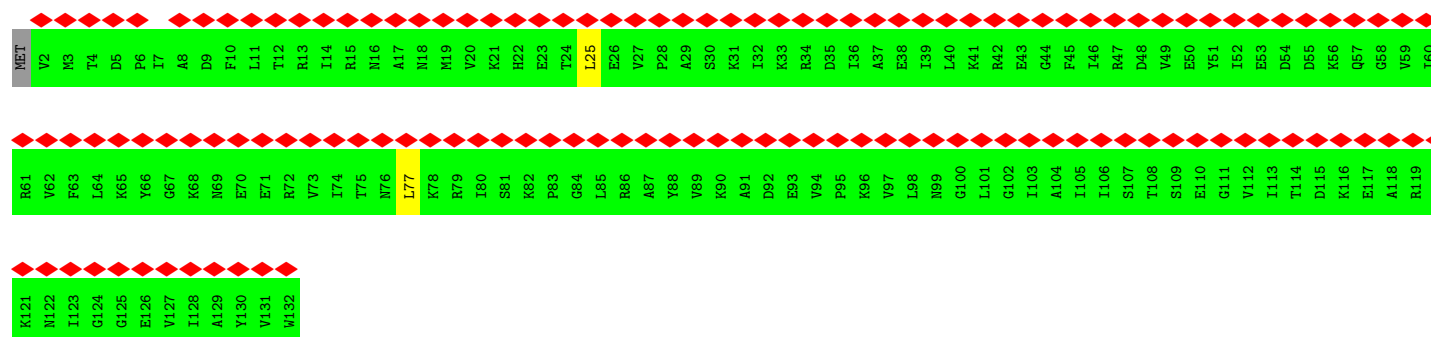
• Molecule 39: 30S ribosomal protein S6



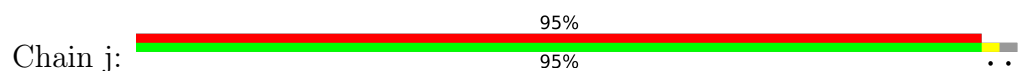
• Molecule 40: 30S ribosomal protein S7

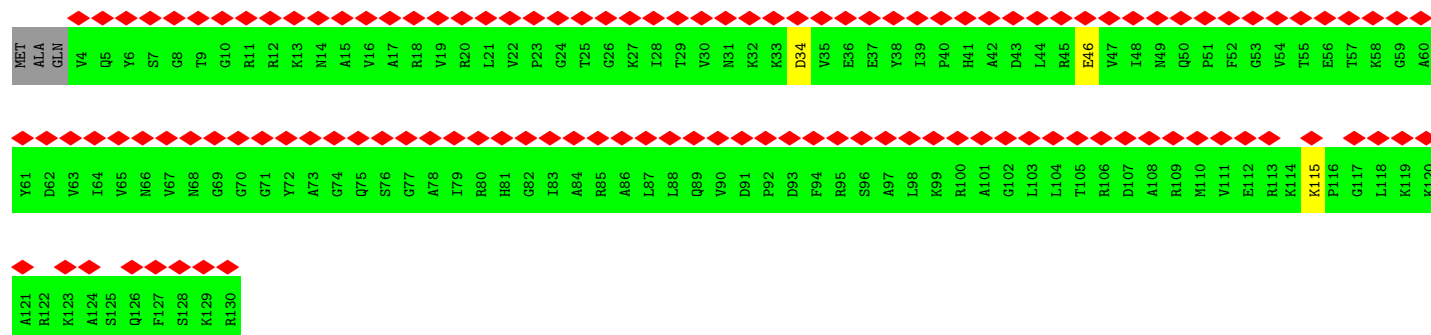


• Molecule 41: 30S ribosomal protein S8

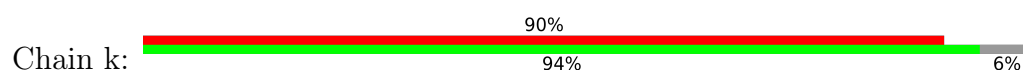


• Molecule 42: 30S ribosomal protein S9

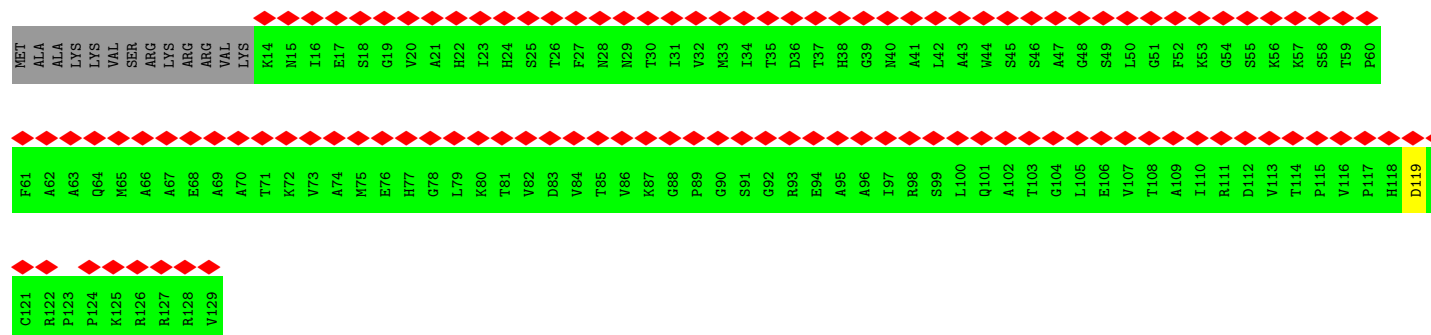
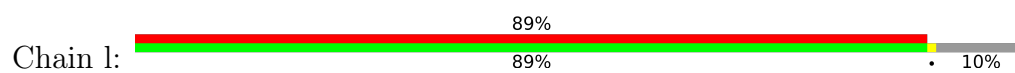




• Molecule 43: 30S ribosomal protein S10



• Molecule 44: 30S ribosomal protein S11

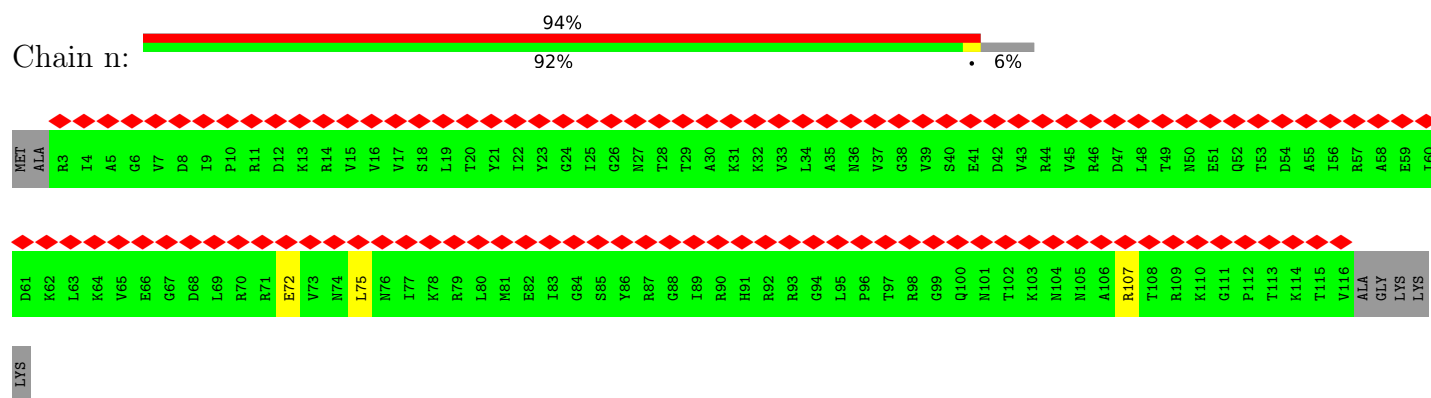


• Molecule 45: 30S ribosomal protein S12

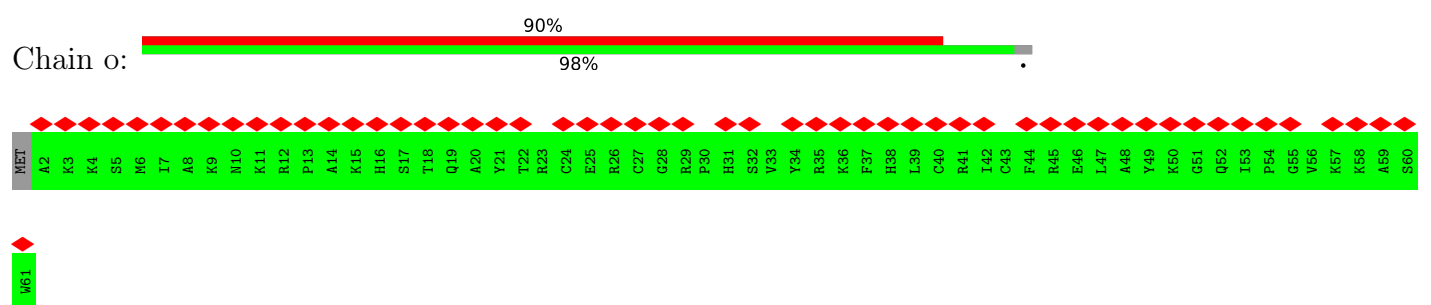




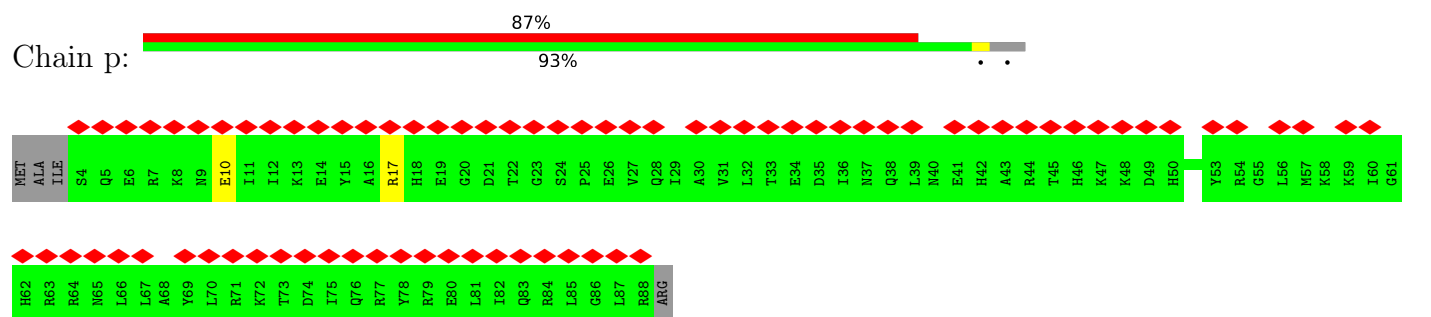
- Molecule 46: 30S ribosomal protein S13



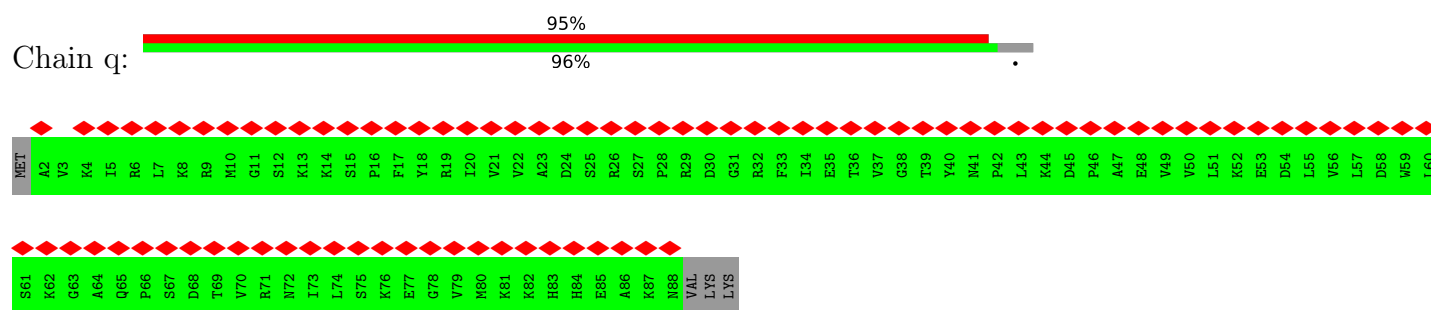
- Molecule 47: 30S ribosomal protein S14 type Z



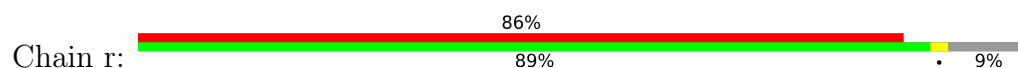
- Molecule 48: 30S ribosomal protein S15

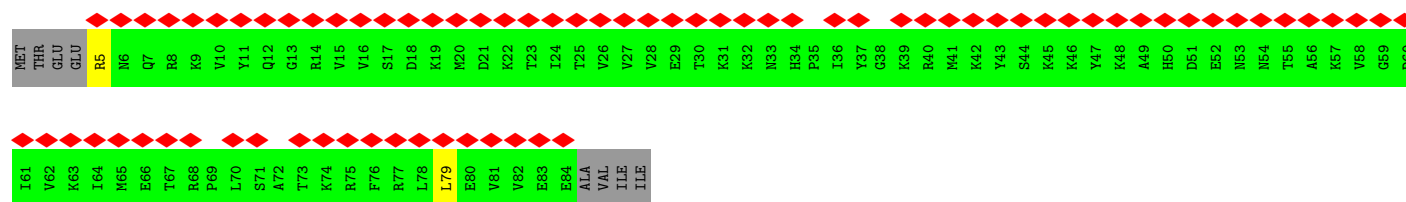


- Molecule 49: 30S ribosomal protein S16

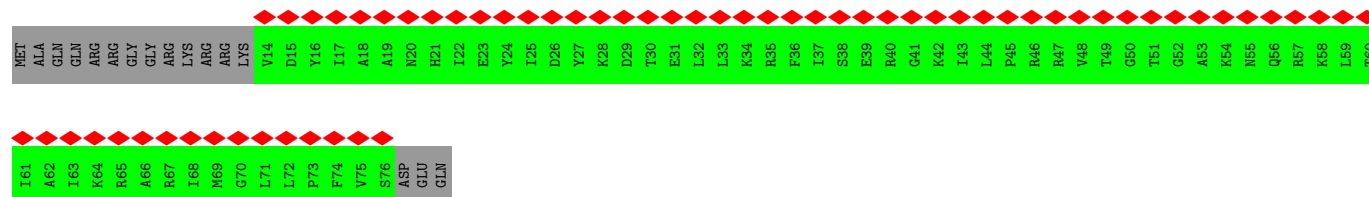
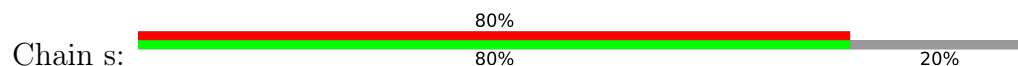


- Molecule 50: 30S ribosomal protein S17

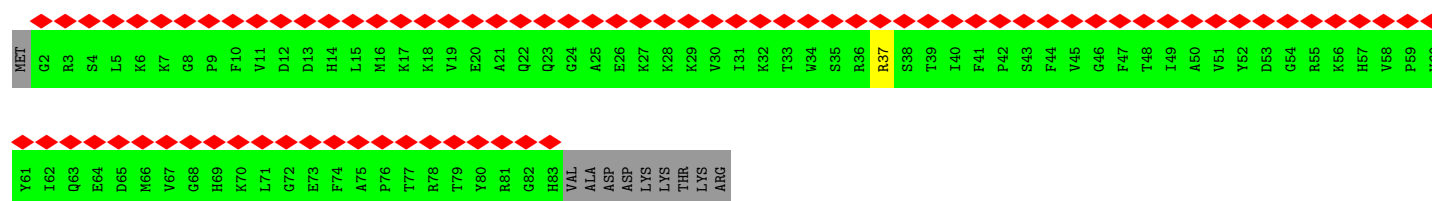
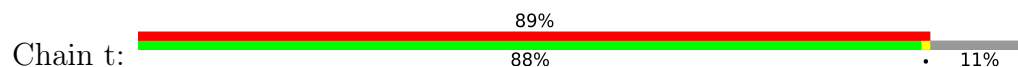




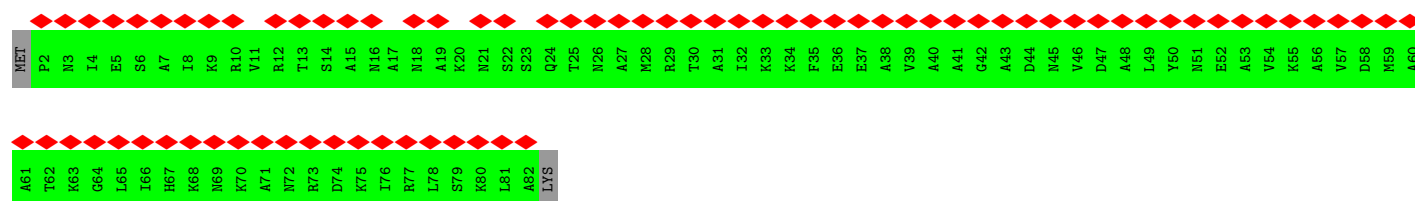
• Molecule 51: 30S ribosomal protein S18



• Molecule 52: 30S ribosomal protein S19



• Molecule 53: 30S ribosomal protein S20



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112877	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 ( $e^-/\text{\AA}^2$ )	30.255	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size ( $\text{\AA}$ )	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.82, 0.82, 0.82	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ATP, MG, MA6, ZN, PUT, 2MG, OMC, SCM, IAS, OMG, K

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	0.25	0/4421	0.44	0/5951
2	1	0.23	0/492	0.50	0/654
3	2	0.23	0/430	0.51	0/579
4	3	0.27	0/664	0.49	0/896
5	4	0.27	0/413	0.55	0/549
6	5	0.28	0/414	0.61	0/552
7	6	0.28	0/377	0.69	0/491
8	7	0.26	0/528	0.66	0/689
9	8	0.31	0/310	0.57	0/409
10	A	0.45	0/69656	0.99	686/108653 (0.6%)
11	B	0.35	0/2728	0.85	25/4252 (0.6%)
12	D	0.29	0/1815	0.77	7/2828 (0.2%)
13	F	0.25	0/1717	0.44	0/2318
14	G	0.28	0/2141	0.56	0/2881
15	H	0.29	0/1594	0.55	0/2140
16	I	0.28	0/1595	0.52	0/2157
17	J	0.26	0/1411	0.49	0/1897
18	K	0.27	0/1355	0.54	0/1825
19	M	0.27	0/1167	0.50	0/1576
20	N	0.28	0/930	0.59	0/1247
21	O	0.27	0/1106	0.55	0/1474
22	P	0.28	0/1093	0.54	0/1457
23	Q	0.26	0/1006	0.58	0/1349
24	R	0.27	0/917	0.54	0/1226
25	S	0.27	0/939	0.61	0/1262
26	T	0.27	0/963	0.50	0/1280
27	U	0.29	0/791	0.48	0/1061
28	V	0.27	0/850	0.54	0/1145
29	W	0.27	0/743	0.53	0/993
30	X	0.28	0/772	0.47	0/1035
31	Y	0.29	0/565	0.57	0/755
32	Z	0.26	0/486	0.56	0/648

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	a	0.39	0/36436	0.96	323/56823 (0.6%)
34	b	0.23	0/319	0.82	3/494 (0.6%)
35	c	0.26	0/1803	0.47	0/2430
36	d	0.26	0/1643	0.52	0/2208
37	e	0.27	0/1641	0.53	0/2206
38	f	0.26	0/1217	0.53	0/1641
39	g	0.26	0/798	0.50	0/1075
40	h	0.25	0/1238	0.50	0/1668
41	i	0.27	0/1054	0.53	0/1417
42	j	0.27	0/993	0.54	0/1331
43	k	0.27	0/785	0.53	0/1059
44	l	0.25	0/860	0.53	0/1160
45	m	0.28	0/1068	0.60	0/1435
46	n	0.25	0/908	0.58	0/1219
47	o	0.28	0/504	0.53	0/669
48	p	0.25	0/726	0.53	0/969
49	q	0.26	0/704	0.52	0/945
50	r	0.26	0/668	0.54	0/891
51	s	0.26	0/518	0.54	0/694
52	t	0.27	0/680	0.51	0/911
53	u	0.23	0/611	0.46	0/818
All	All	0.38	0/159563	0.87	1044/238292 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	F	0	1

There are no bond length outliers.

All (1044) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	226	G	OP1-P-O3'	-40.25	16.64	105.20
33	a	168	A	OP1-P-O3'	-40.10	16.98	105.20
10	A	400	G	OP1-P-O3'	-39.77	17.71	105.20
33	a	491	U	OP1-P-O3'	-39.52	18.26	105.20
10	A	390	C	OP1-P-O3'	-39.48	18.34	105.20
33	a	528	C	OP1-P-O3'	-39.46	18.38	105.20
10	A	181	U	OP1-P-O3'	-39.33	18.68	105.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2118	C	OP1-P-O3'	-39.15	19.06	105.20
10	A	2419	C	OP2-P-O3'	-38.87	19.68	105.20
33	a	180	C	OP1-P-O3'	-38.77	19.90	105.20
10	A	403	G	OP1-P-O3'	-38.14	21.29	105.20
10	A	1584	U	OP2-P-O3'	-37.22	23.31	105.20
10	A	886	G	OP2-P-O3'	-37.03	23.73	105.20
33	a	169	A	OP1-P-OP2	-13.22	99.77	119.60
33	a	227	A	OP1-P-OP2	-12.96	100.16	119.60
10	A	391	A	OP1-P-OP2	-12.70	100.56	119.60
33	a	492	A	OP1-P-OP2	-12.59	100.72	119.60
10	A	182	A	OP1-P-OP2	-12.50	100.85	119.60
10	A	401	A	OP1-P-OP2	-12.43	100.96	119.60
33	a	529	A	OP1-P-OP2	-12.35	101.07	119.60
33	a	181	A	OP1-P-OP2	-12.22	101.27	119.60
10	A	2119	A	OP1-P-OP2	-12.21	101.28	119.60
10	A	1321	A	OP1-P-O3'	11.84	131.25	105.20
10	A	404	A	OP1-P-OP2	-11.29	102.66	119.60
10	A	1644	U	OP1-P-O3'	11.29	130.04	105.20
10	A	832	A	OP1-P-O3'	10.08	127.37	105.20
10	A	1322	A	OP1-P-OP2	-9.91	104.74	119.60
10	A	201	A	O4'-C1'-N9	9.90	116.12	108.20
10	A	1645	A	OP1-P-OP2	-9.61	105.18	119.60
33	a	136	A	OP1-P-OP2	-9.39	105.51	119.60
10	A	833	A	OP1-P-OP2	-9.06	106.01	119.60
33	a	1251	A	OP1-P-OP2	-9.04	106.04	119.60
33	a	1250	U	OP1-P-O3'	8.78	124.52	105.20
33	a	1172	A	OP1-P-OP2	-8.70	106.56	119.60
33	a	621	A	OP1-P-O3'	8.67	124.28	105.20
10	A	569	A	OP1-P-O3'	8.58	124.07	105.20
10	A	905	C	OP1-P-O3'	8.54	123.98	105.20
10	A	906	A	OP1-P-OP2	-8.48	106.88	119.60
10	A	567	A	O4'-C1'-N9	8.47	114.98	108.20
10	A	1309	A	OP1-P-OP2	-8.41	106.98	119.60
33	a	132	A	OP1-P-OP2	-8.35	107.08	119.60
10	A	2761	A	OP1-P-OP2	-8.31	107.13	119.60
33	a	622	A	OP1-P-OP2	-8.24	107.24	119.60
10	A	831	G	OP1-P-O3'	8.19	123.22	105.20
33	a	131	G	OP1-P-O3'	8.19	123.22	105.20
33	a	135	A	OP1-P-O3'	8.17	123.17	105.20
10	A	1089	A	OP1-P-O3'	8.12	123.07	105.20
10	A	832	A	OP1-P-OP2	-8.10	107.45	119.60
10	A	659	A	OP1-P-OP2	-8.09	107.47	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	610	A	OP1-P-O3'	8.06	122.93	105.20
10	A	1090	A	OP1-P-OP2	-8.01	107.59	119.60
10	A	2200	A	OP1-P-OP2	-7.99	107.62	119.60
10	A	611	A	OP1-P-OP2	-7.91	107.73	119.60
10	A	1437	U	OP1-P-O3'	7.89	122.56	105.20
10	A	991	G	OP1-P-O3'	7.86	122.48	105.20
10	A	1308	A	OP1-P-O3'	7.85	122.48	105.20
33	a	1250	U	OP1-P-OP2	-7.82	107.87	119.60
10	A	1531	A	OP1-P-OP2	-7.80	107.89	119.60
10	A	1290	A	OP1-P-OP2	-7.79	107.91	119.60
33	a	398	C	OP1-P-OP2	-7.79	107.91	119.60
33	a	1227	A	OP1-P-OP2	-7.78	107.93	119.60
10	A	551	A	OP1-P-OP2	-7.78	107.94	119.60
33	a	609	A	OP1-P-OP2	-7.75	107.98	119.60
10	A	831	G	OP1-P-OP2	-7.74	107.99	119.60
33	a	1217	A	OP1-P-OP2	-7.74	108.00	119.60
33	a	1171	C	OP1-P-O3'	7.73	122.22	105.20
10	A	2766	A	OP1-P-OP2	-7.73	108.00	119.60
33	a	1045	A	OP1-P-OP2	-7.73	108.01	119.60
10	A	658	G	OP1-P-O3'	7.72	122.17	105.20
10	A	1438	A	OP1-P-OP2	-7.70	108.05	119.60
33	a	976	A	OP1-P-OP2	-7.68	108.07	119.60
10	A	1945	A	OP1-P-OP2	-7.61	108.18	119.60
10	A	708	G	OP1-P-OP2	-7.61	108.19	119.60
10	A	192	A	OP1-P-OP2	-7.60	108.20	119.60
10	A	2904	A	OP1-P-OP2	-7.59	108.21	119.60
10	A	2010	A	OP1-P-OP2	-7.58	108.23	119.60
10	A	335	A	OP1-P-OP2	-7.57	108.25	119.60
10	A	218	A	OP1-P-OP2	-7.54	108.29	119.60
33	a	206	A	OP1-P-OP2	-7.52	108.32	119.60
33	a	404	A	OP1-P-OP2	-7.52	108.32	119.60
10	A	545	A	OP1-P-OP2	-7.51	108.33	119.60
10	A	1273	A	OP1-P-OP2	-7.51	108.33	119.60
10	A	1035	A	OP1-P-OP2	-7.50	108.35	119.60
10	A	2678	A	OP1-P-OP2	-7.50	108.35	119.60
10	A	1555	A	OP1-P-OP2	-7.47	108.40	119.60
10	A	2443	A	OP1-P-OP2	-7.47	108.40	119.60
10	A	1190	A	OP1-P-OP2	-7.46	108.41	119.60
10	A	197	A	OP1-P-OP2	-7.46	108.41	119.60
10	A	1867	A	OP1-P-OP2	-7.45	108.42	119.60
10	A	1799	A	OP1-P-OP2	-7.44	108.44	119.60
10	A	570	A	OP1-P-OP2	-7.44	108.45	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1801	C	OP1-P-OP2	-7.43	108.45	119.60
10	A	2491	A	OP1-P-OP2	-7.43	108.46	119.60
10	A	2531	A	OP1-P-OP2	-7.43	108.46	119.60
33	a	1216	G	OP1-P-O3'	7.42	121.53	105.20
10	A	1321	A	O4'-C1'-N9	7.42	114.13	108.20
10	A	252	G	OP1-P-OP2	-7.41	108.48	119.60
10	A	2866	A	OP1-P-OP2	-7.41	108.49	119.60
33	a	674	A	OP1-P-OP2	-7.40	108.50	119.60
10	A	2796	A	OP1-P-OP2	-7.38	108.53	119.60
11	B	48	A	OP1-P-OP2	-7.37	108.54	119.60
33	a	525	A	OP1-P-OP2	-7.37	108.55	119.60
10	A	2770	A	OP1-P-OP2	-7.37	108.55	119.60
10	A	1249	A	OP1-P-OP2	-7.36	108.55	119.60
10	A	2016	A	OP1-P-OP2	-7.36	108.55	119.60
33	a	991	A	OP1-P-OP2	-7.36	108.55	119.60
10	A	1907	C	OP1-P-OP2	-7.36	108.56	119.60
10	A	2027	A	OP1-P-OP2	-7.36	108.57	119.60
10	A	1014	A	OP1-P-OP2	-7.35	108.58	119.60
10	A	2722	G	OP1-P-OP2	-7.35	108.58	119.60
10	A	1932	A	OP1-P-OP2	-7.34	108.58	119.60
10	A	2670	A	OP1-P-OP2	-7.34	108.58	119.60
33	a	598	A	OP1-P-OP2	-7.32	108.62	119.60
33	a	1164	A	OP1-P-OP2	-7.32	108.62	119.60
10	A	782	A	OP1-P-OP2	-7.31	108.63	119.60
10	A	227	A	OP1-P-OP2	-7.31	108.64	119.60
33	a	258	A	OP1-P-OP2	-7.30	108.65	119.60
10	A	278	A	OP1-P-OP2	-7.30	108.65	119.60
33	a	1010	A	OP1-P-OP2	-7.30	108.65	119.60
33	a	1436	A	OP1-P-OP2	-7.29	108.67	119.60
33	a	1253	A	OP1-P-OP2	-7.29	108.67	119.60
10	A	2203	A	OP1-P-OP2	-7.28	108.67	119.60
33	a	1348	C	OP1-P-OP2	-7.27	108.69	119.60
10	A	1775	A	OP1-P-OP2	-7.27	108.70	119.60
10	A	2872	A	OP1-P-OP2	-7.26	108.71	119.60
10	A	1007	A	OP1-P-OP2	-7.26	108.71	119.60
10	A	791	A	OP1-P-OP2	-7.25	108.72	119.60
10	A	2033	A	OP1-P-OP2	-7.25	108.72	119.60
33	a	138	A	OP1-P-OP2	-7.25	108.72	119.60
10	A	90	A	OP1-P-OP2	-7.25	108.73	119.60
33	a	1202	A	OP1-P-OP2	-7.25	108.73	119.60
33	a	1401	A	OP1-P-OP2	-7.23	108.75	119.60
33	a	1249	C	OP1-P-O3'	7.23	121.10	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2734	A	OP1-P-OP2	-7.23	108.76	119.60
10	A	461	A	OP1-P-OP2	-7.22	108.76	119.60
33	a	1081	C	OP1-P-O3'	7.22	121.09	105.20
10	A	2238	A	OP1-P-OP2	-7.22	108.77	119.60
33	a	196	A	OP1-P-OP2	-7.22	108.77	119.60
33	a	842	A	OP1-P-OP2	-7.22	108.77	119.60
10	A	1692	A	OP1-P-OP2	-7.21	108.78	119.60
10	A	2762	A	OP1-P-OP2	-7.21	108.79	119.60
10	A	1127	A	OP1-P-OP2	-7.21	108.79	119.60
10	A	519	A	OP1-P-OP2	-7.20	108.79	119.60
10	A	967	A	OP1-P-OP2	-7.20	108.80	119.60
10	A	1710	A	OP1-P-OP2	-7.20	108.80	119.60
10	A	997	U	OP1-P-O3'	7.20	121.03	105.20
10	A	2887	A	OP1-P-OP2	-7.20	108.81	119.60
10	A	235	A	OP1-P-OP2	-7.19	108.81	119.60
10	A	274	A	OP1-P-OP2	-7.19	108.81	119.60
10	A	522	A	OP1-P-OP2	-7.19	108.81	119.60
33	a	1495	A	OP1-P-OP2	-7.19	108.82	119.60
10	A	28	A	OP1-P-OP2	-7.18	108.82	119.60
33	a	841	A	OP1-P-OP2	-7.18	108.83	119.60
33	a	1264	A	OP1-P-OP2	-7.18	108.83	119.60
10	A	1589	A	OP1-P-OP2	-7.17	108.85	119.60
10	A	1731	A	OP1-P-OP2	-7.17	108.85	119.60
33	a	1082	A	OP1-P-OP2	-7.16	108.86	119.60
10	A	2107	A	OP1-P-OP2	-7.16	108.86	119.60
33	a	1157	A	OP1-P-OP2	-7.15	108.87	119.60
10	A	1250	A	OP1-P-OP2	-7.15	108.88	119.60
10	A	543	A	OP1-P-OP2	-7.14	108.89	119.60
33	a	451	A	OP1-P-OP2	-7.14	108.89	119.60
10	A	458	C	OP1-P-OP2	-7.13	108.90	119.60
10	A	2445	A	OP1-P-OP2	-7.13	108.90	119.60
10	A	2771	A	OP1-P-OP2	-7.13	108.90	119.60
10	A	478	A	OP1-P-OP2	-7.13	108.90	119.60
10	A	1950	A	OP1-P-OP2	-7.13	108.91	119.60
11	B	76	A	OP1-P-OP2	-7.13	108.91	119.60
33	a	962	A	OP1-P-OP2	-7.12	108.91	119.60
10	A	1931	A	OP1-P-OP2	-7.12	108.92	119.60
10	A	882	A	OP1-P-OP2	-7.12	108.92	119.60
10	A	108	A	OP1-P-OP2	-7.12	108.92	119.60
10	A	1187	A	OP1-P-OP2	-7.11	108.94	119.60
33	a	628	A	OP1-P-OP2	-7.11	108.94	119.60
33	a	1358	A	OP1-P-OP2	-7.11	108.94	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	893	A	OP1-P-OP2	-7.11	108.94	119.60
10	A	1093	A	OP1-P-OP2	-7.11	108.94	119.60
33	a	319	A	OP1-P-OP2	-7.10	108.95	119.60
10	A	1979	A	OP1-P-OP2	-7.09	108.96	119.60
33	a	166	A	OP1-P-OP2	-7.09	108.97	119.60
11	B	25	A	OP1-P-OP2	-7.08	108.98	119.60
33	a	689	A	OP1-P-OP2	-7.08	108.98	119.60
33	a	18	A	OP1-P-OP2	-7.08	108.98	119.60
10	A	918	A	OP1-P-OP2	-7.07	108.99	119.60
10	A	460	C	OP1-P-O3'	7.07	120.75	105.20
10	A	992	A	OP1-P-OP2	-7.07	109.00	119.60
33	a	738	A	OP1-P-OP2	-7.07	109.00	119.60
10	A	744	A	OP1-P-OP2	-7.06	109.01	119.60
33	a	818	A	O4'-C1'-N9	7.06	113.85	108.20
10	A	145	A	OP1-P-OP2	-7.06	109.01	119.60
10	A	1388	A	OP1-P-OP2	-7.06	109.01	119.60
10	A	429	A	OP1-P-OP2	-7.06	109.02	119.60
10	A	1475	A	OP1-P-OP2	-7.05	109.02	119.60
33	a	362	A	OP1-P-OP2	-7.05	109.02	119.60
10	A	3	U	OP1-P-OP2	-7.05	109.03	119.60
10	A	2324	A	OP1-P-OP2	-7.04	109.03	119.60
33	a	456	A	OP1-P-OP2	-7.04	109.05	119.60
10	A	766	A	OP1-P-OP2	-7.03	109.06	119.60
10	A	1630	A	OP1-P-OP2	-7.02	109.06	119.60
10	A	157	A	OP1-P-OP2	-7.02	109.07	119.60
10	A	1908	C	OP1-P-OP2	-7.02	109.07	119.60
33	a	1332	A	OP1-P-OP2	-7.02	109.07	119.60
33	a	1255	A	OP1-P-OP2	-7.02	109.08	119.60
33	a	221	A	OP1-P-OP2	-7.02	109.08	119.60
33	a	732	A	OP1-P-OP2	-7.01	109.08	119.60
10	A	2126	C	OP1-P-OP2	-7.01	109.08	119.60
10	A	2199	U	OP1-P-O3'	7.01	120.62	105.20
10	A	1628	A	OP1-P-OP2	-7.01	109.09	119.60
33	a	478	A	OP1-P-OP2	-7.01	109.09	119.60
10	A	2627	A	OP1-P-OP2	-7.00	109.09	119.60
33	a	1376	A	OP1-P-OP2	-7.00	109.09	119.60
12	D	39	A	OP1-P-OP2	-7.00	109.10	119.60
33	a	9	G	OP1-P-OP2	-7.00	109.10	119.60
10	A	2225	A	OP1-P-OP2	-7.00	109.10	119.60
10	A	493	A	OP1-P-OP2	-7.00	109.10	119.60
10	A	1456	A	OP1-P-OP2	-7.00	109.10	119.60
33	a	165	G	OP1-P-O3'	7.00	120.59	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	328	A	OP1-P-OP2	-7.00	109.11	119.60
10	A	2010	A	O4'-C1'-N9	6.99	113.79	108.20
10	A	2067	A	OP1-P-OP2	-6.99	109.12	119.60
10	A	2645	A	OP1-P-OP2	-6.98	109.13	119.60
10	A	2769	U	OP1-P-O3'	6.98	120.56	105.20
10	A	13	A	OP1-P-OP2	-6.98	109.13	119.60
10	A	1804	A	OP1-P-OP2	-6.98	109.13	119.60
10	A	2554	A	OP1-P-OP2	-6.98	109.13	119.60
10	A	1441	A	OP1-P-OP2	-6.97	109.14	119.60
10	A	1925	A	OP1-P-OP2	-6.97	109.14	119.60
33	a	667	A	OP1-P-OP2	-6.97	109.14	119.60
10	A	394	A	OP1-P-OP2	-6.97	109.15	119.60
10	A	1519	A	OP1-P-OP2	-6.97	109.15	119.60
33	a	472	A	OP1-P-OP2	-6.97	109.15	119.60
10	A	2121	A	OP1-P-OP2	-6.96	109.16	119.60
33	a	125	A	OP1-P-OP2	-6.96	109.16	119.60
33	a	964	A	OP1-P-OP2	-6.96	109.16	119.60
33	a	950	A	OP1-P-OP2	-6.95	109.17	119.60
10	A	1220	A	OP1-P-OP2	-6.95	109.18	119.60
33	a	1129	A	OP1-P-OP2	-6.95	109.18	119.60
33	a	1039	A	OP1-P-OP2	-6.95	109.18	119.60
10	A	413	A	OP1-P-OP2	-6.93	109.20	119.60
10	A	2816	A	OP1-P-OP2	-6.93	109.21	119.60
10	A	1484	A	OP1-P-OP2	-6.92	109.22	119.60
34	b	13	A	OP1-P-OP2	-6.92	109.23	119.60
10	A	986	A	OP1-P-OP2	-6.91	109.23	119.60
10	A	2216	G	OP1-P-OP2	-6.91	109.23	119.60
33	a	666	A	OP1-P-OP2	-6.91	109.24	119.60
10	A	339	A	OP1-P-OP2	-6.91	109.24	119.60
10	A	2149	A	OP1-P-OP2	-6.91	109.24	119.60
33	a	1060	G	OP1-P-OP2	-6.91	109.24	119.60
10	A	133	A	OP1-P-OP2	-6.90	109.24	119.60
10	A	550	G	OP1-P-O3'	6.90	120.39	105.20
33	a	928	A	OP1-P-OP2	-6.90	109.25	119.60
10	A	1575	A	OP1-P-OP2	-6.90	109.25	119.60
11	B	97	A	OP1-P-OP2	-6.90	109.25	119.60
33	a	621	A	OP1-P-OP2	-6.90	109.25	119.60
10	A	1605	A	OP1-P-OP2	-6.90	109.25	119.60
10	A	1949	A	OP1-P-OP2	-6.89	109.26	119.60
33	a	1013	A	OP1-P-OP2	-6.89	109.26	119.60
10	A	2424	A	OP1-P-OP2	-6.89	109.27	119.60
33	a	1314	A	OP1-P-OP2	-6.89	109.27	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2043	A	OP1-P-OP2	-6.88	109.28	119.60
10	A	2839	A	OP1-P-OP2	-6.88	109.28	119.60
10	A	773	A	OP1-P-OP2	-6.88	109.28	119.60
10	A	176	A	OP1-P-OP2	-6.88	109.29	119.60
33	a	934	A	OP1-P-OP2	-6.88	109.29	119.60
11	B	27	A	OP1-P-OP2	-6.88	109.29	119.60
33	a	565	A	OP1-P-OP2	-6.88	109.29	119.60
33	a	111	A	OP1-P-OP2	-6.87	109.29	119.60
10	A	499	A	OP1-P-OP2	-6.87	109.29	119.60
10	A	1530	G	OP1-P-O3'	6.87	120.32	105.20
10	A	774	A	OP1-P-OP2	-6.87	109.30	119.60
10	A	2132	A	OP1-P-OP2	-6.87	109.30	119.60
33	a	299	A	OP1-P-OP2	-6.87	109.30	119.60
10	A	1489	A	OP1-P-OP2	-6.87	109.30	119.60
10	A	1656	A	OP1-P-OP2	-6.87	109.30	119.60
10	A	1895	A	OP1-P-OP2	-6.87	109.30	119.60
10	A	389	A	OP1-P-OP2	-6.86	109.31	119.60
10	A	945	A	OP1-P-OP2	-6.86	109.31	119.60
10	A	2367	A	OP1-P-OP2	-6.86	109.31	119.60
33	a	458	A	OP1-P-OP2	-6.86	109.31	119.60
33	a	308	A	OP1-P-OP2	-6.86	109.31	119.60
10	A	958	A	OP1-P-OP2	-6.85	109.32	119.60
10	A	566	A	OP1-P-OP2	-6.85	109.32	119.60
10	A	1862	G	OP1-P-OP2	-6.85	109.33	119.60
10	A	131	A	OP1-P-OP2	-6.84	109.33	119.60
10	A	2353	A	OP1-P-OP2	-6.84	109.33	119.60
10	A	716	A	OP1-P-OP2	-6.84	109.34	119.60
10	A	936	A	OP1-P-OP2	-6.84	109.34	119.60
10	A	2579	A	O4'-C1'-N9	6.84	113.67	108.20
34	b	1	G	OP1-P-OP2	-6.84	109.34	119.60
10	A	1696	A	OP1-P-OP2	-6.84	109.34	119.60
33	a	1181	A	OP1-P-OP2	-6.84	109.34	119.60
10	A	2314	A	OP1-P-OP2	-6.84	109.34	119.60
10	A	1650	A	OP1-P-OP2	-6.83	109.35	119.60
10	A	5	A	OP1-P-OP2	-6.83	109.35	119.60
10	A	1214	A	OP1-P-OP2	-6.83	109.35	119.60
10	A	2147	A	OP1-P-OP2	-6.83	109.35	119.60
33	a	1561	A	OP1-P-OP2	-6.83	109.35	119.60
10	A	2447	A	OP1-P-OP2	-6.83	109.36	119.60
10	A	2155	A	OP1-P-OP2	-6.83	109.36	119.60
10	A	2218	A	OP1-P-OP2	-6.83	109.36	119.60
33	a	480	A	OP1-P-OP2	-6.83	109.36	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	325	A	OP1-P-OP2	-6.82	109.36	119.60
11	B	17	A	OP1-P-OP2	-6.82	109.36	119.60
33	a	1389	A	OP1-P-OP2	-6.82	109.36	119.60
33	a	158	A	OP1-P-OP2	-6.82	109.37	119.60
10	A	1499	A	OP1-P-OP2	-6.82	109.37	119.60
10	A	535	A	OP1-P-OP2	-6.81	109.38	119.60
33	a	240	G	OP1-P-OP2	-6.81	109.38	119.60
10	A	1707	A	OP1-P-OP2	-6.81	109.39	119.60
33	a	604	A	OP1-P-OP2	-6.81	109.39	119.60
33	a	1365	A	OP1-P-OP2	-6.81	109.39	119.60
10	A	2615	A	OP1-P-OP2	-6.80	109.40	119.60
33	a	734	A	OP1-P-OP2	-6.80	109.40	119.60
10	A	1208	A	OP1-P-OP2	-6.80	109.41	119.60
10	A	655	A	OP1-P-OP2	-6.79	109.41	119.60
33	a	1071	A	OP1-P-OP2	-6.79	109.41	119.60
10	A	1683	A	OP1-P-OP2	-6.79	109.42	119.60
33	a	688	A	OP1-P-OP2	-6.79	109.42	119.60
10	A	941	A	OP1-P-OP2	-6.79	109.42	119.60
10	A	2647	A	OP1-P-OP2	-6.79	109.42	119.60
33	a	228	A	OP1-P-OP2	-6.78	109.42	119.60
10	A	789	A	OP1-P-OP2	-6.78	109.43	119.60
10	A	1762	A	OP1-P-OP2	-6.78	109.43	119.60
33	a	1487	A	OP1-P-OP2	-6.78	109.43	119.60
10	A	2738	A	OP1-P-OP2	-6.78	109.43	119.60
10	A	1516	A	OP1-P-OP2	-6.78	109.44	119.60
33	a	973	A	OP1-P-OP2	-6.78	109.44	119.60
10	A	469	A	OP1-P-OP2	-6.77	109.44	119.60
33	a	375	A	OP1-P-OP2	-6.77	109.45	119.60
10	A	940	A	OP1-P-OP2	-6.77	109.45	119.60
10	A	1054	A	OP1-P-OP2	-6.76	109.45	119.60
33	a	1300	A	OP1-P-OP2	-6.76	109.46	119.60
10	A	1529	A	OP1-P-OP2	-6.76	109.46	119.60
10	A	1802	A	OP1-P-OP2	-6.76	109.46	119.60
10	A	10	A	OP1-P-OP2	-6.76	109.47	119.60
10	A	2286	A	OP1-P-OP2	-6.76	109.47	119.60
10	A	2438	A	OP1-P-OP2	-6.76	109.47	119.60
10	A	1061	G	OP1-P-OP2	-6.75	109.47	119.60
33	a	379	A	OP1-P-OP2	-6.75	109.47	119.60
10	A	2014	A	OP1-P-OP2	-6.75	109.48	119.60
10	A	2186	A	OP1-P-OP2	-6.75	109.48	119.60
10	A	301	A	OP1-P-OP2	-6.74	109.49	119.60
10	A	1739	G	OP1-P-OP2	-6.74	109.49	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	2	G	OP1-P-OP2	-6.74	109.49	119.60
10	A	56	A	OP1-P-OP2	-6.74	109.50	119.60
33	a	854	A	OP1-P-OP2	-6.74	109.50	119.60
10	A	1633	A	OP1-P-OP2	-6.73	109.50	119.60
10	A	1145	A	OP1-P-OP2	-6.73	109.51	119.60
10	A	1768	A	OP1-P-OP2	-6.73	109.51	119.60
10	A	2080	A	OP1-P-OP2	-6.73	109.51	119.60
10	A	2820	A	OP1-P-OP2	-6.72	109.52	119.60
10	A	2084	A	OP1-P-OP2	-6.71	109.53	119.60
10	A	1240	A	OP1-P-OP2	-6.71	109.53	119.60
10	A	280	A	OP1-P-OP2	-6.71	109.53	119.60
10	A	2171	A	OP1-P-OP2	-6.71	109.54	119.60
10	A	1709	G	OP1-P-O3'	6.71	119.95	105.20
11	B	80	A	OP1-P-OP2	-6.70	109.54	119.60
33	a	899	A	OP1-P-OP2	-6.70	109.54	119.60
10	A	1231	A	OP1-P-OP2	-6.70	109.55	119.60
10	A	1515	A	OP1-P-OP2	-6.70	109.55	119.60
10	A	1012	A	OP1-P-OP2	-6.70	109.55	119.60
10	A	1185	A	OP1-P-OP2	-6.70	109.55	119.60
33	a	457	A	OP1-P-OP2	-6.70	109.55	119.60
33	a	1442	A	OP1-P-OP2	-6.70	109.55	119.60
33	a	686	A	OP1-P-OP2	-6.70	109.55	119.60
33	a	818	A	OP1-P-OP2	-6.70	109.56	119.60
33	a	1270	A	OP1-P-OP2	-6.70	109.56	119.60
10	A	64	A	OP1-P-OP2	-6.69	109.57	119.60
33	a	1507	A	OP1-P-OP2	-6.69	109.57	119.60
10	A	1422	A	OP1-P-OP2	-6.69	109.57	119.60
33	a	1196	A	OP1-P-OP2	-6.69	109.57	119.60
10	A	1817	A	OP1-P-OP2	-6.68	109.58	119.60
10	A	1535	A	OP1-P-OP2	-6.68	109.58	119.60
33	a	1315	A	OP1-P-OP2	-6.68	109.58	119.60
10	A	2871	U	OP1-P-O3'	6.68	119.89	105.20
10	A	2127	A	OP1-P-OP2	-6.68	109.58	119.60
10	A	1229	A	OP1-P-OP2	-6.67	109.59	119.60
33	a	694	A	OP1-P-OP2	-6.67	109.59	119.60
10	A	2160	A	OP1-P-OP2	-6.67	109.59	119.60
10	A	1061	G	N9-C4-C5	6.67	108.07	105.40
33	a	775	A	OP1-P-OP2	-6.67	109.60	119.60
10	A	2154	A	OP1-P-OP2	-6.67	109.60	119.60
10	A	2903	G	OP1-P-O3'	6.66	119.85	105.20
10	A	1013	A	OP1-P-O3'	6.66	119.84	105.20
10	A	1869	A	OP1-P-OP2	-6.66	109.62	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2909	A	OP1-P-OP2	-6.66	109.62	119.60
33	a	397	G	OP2-P-O3'	6.66	119.84	105.20
10	A	949	A	OP1-P-OP2	-6.65	109.63	119.60
10	A	2313	A	OP1-P-OP2	-6.65	109.63	119.60
10	A	1308	A	OP1-P-OP2	-6.64	109.64	119.60
33	a	890	A	OP1-P-OP2	-6.64	109.64	119.60
10	A	1743	A	OP1-P-OP2	-6.64	109.64	119.60
10	A	634	A	OP1-P-OP2	-6.63	109.65	119.60
33	a	887	A	OP1-P-OP2	-6.63	109.65	119.60
10	A	2822	A	OP1-P-OP2	-6.63	109.66	119.60
10	A	1636	A	OP1-P-OP2	-6.63	109.66	119.60
33	a	1047	A	OP1-P-OP2	-6.62	109.67	119.60
33	a	1183	A	OP1-P-OP2	-6.62	109.66	119.60
10	A	199	A	OP1-P-OP2	-6.62	109.67	119.60
33	a	696	A	OP1-P-OP2	-6.62	109.67	119.60
10	A	553	A	OP1-P-OP2	-6.62	109.68	119.60
10	A	2590	A	OP1-P-OP2	-6.62	109.68	119.60
33	a	489	A	OP1-P-OP2	-6.62	109.68	119.60
10	A	998	A	OP1-P-OP2	-6.61	109.68	119.60
33	a	1163	U	OP1-P-O3'	6.61	119.74	105.20
10	A	264	A	OP1-P-OP2	-6.60	109.69	119.60
10	A	2755	A	OP1-P-OP2	-6.60	109.69	119.60
10	A	404	A	O5'-P-OP1	-6.60	99.76	105.70
10	A	2181	G	OP1-P-OP2	-6.60	109.70	119.60
33	a	1144	A	OP1-P-OP2	-6.60	109.70	119.60
10	A	2183	G	OP1-P-OP2	-6.60	109.70	119.60
11	B	44	A	OP1-P-OP2	-6.60	109.70	119.60
10	A	2516	A	OP1-P-OP2	-6.60	109.70	119.60
10	A	121	G	OP1-P-OP2	-6.60	109.71	119.60
10	A	410	A	OP1-P-OP2	-6.60	109.71	119.60
10	A	2751	A	OP1-P-OP2	-6.59	109.71	119.60
33	a	942	A	OP1-P-OP2	-6.59	109.71	119.60
33	a	1239	A	OP1-P-OP2	-6.59	109.71	119.60
10	A	2211	A	OP1-P-OP2	-6.59	109.72	119.60
12	D	59	A	OP1-P-OP2	-6.59	109.72	119.60
33	a	1375	A	OP1-P-OP2	-6.59	109.72	119.60
10	A	1635	A	OP1-P-OP2	-6.59	109.72	119.60
33	a	422	A	OP1-P-OP2	-6.58	109.72	119.60
10	A	2684	A	OP1-P-OP2	-6.58	109.72	119.60
33	a	1452	A	OP1-P-OP2	-6.58	109.72	119.60
10	A	1897	A	OP1-P-OP2	-6.58	109.73	119.60
10	A	2182	G	OP1-P-OP2	-6.58	109.74	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	81	A	OP1-P-OP2	-6.58	109.74	119.60
33	a	986	A	OP1-P-OP2	-6.58	109.74	119.60
10	A	574	A	OP1-P-OP2	-6.57	109.74	119.60
33	a	1066	A	OP1-P-OP2	-6.57	109.74	119.60
33	a	707	A	OP1-P-OP2	-6.57	109.75	119.60
10	A	719	A	OP1-P-OP2	-6.57	109.75	119.60
10	A	915	A	OP1-P-OP2	-6.57	109.75	119.60
10	A	1823	A	OP1-P-OP2	-6.56	109.75	119.60
10	A	682	A	OP1-P-OP2	-6.56	109.76	119.60
33	a	1390	C	OP1-P-OP2	-6.56	109.76	119.60
10	A	382	A	OP1-P-OP2	-6.56	109.76	119.60
33	a	498	A	OP1-P-OP2	-6.56	109.76	119.60
10	A	496	A	OP1-P-OP2	-6.56	109.76	119.60
33	a	135	A	OP1-P-OP2	-6.56	109.77	119.60
33	a	1422	A	OP1-P-OP2	-6.56	109.76	119.60
11	B	20	A	OP1-P-OP2	-6.55	109.77	119.60
33	a	470	A	OP1-P-OP2	-6.55	109.78	119.60
10	A	486	A	OP1-P-OP2	-6.55	109.78	119.60
33	a	1094	A	OP1-P-OP2	-6.54	109.78	119.60
10	A	1889	A	OP1-P-OP2	-6.54	109.78	119.60
10	A	2246	A	OP1-P-OP2	-6.54	109.80	119.60
10	A	1866	A	OP1-P-OP2	-6.54	109.80	119.60
10	A	569	A	O4'-C1'-N9	6.53	113.43	108.20
10	A	1526	A	OP1-P-OP2	-6.53	109.80	119.60
11	B	26	C	OP1-P-O3'	6.53	119.56	105.20
10	A	905	C	OP1-P-OP2	-6.53	109.81	119.60
10	A	1052	A	OP1-P-OP2	-6.53	109.81	119.60
12	D	11	A	OP1-P-OP2	-6.53	109.81	119.60
33	a	189	A	OP1-P-OP2	-6.52	109.81	119.60
10	A	2893	A	OP1-P-OP2	-6.52	109.82	119.60
11	B	113	A	OP1-P-OP2	-6.52	109.82	119.60
33	a	1230	A	OP1-P-OP2	-6.52	109.82	119.60
10	A	1544	A	OP1-P-OP2	-6.52	109.82	119.60
10	A	2005	G	OP1-P-OP2	-6.51	109.83	119.60
11	B	19	A	OP1-P-OP2	-6.51	109.83	119.60
10	A	1839	C	OP1-P-OP2	-6.51	109.83	119.60
10	A	2477	C	OP1-P-OP2	-6.51	109.83	119.60
10	A	2472	A	OP1-P-OP2	-6.51	109.84	119.60
10	A	1029	A	OP1-P-OP2	-6.51	109.84	119.60
10	A	2116	A	OP1-P-OP2	-6.51	109.84	119.60
10	A	2753	A	OP1-P-OP2	-6.51	109.84	119.60
33	a	218	A	OP1-P-OP2	-6.50	109.84	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	761	A	OP1-P-OP2	-6.50	109.84	119.60
10	A	2026	A	OP1-P-OP2	-6.50	109.85	119.60
10	A	2240	A	OP1-P-OP2	-6.50	109.85	119.60
10	A	790	A	OP1-P-O3'	6.50	119.50	105.20
10	A	2495	A	OP1-P-OP2	-6.50	109.85	119.60
10	A	2446	A	OP1-P-OP2	-6.50	109.86	119.60
10	A	228	A	OP1-P-OP2	-6.50	109.86	119.60
33	a	124	G	OP1-P-O3'	6.50	119.49	105.20
10	A	259	A	OP1-P-OP2	-6.49	109.87	119.60
10	A	1203	A	OP1-P-OP2	-6.49	109.87	119.60
33	a	459	A	OP1-P-OP2	-6.49	109.87	119.60
33	a	1252	C	OP1-P-O3'	6.49	119.48	105.20
10	A	304	A	OP1-P-OP2	-6.49	109.87	119.60
10	A	1272	G	OP1-P-O3'	6.49	119.47	105.20
10	A	2901	A	OP1-P-OP2	-6.48	109.88	119.60
33	a	1289	A	OP1-P-OP2	-6.48	109.88	119.60
11	B	51	A	OP1-P-OP2	-6.48	109.89	119.60
10	A	441	A	OP1-P-OP2	-6.47	109.89	119.60
10	A	1909	A	OP1-P-OP2	-6.47	109.90	119.60
33	a	517	A	OP1-P-OP2	-6.47	109.90	119.60
10	A	728	A	OP1-P-OP2	-6.47	109.90	119.60
33	a	1526	A	OP1-P-OP2	-6.47	109.90	119.60
10	A	2878	A	OP1-P-OP2	-6.46	109.91	119.60
33	a	284	A	OP1-P-OP2	-6.46	109.91	119.60
33	a	341	A	OP1-P-OP2	-6.46	109.91	119.60
10	A	1682	A	OP1-P-OP2	-6.46	109.91	119.60
33	a	1197	A	OP1-P-OP2	-6.46	109.91	119.60
10	A	67	A	OP1-P-OP2	-6.46	109.92	119.60
10	A	462	A	OP1-P-OP2	-6.46	109.92	119.60
33	a	1505	A	OP1-P-OP2	-6.46	109.92	119.60
33	a	188	A	OP1-P-OP2	-6.45	109.92	119.60
33	a	803	A	OP1-P-OP2	-6.45	109.92	119.60
10	A	2189	A	OP1-P-OP2	-6.45	109.93	119.60
10	A	2484	A	OP1-P-OP2	-6.45	109.93	119.60
10	A	2845	A	OP1-P-OP2	-6.45	109.93	119.60
33	a	1034	A	OP1-P-OP2	-6.45	109.93	119.60
33	a	300	A	OP1-P-OP2	-6.44	109.94	119.60
10	A	901	A	OP1-P-OP2	-6.44	109.94	119.60
10	A	347	A	OP1-P-OP2	-6.44	109.94	119.60
10	A	2073	A	OP1-P-OP2	-6.44	109.94	119.60
33	a	559	A	OP1-P-OP2	-6.44	109.94	119.60
10	A	2280	A	OP1-P-OP2	-6.43	109.95	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	890	A	OP1-P-OP2	-6.43	109.96	119.60
10	A	1688	A	OP1-P-OP2	-6.43	109.96	119.60
10	A	2754	A	OP1-P-OP2	-6.43	109.95	119.60
33	a	523	A	OP1-P-OP2	-6.43	109.96	119.60
10	A	53	A	OP1-P-OP2	-6.43	109.96	119.60
10	A	588	A	OP1-P-OP2	-6.43	109.96	119.60
10	A	2836	A	OP1-P-OP2	-6.42	109.96	119.60
33	a	833	A	OP1-P-OP2	-6.42	109.97	119.60
10	A	1631	A	OP1-P-OP2	-6.42	109.97	119.60
33	a	353	A	OP1-P-OP2	-6.42	109.97	119.60
10	A	166	A	OP1-P-OP2	-6.42	109.97	119.60
11	B	54	U	OP1-P-OP2	-6.42	109.97	119.60
10	A	550	G	O4'-C1'-N9	6.42	113.33	108.20
10	A	1644	U	OP1-P-OP2	-6.41	109.98	119.60
12	D	52	A	OP1-P-OP2	-6.41	109.98	119.60
10	A	707	A	OP1-P-OP2	-6.41	109.98	119.60
10	A	874	A	OP1-P-OP2	-6.41	109.98	119.60
10	A	130	A	OP1-P-OP2	-6.41	109.98	119.60
10	A	1898	A	OP1-P-OP2	-6.41	109.98	119.60
33	a	1150	A	OP1-P-OP2	-6.41	109.98	119.60
10	A	629	A	OP1-P-OP2	-6.41	109.99	119.60
12	D	36	A	OP1-P-OP2	-6.41	109.99	119.60
10	A	1664	A	OP1-P-OP2	-6.40	110.00	119.60
33	a	1287	A	OP1-P-OP2	-6.40	110.00	119.60
10	A	178	A	OP1-P-OP2	-6.40	110.00	119.60
10	A	539	A	OP1-P-OP2	-6.40	110.00	119.60
10	A	862	A	OP1-P-OP2	-6.40	110.00	119.60
10	A	1280	A	OP1-P-OP2	-6.39	110.01	119.60
12	D	44	A	OP1-P-OP2	-6.39	110.01	119.60
33	a	117	A	OP1-P-OP2	-6.39	110.01	119.60
33	a	539	A	OP1-P-OP2	-6.39	110.01	119.60
10	A	2688	A	OP1-P-OP2	-6.39	110.01	119.60
33	a	57	A	OP1-P-OP2	-6.39	110.01	119.60
10	A	510	A	OP1-P-OP2	-6.39	110.01	119.60
33	a	1271	A	OP1-P-OP2	-6.39	110.01	119.60
33	a	223	A	OP1-P-OP2	-6.39	110.02	119.60
33	a	1276	A	OP1-P-OP2	-6.39	110.02	119.60
33	a	1280	A	OP1-P-OP2	-6.39	110.02	119.60
10	A	118	A	OP1-P-OP2	-6.39	110.02	119.60
10	A	317	A	OP1-P-OP2	-6.38	110.03	119.60
10	A	1108	A	OP1-P-OP2	-6.38	110.03	119.60
10	A	2136	A	OP1-P-OP2	-6.38	110.03	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2585	A	OP1-P-OP2	-6.38	110.03	119.60
33	a	433	A	OP1-P-OP2	-6.38	110.03	119.60
10	A	65	A	OP1-P-OP2	-6.38	110.03	119.60
10	A	1512	A	OP1-P-OP2	-6.38	110.03	119.60
10	A	1061	G	C8-N9-C1'	6.37	135.28	127.00
33	a	922	A	OP1-P-OP2	-6.37	110.04	119.60
11	B	47	C	OP1-P-O3'	6.37	119.20	105.20
33	a	635	A	OP1-P-OP2	-6.37	110.05	119.60
10	A	1048	A	OP1-P-OP2	-6.36	110.05	119.60
33	a	648	A	OP1-P-OP2	-6.36	110.05	119.60
10	A	2721	G	OP1-P-O3'	6.36	119.19	105.20
10	A	957	A	OP1-P-OP2	-6.36	110.06	119.60
10	A	1287	A	OP1-P-OP2	-6.36	110.07	119.60
10	A	2366	G	OP1-P-O3'	6.36	119.18	105.20
10	A	2103	A	OP1-P-OP2	-6.35	110.07	119.60
33	a	848	A	OP1-P-OP2	-6.35	110.07	119.60
10	A	626	A	OP1-P-OP2	-6.35	110.08	119.60
10	A	6	A	OP1-P-OP2	-6.35	110.08	119.60
34	b	3	A	OP1-P-OP2	-6.35	110.08	119.60
33	a	1262	A	OP1-P-OP2	-6.34	110.08	119.60
10	A	1464	A	OP1-P-OP2	-6.34	110.09	119.60
10	A	454	A	OP1-P-OP2	-6.34	110.09	119.60
33	a	400	A	OP1-P-OP2	-6.34	110.10	119.60
33	a	1041	A	OP1-P-OP2	-6.33	110.10	119.60
10	A	2677	G	OP1-P-O3'	6.33	119.13	105.20
33	a	828	A	OP1-P-OP2	-6.33	110.11	119.60
33	a	296	A	OP1-P-OP2	-6.32	110.11	119.60
10	A	2011	A	OP1-P-OP2	-6.32	110.12	119.60
33	a	807	A	OP1-P-OP2	-6.32	110.12	119.60
33	a	1109	A	OP1-P-OP2	-6.32	110.12	119.60
10	A	1825	A	OP1-P-OP2	-6.32	110.13	119.60
10	A	2815	A	OP1-P-OP2	-6.32	110.13	119.60
10	A	1343	A	OP1-P-OP2	-6.31	110.13	119.60
10	A	2374	A	OP1-P-OP2	-6.31	110.13	119.60
33	a	524	A	OP1-P-O3'	6.31	119.08	105.20
10	A	622	A	OP1-P-OP2	-6.30	110.15	119.60
10	A	803	A	OP1-P-OP2	-6.30	110.15	119.60
33	a	1226	C	OP1-P-O3'	6.30	119.06	105.20
10	A	1061	G	N3-C4-N9	-6.30	122.22	126.00
10	A	2050	A	OP1-P-OP2	-6.30	110.16	119.60
10	A	2341	A	OP1-P-OP2	-6.30	110.16	119.60
33	a	992	A	OP1-P-OP2	-6.29	110.16	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	44	A	OP1-P-OP2	-6.29	110.16	119.60
10	A	1949	A	C1'-O4'-C4'	-6.29	104.87	109.90
33	a	855	A	OP1-P-OP2	-6.29	110.16	119.60
33	a	1306	A	OP1-P-OP2	-6.29	110.16	119.60
33	a	114	A	OP1-P-OP2	-6.29	110.17	119.60
10	A	2248	A	OP1-P-OP2	-6.29	110.17	119.60
10	A	2692	A	OP1-P-OP2	-6.29	110.17	119.60
10	A	2794	A	OP1-P-OP2	-6.29	110.17	119.60
10	A	2847	A	OP1-P-OP2	-6.28	110.17	119.60
10	A	1336	A	O4'-C1'-N9	6.28	113.23	108.20
33	a	385	A	OP1-P-OP2	-6.28	110.18	119.60
10	A	2789	A	OP1-P-OP2	-6.28	110.18	119.60
33	a	1454	A	OP1-P-OP2	-6.28	110.19	119.60
10	A	1879	A	OP1-P-OP2	-6.27	110.19	119.60
11	B	64	A	OP1-P-OP2	-6.27	110.19	119.60
11	B	46	A	OP1-P-OP2	-6.27	110.20	119.60
10	A	383	A	OP1-P-OP2	-6.27	110.20	119.60
10	A	1154	A	OP1-P-OP2	-6.27	110.20	119.60
33	a	1242	A	OP1-P-OP2	-6.27	110.20	119.60
10	A	2555	A	OP1-P-OP2	-6.27	110.20	119.60
10	A	217	G	OP1-P-O3'	6.26	118.98	105.20
33	a	1265	A	OP1-P-OP2	-6.26	110.20	119.60
10	A	615	A	OP1-P-OP2	-6.26	110.20	119.60
33	a	785	A	OP1-P-OP2	-6.26	110.21	119.60
10	A	147	A	OP1-P-OP2	-6.26	110.21	119.60
10	A	2390	A	OP1-P-OP2	-6.26	110.21	119.60
10	A	1906	C	OP1-P-OP2	-6.26	110.21	119.60
10	A	2342	A	OP1-P-OP2	-6.26	110.21	119.60
10	A	2291	A	OP1-P-OP2	-6.25	110.22	119.60
33	a	250	A	OP1-P-OP2	-6.25	110.22	119.60
33	a	1156	C	OP1-P-O3'	6.25	118.96	105.20
10	A	1672	A	OP1-P-OP2	-6.25	110.23	119.60
10	A	2703	A	OP1-P-OP2	-6.25	110.23	119.60
10	A	541	A	OP1-P-OP2	-6.25	110.23	119.60
10	A	2814	A	OP1-P-OP2	-6.25	110.23	119.60
33	a	35	A	OP1-P-OP2	-6.25	110.23	119.60
10	A	1632	A	OP1-P-OP2	-6.24	110.24	119.60
10	A	2281	A	OP1-P-OP2	-6.24	110.24	119.60
10	A	889	A	OP1-P-OP2	-6.23	110.25	119.60
10	A	1168	A	OP1-P-OP2	-6.22	110.26	119.60
10	A	2311	A	OP1-P-OP2	-6.22	110.27	119.60
10	A	2346	A	OP1-P-OP2	-6.22	110.28	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1503	A	OP1-P-OP2	-6.22	110.28	119.60
10	A	1468	A	OP1-P-OP2	-6.21	110.28	119.60
10	A	518	A	OP1-P-OP2	-6.21	110.28	119.60
33	a	1451	A	OP1-P-O3'	6.21	118.86	105.20
10	A	106	A	OP1-P-OP2	-6.21	110.29	119.60
33	a	936	A	OP1-P-OP2	-6.21	110.29	119.60
33	a	1383	A	OP1-P-OP2	-6.20	110.29	119.60
10	A	1652	A	OP1-P-OP2	-6.20	110.30	119.60
33	a	497	A	OP1-P-OP2	-6.20	110.30	119.60
10	A	2263	G	OP1-P-OP2	-6.19	110.32	119.60
10	A	1558	A	OP1-P-OP2	-6.19	110.32	119.60
10	A	191	G	OP1-P-O3'	6.18	118.80	105.20
10	A	224	A	OP1-P-OP2	-6.18	110.33	119.60
10	A	1183	A	OP1-P-OP2	-6.18	110.33	119.60
33	a	1067	A	OP1-P-OP2	-6.18	110.33	119.60
33	a	810	A	OP1-P-OP2	-6.18	110.33	119.60
10	A	1282	A	OP1-P-OP2	-6.17	110.34	119.60
10	A	1394	A	OP1-P-OP2	-6.17	110.34	119.60
10	A	2221	A	OP1-P-OP2	-6.17	110.34	119.60
10	A	860	A	OP1-P-OP2	-6.17	110.35	119.60
33	a	1224	A	OP1-P-OP2	-6.17	110.35	119.60
10	A	1430	A	OP1-P-OP2	-6.16	110.36	119.60
33	a	269	A	OP1-P-OP2	-6.16	110.36	119.60
10	A	198	A	OP1-P-OP2	-6.16	110.36	119.60
10	A	368	A	OP1-P-OP2	-6.16	110.37	119.60
11	B	71	A	OP1-P-OP2	-6.16	110.36	119.60
10	A	1982	A	OP1-P-OP2	-6.15	110.37	119.60
10	A	500	C	OP1-P-OP2	-6.15	110.38	119.60
33	a	415	A	OP1-P-OP2	-6.15	110.38	119.60
10	A	1189	U	OP1-P-O3'	6.14	118.72	105.20
10	A	1883	U	C2-N1-C1'	6.14	125.07	117.70
10	A	2886	A	OP1-P-OP2	-6.14	110.38	119.60
33	a	168	A	OP1-P-OP2	-6.14	110.39	119.60
10	A	1206	A	OP1-P-OP2	-6.13	110.40	119.60
10	A	1400	A	OP1-P-OP2	-6.13	110.40	119.60
10	A	215	A	OP1-P-OP2	-6.13	110.41	119.60
10	A	223	A	OP1-P-OP2	-6.13	110.41	119.60
10	A	1430	A	O4'-C1'-N9	6.13	113.10	108.20
10	A	1571	A	OP1-P-OP2	-6.13	110.41	119.60
10	A	1931	A	OP1-P-O3'	6.12	118.67	105.20
33	a	1023	A	OP1-P-OP2	-6.12	110.42	119.60
10	A	117	A	OP1-P-OP2	-6.12	110.42	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	392	A	OP1-P-OP2	-6.12	110.42	119.60
33	a	1372	A	OP1-P-OP2	-6.12	110.42	119.60
10	A	2327	A	OP1-P-OP2	-6.12	110.43	119.60
10	A	841	A	OP1-P-OP2	-6.11	110.44	119.60
10	A	281	A	OP1-P-OP2	-6.11	110.44	119.60
10	A	162	A	OP1-P-OP2	-6.10	110.44	119.60
33	a	131	G	O4'-C1'-N9	6.10	113.08	108.20
33	a	666	A	OP1-P-O3'	6.10	118.63	105.20
33	a	900	A	OP1-P-OP2	-6.10	110.44	119.60
10	A	1505	A	OP1-P-OP2	-6.10	110.45	119.60
10	A	334	G	OP1-P-O3'	6.10	118.62	105.20
10	A	2359	A	OP1-P-OP2	-6.10	110.45	119.60
10	A	364	U	OP1-P-OP2	-6.10	110.45	119.60
10	A	430	A	OP1-P-OP2	-6.10	110.45	119.60
33	a	31	A	OP1-P-OP2	-6.10	110.45	119.60
10	A	516	A	OP1-P-OP2	-6.10	110.46	119.60
10	A	277	A	OP1-P-OP2	-6.09	110.47	119.60
10	A	2026	A	OP1-P-O3'	6.09	118.59	105.20
10	A	1067	A	OP1-P-OP2	-6.08	110.47	119.60
10	A	2260	A	OP1-P-OP2	-6.08	110.48	119.60
33	a	589	A	OP1-P-OP2	-6.08	110.48	119.60
10	A	610	A	OP1-P-OP2	-6.08	110.48	119.60
10	A	2254	A	OP1-P-OP2	-6.08	110.48	119.60
10	A	1298	A	OP1-P-OP2	-6.08	110.49	119.60
10	A	1598	A	OP1-P-OP2	-6.08	110.49	119.60
10	A	2279	A	OP1-P-OP2	-6.08	110.49	119.60
10	A	917	U	OP1-P-O3'	6.07	118.56	105.20
33	a	634	A	OP1-P-OP2	-6.07	110.49	119.60
10	A	1799	A	O4'-C1'-N9	6.07	113.06	108.20
10	A	2391	A	OP1-P-OP2	-6.07	110.50	119.60
33	a	220	A	OP1-P-OP2	-6.06	110.50	119.60
10	A	765	G	OP1-P-O3'	6.06	118.53	105.20
33	a	608	C	OP1-P-O3'	6.06	118.53	105.20
10	A	1377	A	OP1-P-OP2	-6.05	110.52	119.60
10	A	376	A	OP1-P-OP2	-6.05	110.52	119.60
33	a	68	A	OP1-P-OP2	-6.05	110.53	119.60
10	A	1283	A	OP1-P-OP2	-6.05	110.53	119.60
10	A	980	A	OP1-P-OP2	-6.04	110.54	119.60
10	A	1914	A	OP1-P-OP2	-6.04	110.54	119.60
33	a	62	A	OP1-P-OP2	-6.04	110.54	119.60
33	a	1274	A	O4'-C1'-N9	6.04	113.03	108.20
10	A	421	A	OP1-P-OP2	-6.03	110.55	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1132	A	OP1-P-OP2	-6.03	110.55	119.60
10	A	1796	A	OP1-P-OP2	-6.03	110.55	119.60
33	a	440	A	OP1-P-OP2	-6.03	110.56	119.60
10	A	1629	G	OP1-P-O3'	6.03	118.45	105.20
10	A	1357	A	OP1-P-OP2	-6.02	110.56	119.60
10	A	2371	A	OP1-P-OP2	-6.02	110.56	119.60
10	A	2669	U	OP1-P-O3'	6.02	118.45	105.20
33	a	272	A	OP1-P-OP2	-6.02	110.57	119.60
33	a	1004	A	OP1-P-OP2	-6.02	110.57	119.60
10	A	1336	A	OP1-P-OP2	-6.02	110.57	119.60
10	A	2892	A	OP1-P-OP2	-6.02	110.57	119.60
33	a	1160	A	OP1-P-OP2	-6.02	110.57	119.60
10	A	1331	A	OP1-P-OP2	-6.01	110.58	119.60
10	A	1994	A	OP1-P-OP2	-6.01	110.58	119.60
10	A	1022	A	OP1-P-OP2	-6.01	110.58	119.60
33	a	742	A	OP1-P-OP2	-6.01	110.59	119.60
33	a	131	G	OP1-P-OP2	-6.00	110.60	119.60
10	A	701	A	OP1-P-OP2	-6.00	110.60	119.60
10	A	830	C	OP1-P-O3'	6.00	118.40	105.20
10	A	2018	A	OP1-P-OP2	-6.00	110.61	119.60
10	A	2384	G	OP1-P-OP2	-6.00	110.61	119.60
33	a	1366	A	OP1-P-OP2	-5.99	110.61	119.60
33	a	12	A	OP1-P-OP2	-5.99	110.62	119.60
33	a	1337	A	OP1-P-OP2	-5.99	110.62	119.60
10	A	608	A	OP1-P-OP2	-5.99	110.62	119.60
10	A	839	A	OP1-P-OP2	-5.99	110.62	119.60
10	A	1944	U	OP1-P-O3'	5.99	118.37	105.20
10	A	1239	A	OP1-P-OP2	-5.98	110.63	119.60
10	A	1815	A	OP1-P-OP2	-5.98	110.63	119.60
33	a	903	A	OP1-P-OP2	-5.98	110.63	119.60
33	a	450	G	OP1-P-O3'	5.98	118.35	105.20
33	a	484	A	OP1-P-OP2	-5.98	110.63	119.60
33	a	702	A	OP1-P-OP2	-5.98	110.64	119.60
33	a	408	A	OP1-P-OP2	-5.98	110.64	119.60
33	a	691	A	OP1-P-OP2	-5.98	110.64	119.60
10	A	1627	G	OP1-P-O3'	5.97	118.34	105.20
33	a	990	G	OP1-P-O3'	5.97	118.34	105.20
10	A	681	A	OP1-P-OP2	-5.97	110.64	119.60
10	A	2742	A	OP1-P-OP2	-5.97	110.65	119.60
33	a	355	A	OP1-P-OP2	-5.97	110.65	119.60
10	A	1001	A	OP1-P-OP2	-5.96	110.65	119.60
33	a	975	C	OP1-P-O3'	5.96	118.32	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1496	A	OP1-P-OP2	-5.96	110.66	119.60
10	A	1371	A	OP1-P-OP2	-5.96	110.66	119.60
10	A	173	A	OP1-P-OP2	-5.96	110.66	119.60
10	A	2855	A	OP1-P-OP2	-5.95	110.68	119.60
10	A	2760	G	OP1-P-O3'	5.95	118.28	105.20
33	a	347	A	OP1-P-OP2	-5.95	110.68	119.60
10	A	1061	G	C6-C5-N7	5.95	133.97	130.40
10	A	38	A	OP1-P-OP2	-5.94	110.69	119.60
10	A	378	A	OP1-P-OP2	-5.94	110.69	119.60
33	a	521	A	OP1-P-OP2	-5.94	110.69	119.60
33	a	419	A	OP1-P-OP2	-5.94	110.69	119.60
10	A	2036	A	OP1-P-OP2	-5.93	110.70	119.60
10	A	2719	A	OP1-P-OP2	-5.93	110.70	119.60
10	A	448	G	OP1-P-OP2	-5.93	110.70	119.60
10	A	1650	A	O4'-C1'-N9	5.93	112.94	108.20
10	A	1863	G	OP1-P-OP2	-5.93	110.70	119.60
33	a	961	C	OP1-P-O3'	5.92	118.23	105.20
10	A	1973	A	OP1-P-OP2	-5.92	110.72	119.60
10	A	2603	A	OP1-P-OP2	-5.92	110.72	119.60
10	A	196	G	OP1-P-O3'	5.92	118.21	105.20
10	A	2490	C	OP1-P-O3'	5.91	118.21	105.20
10	A	488	A	OP1-P-OP2	-5.91	110.73	119.60
10	A	517	A	OP1-P-OP2	-5.91	110.73	119.60
10	A	1711	A	OP1-P-OP2	-5.91	110.73	119.60
10	A	2382	A	OP1-P-OP2	-5.91	110.73	119.60
33	a	633	A	OP1-P-OP2	-5.91	110.73	119.60
10	A	400	G	OP2-P-O3'	5.91	118.20	105.20
10	A	903	A	OP1-P-OP2	-5.91	110.74	119.60
10	A	2431	A	OP1-P-OP2	-5.91	110.74	119.60
33	a	1355	A	OP1-P-OP2	-5.90	110.74	119.60
10	A	947	A	OP1-P-OP2	-5.90	110.75	119.60
10	A	2482	A	OP1-P-OP2	-5.90	110.75	119.60
33	a	1137	A	OP1-P-OP2	-5.90	110.75	119.60
10	A	2064	A	OP1-P-OP2	-5.90	110.75	119.60
33	a	312	A	OP1-P-OP2	-5.89	110.76	119.60
10	A	1554	G	OP1-P-O3'	5.89	118.16	105.20
10	A	1842	A	OP1-P-OP2	-5.89	110.77	119.60
33	a	806	A	OP1-P-OP2	-5.89	110.77	119.60
10	A	2553	C	OP1-P-O3'	5.88	118.15	105.20
10	A	2613	A	OP1-P-OP2	-5.88	110.78	119.60
10	A	2777	A	OP1-P-OP2	-5.88	110.78	119.60
33	a	845	A	OP1-P-OP2	-5.88	110.78	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	707	A	OP1-P-O3'	5.88	118.13	105.20
10	A	950	A	OP1-P-OP2	-5.88	110.79	119.60
10	A	645	A	OP1-P-OP2	-5.87	110.79	119.60
10	A	1485	A	OP1-P-OP2	-5.87	110.80	119.60
33	a	398	C	N1-C1'-C2'	5.86	121.62	114.00
10	A	420	A	OP1-P-OP2	-5.86	110.81	119.60
10	A	544	G	OP1-P-O3'	5.86	118.09	105.20
10	A	2386	A	OP1-P-OP2	-5.86	110.81	119.60
33	a	455	U	OP1-P-O3'	5.86	118.09	105.20
33	a	1348	C	O4'-C1'-N1	5.85	112.88	108.20
10	A	1472	A	OP1-P-OP2	-5.85	110.83	119.60
33	a	423	A	OP1-P-OP2	-5.85	110.83	119.60
33	a	477	A	OP1-P-OP2	-5.84	110.84	119.60
10	A	2865	U	OP1-P-O3'	5.84	118.05	105.20
33	a	339	A	OP1-P-OP2	-5.84	110.84	119.60
33	a	840	A	OP1-P-OP2	-5.83	110.85	119.60
33	a	1534	A	OP1-P-OP2	-5.83	110.85	119.60
10	A	530	A	OP1-P-OP2	-5.83	110.86	119.60
10	A	107	G	OP1-P-O3'	5.83	118.02	105.20
10	A	457	C	OP1-P-O3'	5.82	118.00	105.20
10	A	2202	G	OP1-P-O3'	5.82	118.00	105.20
33	a	364	A	OP1-P-OP2	-5.81	110.88	119.60
33	a	794	A	OP1-P-OP2	-5.81	110.88	119.60
10	A	1834	A	OP1-P-OP2	-5.81	110.89	119.60
10	A	2501	A	OP1-P-OP2	-5.81	110.89	119.60
10	A	1966	A	OP1-P-OP2	-5.80	110.90	119.60
10	A	1822	A	OP1-P-OP2	-5.80	110.91	119.60
33	a	863	A	OP1-P-OP2	-5.80	110.91	119.60
10	A	1781	A	OP1-P-OP2	-5.79	110.92	119.60
33	a	508	A	OP1-P-OP2	-5.78	110.93	119.60
10	A	1420	A	OP1-P-OP2	-5.78	110.93	119.60
10	A	2046	A	OP1-P-OP2	-5.76	110.96	119.60
10	A	89	U	OP1-P-O3'	5.76	117.87	105.20
10	A	193	A	OP1-P-OP2	-5.76	110.96	119.60
10	A	743	G	OP1-P-O3'	5.76	117.87	105.20
10	A	2515	G	OP1-P-O3'	5.76	117.87	105.20
33	a	399	A	OP1-P-OP2	-5.76	110.97	119.60
33	a	1177	A	OP1-P-OP2	-5.75	110.97	119.60
33	a	668	A	OP1-P-OP2	-5.75	110.98	119.60
10	A	257	A	OP1-P-OP2	-5.74	110.99	119.60
10	A	1032	A	OP1-P-OP2	-5.74	110.99	119.60
10	A	1413	A	OP1-P-OP2	-5.73	111.00	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2646	A	OP1-P-OP2	-5.73	111.00	119.60
33	a	1510	A	OP1-P-OP2	-5.73	111.01	119.60
11	B	24	U	OP1-P-O3'	5.72	117.79	105.20
10	A	2095	A	OP1-P-OP2	-5.72	111.02	119.60
33	a	205	U	OP1-P-O3'	5.72	117.78	105.20
10	A	348	A	OP1-P-OP2	-5.72	111.03	119.60
10	A	272	A	OP1-P-OP2	-5.71	111.03	119.60
33	a	155	A	OP1-P-OP2	-5.71	111.03	119.60
10	A	654	G	OP1-P-O3'	5.71	117.76	105.20
10	A	1289	A	OP1-P-O3'	5.71	117.76	105.20
10	A	1195	A	OP1-P-OP2	-5.71	111.03	119.60
10	A	1782	A	OP1-P-OP2	-5.70	111.05	119.60
10	A	2795	G	OP1-P-O3'	5.70	117.75	105.20
33	a	673	G	OP1-P-O3'	5.70	117.75	105.20
33	a	1005	A	OP1-P-OP2	-5.70	111.05	119.60
10	A	1060	A	OP1-P-OP2	-5.70	111.06	119.60
10	A	1034	C	OP1-P-O3'	5.69	117.72	105.20
10	A	542	U	OP1-P-O3'	5.68	117.70	105.20
10	A	569	A	OP1-P-OP2	-5.67	111.10	119.60
10	A	2584	C	OP1-P-O3'	5.67	117.66	105.20
33	a	28	A	OP1-P-OP2	-5.66	111.10	119.60
10	A	1798	A	OP1-P-OP2	-5.66	111.11	119.60
10	A	1691	G	OP1-P-O3'	5.66	117.64	105.20
10	A	2009	C	OP1-P-O3'	5.66	117.64	105.20
10	A	390	C	OP2-P-O3'	5.65	117.63	105.20
10	A	1304	A	OP1-P-OP2	-5.64	111.13	119.60
11	B	56	A	OP1-P-OP2	-5.64	111.13	119.60
10	A	2706	A	OP1-P-OP2	-5.64	111.14	119.60
33	a	1400	A	OP1-P-O3'	5.64	117.60	105.20
10	A	41	A	OP1-P-OP2	-5.63	111.16	119.60
10	A	181	U	OP2-P-O3'	5.62	117.58	105.20
33	a	681	A	OP1-P-OP2	-5.62	111.17	119.60
10	A	1125	A	OP1-P-OP2	-5.62	111.17	119.60
10	A	2654	A	OP1-P-OP2	-5.62	111.17	119.60
10	A	1314	A	OP1-P-OP2	-5.62	111.17	119.60
10	A	1949	A	OP1-P-O3'	5.62	117.56	105.20
10	A	188	A	OP1-P-OP2	-5.62	111.17	119.60
10	A	1319	A	OP1-P-OP2	-5.62	111.18	119.60
10	A	2644	G	OP1-P-O3'	5.62	117.55	105.20
10	A	2829	A	OP1-P-OP2	-5.62	111.18	119.60
10	A	769	A	OP1-P-OP2	-5.61	111.19	119.60
10	A	1649	U	OP1-P-O3'	5.60	117.53	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	589	A	O4'-C1'-N9	5.60	112.68	108.20
10	A	2761	A	OP1-P-O3'	5.60	117.52	105.20
10	A	715	A	OP1-P-O3'	5.60	117.52	105.20
10	A	440	A	OP1-P-OP2	-5.59	111.21	119.60
10	A	367	A	OP1-P-OP2	-5.59	111.22	119.60
10	A	1061	G	C4-N9-C1'	-5.58	119.24	126.50
33	a	730	A	OP1-P-OP2	-5.58	111.23	119.60
10	A	1050	A	OP1-P-OP2	-5.58	111.23	119.60
33	a	879	A	OP1-P-OP2	-5.58	111.23	119.60
10	A	2101	A	OP1-P-OP2	-5.57	111.24	119.60
10	A	482	A	OP1-P-OP2	-5.57	111.24	119.60
10	A	1753	A	OP1-P-OP2	-5.56	111.25	119.60
10	A	1866	A	OP1-P-O3'	5.56	117.44	105.20
10	A	651	A	OP1-P-OP2	-5.55	111.28	119.60
33	a	354	C	OP1-P-O3'	5.55	117.40	105.20
33	a	195	C	OP1-P-O3'	5.54	117.39	105.20
10	A	2090	A	OP1-P-OP2	-5.53	111.30	119.60
10	A	714	A	OP1-P-OP2	-5.53	111.31	119.60
10	A	156	C	OP1-P-O3'	5.53	117.36	105.20
33	a	916	A	OP1-P-OP2	-5.53	111.31	119.60
10	A	1339	A	OP1-P-OP2	-5.52	111.31	119.60
10	A	201	A	OP1-P-OP2	-5.52	111.32	119.60
33	a	963	C	OP1-P-O3'	5.51	117.33	105.20
33	a	1129	A	O5'-P-OP2	5.51	117.31	110.70
33	a	1274	A	OP1-P-OP2	-5.51	111.34	119.60
33	a	945	A	OP1-P-OP2	-5.50	111.34	119.60
33	a	1540	A	OP1-P-OP2	-5.50	111.35	119.60
10	A	226	G	OP1-P-O3'	5.50	117.29	105.20
33	a	1548	G	OP1-P-OP2	-5.49	111.37	119.60
10	A	1248	G	OP1-P-O3'	5.48	117.26	105.20
10	A	2118	C	OP2-P-O3'	5.48	117.26	105.20
10	A	2579	A	OP1-P-OP2	-5.48	111.39	119.60
10	A	1786	A	OP1-P-OP2	-5.47	111.39	119.60
10	A	518	A	OP1-P-O3'	5.45	117.18	105.20
10	A	2015	G	OP1-P-O3'	5.45	117.18	105.20
10	A	21	A	OP1-P-OP2	-5.44	111.43	119.60
33	a	1357	G	OP1-P-O3'	5.43	117.15	105.20
10	A	1761	C	OP1-P-O3'	5.43	117.14	105.20
10	A	4	U	OP1-P-O3'	5.42	117.13	105.20
33	a	34	A	OP1-P-OP2	-5.42	111.46	119.60
10	A	175	U	OP1-P-O3'	5.42	117.13	105.20
10	A	1020	A	OP1-P-OP2	-5.42	111.47	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1740	A	OP1-P-OP2	-5.42	111.47	119.60
10	A	246	A	OP1-P-OP2	-5.41	111.49	119.60
33	a	491	U	OP2-P-O3'	5.40	117.09	105.20
33	a	896	A	OP1-P-OP2	-5.40	111.49	119.60
10	A	2237	G	OP1-P-O3'	5.40	117.08	105.20
10	A	251	C	OP1-P-O3'	5.39	117.06	105.20
10	A	1474	U	OP1-P-O3'	5.39	117.06	105.20
33	a	1424	A	OP1-P-OP2	-5.39	111.51	119.60
33	a	1223	A	OP1-P-OP2	-5.39	111.52	119.60
33	a	257	G	OP1-P-O3'	5.38	117.04	105.20
10	A	2352	G	OP1-P-O3'	5.37	117.02	105.20
10	A	2405	A	OP1-P-OP2	-5.37	111.55	119.60
33	a	137	C	OP1-P-O3'	5.37	117.01	105.20
10	A	1494	A	O4'-C1'-N9	5.36	112.49	108.20
10	A	881	G	OP1-P-O3'	5.36	116.99	105.20
10	A	966	C	OP1-P-O3'	5.36	116.99	105.20
10	A	1906	C	OP1-P-O3'	5.36	116.99	105.20
33	a	1386	A	OP1-P-OP2	-5.36	111.56	119.60
10	A	939	G	OP1-P-O3'	5.36	116.98	105.20
33	a	1494	U	OP1-P-O3'	5.35	116.98	105.20
33	a	1177	A	O4'-C1'-N9	5.35	112.48	108.20
33	a	1375	A	OP1-P-O3'	5.35	116.97	105.20
10	A	2815	A	OP1-P-O3'	5.34	116.95	105.20
12	D	38	A	OP1-P-O3'	5.34	116.94	105.20
10	A	2861	A	OP1-P-OP2	-5.34	111.59	119.60
10	A	234	G	OP1-P-O3'	5.33	116.93	105.20
11	B	75	U	OP1-P-O3'	5.33	116.93	105.20
10	A	1828	A	OP1-P-OP2	-5.33	111.61	119.60
10	A	61	A	OP1-P-OP2	-5.32	111.61	119.60
10	A	1730	U	OP1-P-O3'	5.32	116.91	105.20
10	A	2510	A	OP1-P-OP2	-5.32	111.62	119.60
33	a	1263	C	OP1-P-O3'	5.32	116.90	105.20
10	A	892	G	OP1-P-O3'	5.31	116.89	105.20
10	A	822	A	OP1-P-OP2	-5.31	111.63	119.60
10	A	1092	U	OP1-P-O3'	5.31	116.89	105.20
33	a	528	C	OP2-P-O3'	5.31	116.89	105.20
10	A	1312	A	OP1-P-OP2	-5.31	111.64	119.60
10	A	671	A	OP1-P-OP2	-5.30	111.64	119.60
10	A	1167	A	OP1-P-O3'	5.30	116.86	105.20
33	a	737	G	OP1-P-O3'	5.30	116.86	105.20
10	A	567	A	OP1-P-OP2	-5.30	111.65	119.60
33	a	1345	A	OP1-P-OP2	-5.30	111.66	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	180	C	OP2-P-O3'	5.29	116.83	105.20
10	A	1488	C	OP1-P-O3'	5.28	116.83	105.20
10	A	1588	G	OP1-P-O3'	5.28	116.82	105.20
10	A	273	A	OP1-P-O3'	5.28	116.81	105.20
10	A	1677	A	OP1-P-OP2	-5.27	111.69	119.60
10	A	697	A	OP1-P-OP2	-5.27	111.69	119.60
33	a	353	A	O4'-C1'-N9	5.27	112.41	108.20
33	a	1331	G	OP1-P-O3'	5.27	116.78	105.20
10	A	129	C	OP1-P-O3'	5.26	116.77	105.20
10	A	1226	A	OP1-P-OP2	-5.26	111.71	119.60
33	a	17	G	OP1-P-O3'	5.26	116.77	105.20
10	A	1534	U	OP1-P-O3'	5.25	116.76	105.20
10	A	300	U	OP1-P-O3'	5.24	116.72	105.20
10	A	2724	A	OP1-P-OP2	-5.24	111.74	119.60
10	A	732	A	OP1-P-OP2	-5.22	111.77	119.60
10	A	1321	A	OP1-P-OP2	-5.22	111.77	119.60
33	a	1195	A	OP1-P-O3'	5.22	116.68	105.20
10	A	486	A	P-O3'-C3'	5.21	125.96	119.70
10	A	2886	A	OP1-P-O3'	5.21	116.67	105.20
10	A	996	A	OP1-P-OP2	-5.20	111.79	119.60
33	a	564	U	OP1-P-O3'	5.20	116.64	105.20
10	A	2589	G	OP1-P-O3'	5.19	116.62	105.20
10	A	206	A	OP1-P-OP2	-5.19	111.81	119.60
10	A	403	G	OP2-P-O3'	5.19	116.62	105.20
33	a	168	A	OP2-P-O3'	5.19	116.62	105.20
10	A	12	U	OP1-P-O3'	5.19	116.62	105.20
33	a	1038	U	OP1-P-O3'	5.19	116.61	105.20
10	A	541	A	O4'-C1'-N9	5.18	112.35	108.20
33	a	731	U	OP1-P-O3'	5.18	116.61	105.20
10	A	1949	A	O4'-C1'-N9	5.18	112.34	108.20
10	A	1051	U	OP1-P-O3'	5.18	116.59	105.20
10	A	2144	A	OP1-P-OP2	-5.18	111.84	119.60
10	A	2032	U	OP1-P-O3'	5.17	116.58	105.20
33	a	1345	A	O4'-C1'-N9	5.17	112.34	108.20
10	A	1687	G	OP1-P-O3'	5.17	116.58	105.20
11	B	96	G	OP1-P-O3'	5.15	116.54	105.20
10	A	1249	A	OP1-P-O3'	5.15	116.54	105.20
10	A	161	A	OP1-P-OP2	-5.15	111.88	119.60
10	A	715	A	OP1-P-OP2	-5.15	111.87	119.60
10	A	1061	G	P-O3'-C3'	5.15	125.88	119.70
10	A	521	C	OP1-P-O3'	5.15	116.53	105.20
10	A	477	U	OP1-P-O3'	5.14	116.52	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1799	A	C1'-O4'-C4'	-5.14	105.79	109.90
33	a	687	G	OP1-P-O3'	5.14	116.50	105.20
33	a	892	A	OP1-P-OP2	-5.13	111.90	119.60
10	A	2463	A	OP1-P-OP2	-5.13	111.91	119.60
10	A	1195	A	P-O5'-C5'	5.12	129.10	120.90
10	A	346	A	OP1-P-OP2	-5.12	111.92	119.60
11	B	54	U	N1-C1'-C2'	5.12	120.65	114.00
10	A	1644	U	O4'-C1'-N1	5.11	112.29	108.20
10	A	709	A	OP1-P-OP2	-5.10	111.95	119.60
10	A	1186	U	OP1-P-O3'	5.10	116.42	105.20
10	A	55	G	OP1-P-O3'	5.09	116.40	105.20
10	A	2892	A	OP1-P-O3'	5.09	116.39	105.20
10	A	2574	A	OP1-P-OP2	-5.08	111.98	119.60
10	A	1040	A	OP1-P-OP2	-5.07	111.99	119.60
33	a	300	A	O4'-C1'-N9	5.07	112.25	108.20
33	a	886	C	OP1-P-O3'	5.05	116.32	105.20
33	a	1201	G	OP1-P-O3'	5.05	116.31	105.20
10	A	2646	A	OP1-P-O3'	5.04	116.29	105.20
33	a	1372	A	O4'-C1'-N9	5.04	112.23	108.20
10	A	2125	A	OP1-P-O3'	5.03	116.27	105.20
10	A	1219	U	OP1-P-O3'	5.03	116.25	105.20
10	A	2442	G	OP1-P-O3'	5.02	116.25	105.20
10	A	2062	A	OP1-P-OP2	-5.02	112.07	119.60
33	a	479	C	OP1-P-O3'	5.02	116.25	105.20
33	a	471	G	OP1-P-O3'	5.01	116.23	105.20
10	A	227	A	OP1-P-O3'	5.01	116.23	105.20
10	A	1861	A	OP1-P-O3'	5.00	116.20	105.20
10	A	2046	A	O4'-C1'-N9	5.00	112.20	108.20
33	a	933	G	OP1-P-O3'	5.00	116.20	105.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	F	117	THR	Peptide

## 5.2 Too-close contacts

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	532/586 (91%)	521 (98%)	11 (2%)	0	100	100
2	1	57/62 (92%)	57 (100%)	0	0	100	100
3	2	55/59 (93%)	55 (100%)	0	0	100	100
4	3	78/89 (88%)	75 (96%)	3 (4%)	0	100	100
5	4	51/59 (86%)	49 (96%)	2 (4%)	0	100	100
6	5	46/49 (94%)	46 (100%)	0	0	100	100
7	6	42/44 (96%)	42 (100%)	0	0	100	100
8	7	62/66 (94%)	61 (98%)	1 (2%)	0	100	100
9	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	F	224/229 (98%)	214 (96%)	10 (4%)	0	100	100
14	G	272/275 (99%)	266 (98%)	6 (2%)	0	100	100
15	H	204/209 (98%)	197 (97%)	7 (3%)	0	100	100
16	I	203/207 (98%)	200 (98%)	3 (2%)	0	100	100
17	J	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
18	K	172/178 (97%)	161 (94%)	11 (6%)	0	100	100
19	M	145/147 (99%)	145 (100%)	0	0	100	100
20	N	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
21	O	144/146 (99%)	139 (96%)	4 (3%)	1 (1%)	22	32
22	P	132/144 (92%)	131 (99%)	1 (1%)	0	100	100
23	Q	123/127 (97%)	118 (96%)	5 (4%)	0	100	100
24	R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
25	S	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
26	T	116/119 (98%)	116 (100%)	0	0	100	100
27	U	99/102 (97%)	98 (99%)	1 (1%)	0	100	100
28	V	109/115 (95%)	109 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	W	89/96 (93%)	88 (99%)	1 (1%)	0	100	100
30	X	99/103 (96%)	93 (94%)	6 (6%)	0	100	100
31	Y	72/95 (76%)	67 (93%)	5 (7%)	0	100	100
32	Z	59/62 (95%)	59 (100%)	0	0	100	100
35	c	220/261 (84%)	213 (97%)	7 (3%)	0	100	100
36	d	203/218 (93%)	198 (98%)	5 (2%)	0	100	100
37	e	198/203 (98%)	194 (98%)	4 (2%)	0	100	100
38	f	161/166 (97%)	159 (99%)	2 (1%)	0	100	100
39	g	94/100 (94%)	92 (98%)	2 (2%)	0	100	100
40	h	151/156 (97%)	149 (99%)	2 (1%)	0	100	100
41	i	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
42	j	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
43	k	94/102 (92%)	92 (98%)	2 (2%)	0	100	100
44	l	112/129 (87%)	109 (97%)	3 (3%)	0	100	100
45	m	132/137 (96%)	124 (94%)	8 (6%)	0	100	100
46	n	112/121 (93%)	110 (98%)	2 (2%)	0	100	100
47	o	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
48	p	83/89 (93%)	81 (98%)	2 (2%)	0	100	100
49	q	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
50	r	78/88 (89%)	75 (96%)	3 (4%)	0	100	100
51	s	61/79 (77%)	58 (95%)	3 (5%)	0	100	100
52	t	80/92 (87%)	78 (98%)	2 (2%)	0	100	100
53	u	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
All	All	5999/6378 (94%)	5840 (97%)	158 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	O	29	LYS

### 5.3.2 Protein sidechains ⓘ

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



entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	489/533 (92%)	483 (99%)	6 (1%)	71	85
2	1	54/56 (96%)	53 (98%)	1 (2%)	57	75
3	2	48/50 (96%)	48 (100%)	0	100	100
4	3	72/79 (91%)	72 (100%)	0	100	100
5	4	43/48 (90%)	43 (100%)	0	100	100
6	5	48/49 (98%)	47 (98%)	1 (2%)	53	72
7	6	39/39 (100%)	39 (100%)	0	100	100
8	7	51/53 (96%)	50 (98%)	1 (2%)	55	74
9	8	35/35 (100%)	34 (97%)	1 (3%)	42	62
13	F	181/183 (99%)	179 (99%)	2 (1%)	73	87
14	G	224/225 (100%)	224 (100%)	0	100	100
15	H	169/172 (98%)	167 (99%)	2 (1%)	71	85
16	I	172/173 (99%)	171 (99%)	1 (1%)	86	94
17	J	154/156 (99%)	153 (99%)	1 (1%)	86	94
18	K	145/148 (98%)	141 (97%)	4 (3%)	43	63
19	M	124/124 (100%)	122 (98%)	2 (2%)	62	79
20	N	98/98 (100%)	98 (100%)	0	100	100
21	O	112/112 (100%)	110 (98%)	2 (2%)	59	76
22	P	107/114 (94%)	107 (100%)	0	100	100
23	Q	107/109 (98%)	105 (98%)	2 (2%)	57	75
24	R	92/92 (100%)	92 (100%)	0	100	100
25	S	97/98 (99%)	97 (100%)	0	100	100
26	T	94/95 (99%)	93 (99%)	1 (1%)	73	87
27	U	83/83 (100%)	83 (100%)	0	100	100
28	V	94/98 (96%)	90 (96%)	4 (4%)	29	46
29	W	82/85 (96%)	80 (98%)	2 (2%)	49	68
30	X	85/87 (98%)	85 (100%)	0	100	100
31	Y	59/75 (79%)	58 (98%)	1 (2%)	60	78
32	Z	54/55 (98%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	c	187/220 (85%)	182 (97%)	5 (3%)	44	65
36	d	163/174 (94%)	163 (100%)	0	100	100
37	e	174/177 (98%)	166 (95%)	8 (5%)	27	43
38	f	126/128 (98%)	125 (99%)	1 (1%)	81	91
39	g	85/88 (97%)	85 (100%)	0	100	100
40	h	130/133 (98%)	127 (98%)	3 (2%)	50	70
41	i	112/113 (99%)	110 (98%)	2 (2%)	59	76
42	j	100/102 (98%)	97 (97%)	3 (3%)	41	61
43	k	87/92 (95%)	87 (100%)	0	100	100
44	l	89/100 (89%)	89 (100%)	0	100	100
45	m	117/119 (98%)	113 (97%)	4 (3%)	37	56
46	n	98/102 (96%)	95 (97%)	3 (3%)	40	60
47	o	51/52 (98%)	51 (100%)	0	100	100
48	p	76/79 (96%)	74 (97%)	2 (3%)	46	66
49	q	77/81 (95%)	77 (100%)	0	100	100
50	r	74/81 (91%)	72 (97%)	2 (3%)	44	65
51	s	54/67 (81%)	54 (100%)	0	100	100
52	t	70/79 (89%)	69 (99%)	1 (1%)	67	82
53	u	62/64 (97%)	62 (100%)	0	100	100
All	All	5144/5375 (96%)	5076 (99%)	68 (1%)	70	84

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	13	GLU
1	0	88	ARG
1	0	152	PHE
1	0	245	TYR
1	0	346	TYR
1	0	414	ASN
2	1	19	LYS
6	5	32	LYS
8	7	31	HIS
9	8	4	ARG
13	F	6	LYS

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Mol	Chain	Res	Type
13	F	205	LYS
15	H	125	ARG
15	H	191	ASN
16	I	13	GLN
17	J	143	TYR
18	K	69	ARG
18	K	81	GLU
18	K	102	LYS
18	K	119	GLU
19	M	14	ARG
19	M	118	LYS
21	O	1	MET
21	O	73	ASP
23	Q	24	LEU
23	Q	74	ARG
26	T	51	ARG
28	V	26	ILE
28	V	27	ASP
28	V	91	ARG
28	V	114	GLU
29	W	37	LEU
29	W	56	LEU
31	Y	80	ARG
35	c	23	TRP
35	c	129	LEU
35	c	208	ARG
35	c	221	PHE
35	c	223	GLU
37	e	13	ARG
37	e	14	ARG
37	e	24	LYS
37	e	54	LYS
37	e	60	MET
37	e	83	HIS
37	e	95	LEU
37	e	151	THR
38	f	163	GLU
40	h	60	GLU
40	h	143	LYS
40	h	149	ARG
41	i	25	LEU
41	i	77	LEU

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Mol	Chain	Res	Type
42	j	34	ASP
42	j	46	GLU
42	j	115	LYS
45	m	67	ARG
45	m	94	LEU
45	m	103	LEU
45	m	133	LYS
46	n	72	GLU
46	n	75	LEU
46	n	107	ARG
48	p	10	GLU
48	p	17	ARG
50	r	5	ARG
50	r	79	LEU
52	t	37	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2898/2910 (99%)	460 (15%)	91 (3%)
11	B	113/116 (97%)	24 (21%)	3 (2%)
12	D	75/77 (97%)	15 (20%)	1 (1%)
33	a	1516/1558 (97%)	229 (15%)	0
34	b	11/19 (57%)	2 (18%)	0
All	All	4613/4680 (98%)	730 (15%)	95 (2%)

All (730) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	10	A
10	A	14	A
10	A	34	U
10	A	36	G
10	A	46	C
10	A	49	A
10	A	55	G
10	A	62	C
10	A	64	A

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Mol	Chain	Res	Type
10	A	71	A
10	A	75	G
10	A	90	A
10	A	91	A
10	A	92	G
10	A	93	U
10	A	101	G
10	A	109	G
10	A	117	A
10	A	118	A
10	A	119	U
10	A	161	A
10	A	164	A
10	A	169	G
10	A	179	G
10	A	182	A
10	A	183	G
10	A	198	A
10	A	206	A
10	A	207	G
10	A	215	A
10	A	218	A
10	A	223	A
10	A	224	A
10	A	230	A
10	A	231	U
10	A	232	U
10	A	247	G
10	A	250	G
10	A	251	C
10	A	252	G
10	A	257	A
10	A	269	C
10	A	270	C
10	A	271	C
10	A	282	G
10	A	289	U
10	A	290	G
10	A	298	U
10	A	300	U
10	A	301	A
10	A	308	C

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Mol	Chain	Res	Type
10	A	309	G
10	A	310	A
10	A	311	U
10	A	318	G
10	A	320	C
10	A	321	U
10	A	322	G
10	A	347	A
10	A	352	C
10	A	353	G
10	A	355	U
10	A	366	A
10	A	398	A
10	A	399	G
10	A	403	G
10	A	404	A
10	A	410	A
10	A	411	G
10	A	425	G
10	A	430	A
10	A	440	A
10	A	442	U
10	A	450	G
10	A	451	A
10	A	459	G
10	A	479	G
10	A	487	U
10	A	490	U
10	A	494	C
10	A	495	C
10	A	496	A
10	A	497	G
10	A	509	A
10	A	519	A
10	A	520	G
10	A	529	A
10	A	542	U
10	A	543	A
10	A	546	U
10	A	556	G
10	A	560	G
10	A	568	C

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Mol	Chain	Res	Type
10	A	569	A
10	A	571	G
10	A	576	A
10	A	581	G
10	A	584	A
10	A	585	A
10	A	587	G
10	A	599	G
10	A	609	G
10	A	611	A
10	A	639	A
10	A	652	G
10	A	665	A
10	A	675	A
10	A	683	U
10	A	684	A
10	A	692	U
10	A	694	A
10	A	725	U
10	A	740	G
10	A	756	A
10	A	768	G
10	A	769	A
10	A	786	U
10	A	792	G
10	A	803	A
10	A	804	G
10	A	814	G
10	A	821	A
10	A	823	U
10	A	829	A
10	A	832	A
10	A	833	A
10	A	840	G
10	A	844	G
10	A	851	C
10	A	858	A
10	A	866	U
10	A	867	U
10	A	886	G
10	A	906	A
10	A	922	G

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Mol	Chain	Res	Type
10	A	926	A
10	A	928	C
10	A	929	U
10	A	930	C
10	A	931	G
10	A	933	G
10	A	935	U
10	A	936	A
10	A	950	A
10	A	952	C
10	A	957	A
10	A	965	U
10	A	966	C
10	A	972	U
10	A	974	U
10	A	984	A
10	A	985	G
10	A	997	U
10	A	1000	G
10	A	1013	A
10	A	1022	A
10	A	1035	A
10	A	1050	A
10	A	1051	U
10	A	1052	A
10	A	1056	G
10	A	1061	G
10	A	1062	U
10	A	1066	A
10	A	1072	U
10	A	1086	G
10	A	1101	G
10	A	1109	A
10	A	1110	G
10	A	1111	C
10	A	1115	C
10	A	1122	U
10	A	1123	A
10	A	1124	A
10	A	1126	G
10	A	1127	A
10	A	1128	G

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Mol	Chain	Res	Type
10	A	1150	A
10	A	1151	G
10	A	1166	A
10	A	1167	A
10	A	1168	A
10	A	1171	U
10	A	1172	A
10	A	1174	C
10	A	1175	G
10	A	1181	A
10	A	1182	A
10	A	1190	A
10	A	1196	G
10	A	1209	C
10	A	1212	U
10	A	1213	U
10	A	1232	G
10	A	1248	G
10	A	1274	G
10	A	1284	G
10	A	1289	A
10	A	1292	G
10	A	1301	A
10	A	1302	G
10	A	1307	G
10	A	1308	A
10	A	1309	A
10	A	1310	A
10	A	1311	G
10	A	1322	A
10	A	1335	U
10	A	1337	U
10	A	1340	C
10	A	1348	U
10	A	1373	G
10	A	1378	G
10	A	1380	C
10	A	1385	C
10	A	1387	U
10	A	1395	G
10	A	1400	A
10	A	1414	U

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Mol	Chain	Res	Type
10	A	1420	A
10	A	1421	C
10	A	1451	G
10	A	1454	U
10	A	1455	G
10	A	1460	A
10	A	1461	U
10	A	1468	A
10	A	1469	C
10	A	1474	U
10	A	1475	A
10	A	1480	A
10	A	1486	U
10	A	1487	G
10	A	1494	A
10	A	1495	U
10	A	1496	U
10	A	1497	G
10	A	1500	A
10	A	1501	G
10	A	1503	G
10	A	1510	C
10	A	1511	A
10	A	1517	U
10	A	1520	G
10	A	1524	U
10	A	1526	A
10	A	1530	G
10	A	1534	U
10	A	1535	A
10	A	1537	A
10	A	1538	U
10	A	1551	A
10	A	1564	G
10	A	1567	G
10	A	1569	G
10	A	1575	A
10	A	1583	G
10	A	1584	U
10	A	1585	A
10	A	1611	A
10	A	1613	G

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Mol	Chain	Res	Type
10	A	1614	A
10	A	1623	U
10	A	1627	G
10	A	1628	A
10	A	1629	G
10	A	1645	A
10	A	1649	U
10	A	1650	A
10	A	1651	A
10	A	1652	A
10	A	1653	C
10	A	1659	C
10	A	1689	G
10	A	1690	C
10	A	1705	U
10	A	1711	A
10	A	1716	G
10	A	1740	A
10	A	1741	G
10	A	1742	A
10	A	1756	U
10	A	1757	C
10	A	1758	G
10	A	1759	G
10	A	1769	G
10	A	1776	G
10	A	1777	G
10	A	1786	A
10	A	1795	C
10	A	1804	A
10	A	1813	C
10	A	1814	A
10	A	1828	A
10	A	1829	A
10	A	1833	U
10	A	1842	A
10	A	1855	G
10	A	1860	A
10	A	1861	A
10	A	1871	G
10	A	1872	A
10	A	1873	U

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Mol	Chain	Res	Type
10	A	1883	U
10	A	1884	C
10	A	1885	G
10	A	1919	G
10	A	1926	A
10	A	1927	C
10	A	1929	A
10	A	1932	A
10	A	1942	G
10	A	1943	G
10	A	1950	A
10	A	1951	A
10	A	1968	U
10	A	1976	C
10	A	1978	C
10	A	1980	C
10	A	1983	A
10	A	1984	A
10	A	1985	G
10	A	2004	U
10	A	2005	G
10	A	2006	U
10	A	2009	C
10	A	2010	A
10	A	2036	A
10	A	2044	A
10	A	2045	G
10	A	2046	A
10	A	2047	U
10	A	2056	C
10	A	2068	C
10	A	2069	G
10	A	2073	A
10	A	2074	G
10	A	2075	A
10	A	2076	C
10	A	2081	U
10	A	2082	G
10	A	2106	G
10	A	2108	G
10	A	2112	U
10	A	2120	C

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Mol	Chain	Res	Type
10	A	2121	A
10	A	2129	G
10	A	2130	A
10	A	2144	A
10	A	2145	U
10	A	2146	G
10	A	2160	A
10	A	2161	G
10	A	2171	A
10	A	2172	G
10	A	2191	C
10	A	2196	U
10	A	2201	U
10	A	2207	C
10	A	2211	A
10	A	2212	A
10	A	2216	G
10	A	2217	C
10	A	2224	A
10	A	2225	A
10	A	2226	U
10	A	2233	G
10	A	2239	C
10	A	2251	G
10	A	2252	G
10	A	2259	G
10	A	2264	OMG
10	A	2281	A
10	A	2292	G
10	A	2296	C
10	A	2300	A
10	A	2318	U
10	A	2319	U
10	A	2321	G
10	A	2324	A
10	A	2325	U
10	A	2333	A
10	A	2334	G
10	A	2335	A
10	A	2338	G
10	A	2346	A
10	A	2347	G

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Mol	Chain	Res	Type
10	A	2348	A
10	A	2360	C
10	A	2363	C
10	A	2392	G
10	A	2396	G
10	A	2398	C
10	A	2415	U
10	A	2419	C
10	A	2435	C
10	A	2437	C
10	A	2438	A
10	A	2439	A
10	A	2441	G
10	A	2442	G
10	A	2443	A
10	A	2448	A
10	A	2454	C
10	A	2458	2MG
10	A	2461	A
10	A	2462	U
10	A	2489	A
10	A	2515	G
10	A	2516	A
10	A	2517	U
10	A	2518	G
10	A	2531	A
10	A	2532	U
10	A	2533	C
10	A	2542	G
10	A	2548	G
10	A	2580	G
10	A	2586	C
10	A	2591	G
10	A	2598	U
10	A	2615	A
10	A	2622	U
10	A	2626	U
10	A	2628	U
10	A	2642	U
10	A	2674	G
10	A	2695	G
10	A	2702	U

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Mol	Chain	Res	Type
10	A	2704	C
10	A	2727	G
10	A	2739	U
10	A	2746	A
10	A	2749	G
10	A	2757	G
10	A	2770	A
10	A	2778	A
10	A	2779	G
10	A	2790	G
10	A	2791	A
10	A	2792	U
10	A	2793	G
10	A	2804	U
10	A	2809	U
10	A	2810	U
10	A	2811	A
10	A	2812	A
10	A	2818	U
10	A	2830	G
10	A	2843	A
10	A	2845	A
10	A	2846	U
10	A	2853	G
10	A	2859	G
10	A	2871	U
10	A	2877	G
10	A	2882	G
10	A	2890	C
10	A	2903	G
10	A	2909	A
11	B	7	G
11	B	10	G
11	B	11	A
11	B	13	A
11	B	23	A
11	B	35	C
11	B	39	G
11	B	43	A
11	B	49	G
11	B	50	A
11	B	55	A

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Mol	Chain	Res	Type
11	B	59	U
11	B	64	A
11	B	65	G
11	B	66	C
11	B	87	U
11	B	88	C
11	B	97	A
11	B	101	U
11	B	103	G
11	B	106	C
11	B	107	G
11	B	108	U
11	B	110	G
12	D	6	G
12	D	8	U
12	D	14	A
12	D	16	U
12	D	17	C
12	D	19	G
12	D	21	U
12	D	22	A
12	D	23	G
12	D	47	G
12	D	48	U
12	D	50	G
12	D	60	A
12	D	71	G
12	D	72	C
33	a	11	G
33	a	34	A
33	a	41	G
33	a	49	C
33	a	50	C
33	a	52	A
33	a	53	A
33	a	57	A
33	a	58	U
33	a	63	G
33	a	74	C
33	a	117	A
33	a	118	G
33	a	126	C

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Mol	Chain	Res	Type
33	a	132	A
33	a	135	A
33	a	136	A
33	a	137	C
33	a	146	A
33	a	154	C
33	a	159	G
33	a	163	G
33	a	168	A
33	a	172	C
33	a	177	A
33	a	180	C
33	a	181	A
33	a	182	G
33	a	191	A
33	a	198	A
33	a	199	A
33	a	200	C
33	a	213	A
33	a	215	G
33	a	230	G
33	a	267	G
33	a	270	U
33	a	271	U
33	a	272	A
33	a	273	G
33	a	276	A
33	a	277	G
33	a	292	G
33	a	293	C
33	a	301	G
33	a	315	G
33	a	332	A
33	a	342	C
33	a	354	C
33	a	355	A
33	a	356	C
33	a	358	G
33	a	370	A
33	a	373	G
33	a	378	C
33	a	380	G

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Mol	Chain	Res	Type
33	a	391	U
33	a	393	U
33	a	398	C
33	a	399	A
33	a	418	G
33	a	424	C
33	a	430	G
33	a	432	G
33	a	438	A
33	a	439	G
33	a	440	A
33	a	441	A
33	a	447	U
33	a	448	C
33	a	450	G
33	a	455	U
33	a	465	U
33	a	470	A
33	a	474	A
33	a	478	A
33	a	479	C
33	a	485	C
33	a	494	C
33	a	495	U
33	a	510	G
33	a	511	G
33	a	522	G
33	a	526	G
33	a	537	C
33	a	540	C
33	a	544	C
33	a	553	G
33	a	556	G
33	a	557	U
33	a	560	U
33	a	573	A
33	a	576	G
33	a	585	A
33	a	588	U
33	a	590	U
33	a	598	A
33	a	599	A

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Mol	Chain	Res	Type
33	a	602	C
33	a	603	G
33	a	605	G
33	a	622	A
33	a	640	C
33	a	644	C
33	a	658	G
33	a	659	U
33	a	665	G
33	a	668	A
33	a	679	U
33	a	687	G
33	a	691	A
33	a	713	A
33	a	721	A
33	a	729	G
33	a	730	A
33	a	736	G
33	a	749	U
33	a	750	G
33	a	757	G
33	a	781	G
33	a	787	G
33	a	803	A
33	a	819	U
33	a	820	A
33	a	841	A
33	a	842	A
33	a	843	C
33	a	846	U
33	a	862	G
33	a	866	G
33	a	873	C
33	a	882	G
33	a	899	A
33	a	901	G
33	a	916	A
33	a	917	G
33	a	941	A
33	a	953	G
33	a	954	G
33	a	961	C

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Mol	Chain	Res	Type
33	a	962	A
33	a	972	G
33	a	987	U
33	a	993	G
33	a	995	A
33	a	996	A
33	a	998	G
33	a	1002	A
33	a	1003	G
33	a	1004	A
33	a	1019	U
33	a	1020	G
33	a	1028	U
33	a	1030	G
33	a	1031	A
33	a	1033	C
33	a	1036	U
33	a	1045	A
33	a	1050	U
33	a	1051	U
33	a	1052	U
33	a	1055	C
33	a	1058	C
33	a	1059	G
33	a	1060	G
33	a	1063	A
33	a	1065	A
33	a	1073	A
33	a	1080	G
33	a	1081	C
33	a	1092	U
33	a	1095	G
33	a	1121	G
33	a	1122	U
33	a	1128	A
33	a	1129	A
33	a	1165	G
33	a	1166	U
33	a	1172	A
33	a	1178	G
33	a	1183	A
33	a	1184	C

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Mol	Chain	Res	Type
33	a	1185	U
33	a	1194	C
33	a	1210	G
33	a	1222	A
33	a	1223	A
33	a	1228	U
33	a	1250	U
33	a	1251	A
33	a	1253	A
33	a	1264	A
33	a	1266	U
33	a	1283	C
33	a	1286	U
33	a	1306	A
33	a	1307	U
33	a	1326	G
33	a	1328	U
33	a	1344	A
33	a	1346	C
33	a	1348	C
33	a	1349	G
33	a	1364	G
33	a	1373	G
33	a	1379	G
33	a	1389	A
33	a	1390	C
33	a	1420	A
33	a	1423	C
33	a	1424	A
33	a	1448	U
33	a	1468	A
33	a	1472	A
33	a	1478	U
33	a	1479	U
33	a	1480	U
33	a	1481	G
33	a	1517	U
33	a	1519	A
33	a	1521	G
33	a	1524	G
33	a	1530	A
33	a	1533	U

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Mol	Chain	Res	Type
33	a	1544	G
33	a	1556	G
33	a	1557	G
33	a	1558	A
33	a	1564	U
34	b	6	U
34	b	16	A

All (95) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	13	A
10	A	90	A
10	A	118	A
10	A	125	A
10	A	178	A
10	A	182	A
10	A	198	A
10	A	206	A
10	A	223	A
10	A	251	C
10	A	272	A
10	A	281	A
10	A	288	U
10	A	354	C
10	A	410	A
10	A	429	A
10	A	486	A
10	A	496	A
10	A	518	A
10	A	541	A
10	A	550	G
10	A	570	A
10	A	651	A
10	A	791	A
10	A	803	A
10	A	818	A
10	A	832	A
10	A	839	A
10	A	840	G
10	A	841	A
10	A	905	C

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Mol	Chain	Res	Type
10	A	992	A
10	A	996	A
10	A	1050	A
10	A	1057	U
10	A	1061	G
10	A	1108	A
10	A	1127	A
10	A	1183	A
10	A	1189	U
10	A	1195	A
10	A	1265	A
10	A	1273	A
10	A	1283	A
10	A	1301	A
10	A	1308	A
10	A	1321	A
10	A	1336	A
10	A	1347	U
10	A	1377	A
10	A	1389	A
10	A	1413	A
10	A	1420	A
10	A	1494	A
10	A	1536	A
10	A	1583	G
10	A	1612	A
10	A	1628	A
10	A	1644	U
10	A	1650	A
10	A	1652	A
10	A	1658	A
10	A	1710	A
10	A	1740	A
10	A	1828	A
10	A	1926	A
10	A	1949	A
10	A	2046	A
10	A	2080	A
10	A	2111	U
10	A	2171	A
10	A	2211	A
10	A	2216	G

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Mol	Chain	Res	Type
10	A	2225	A
10	A	2238	A
10	A	2318	U
10	A	2324	A
10	A	2359	A
10	A	2435	C
10	A	2438	A
10	A	2443	A
10	A	2516	A
10	A	2531	A
10	A	2579	A
10	A	2585	A
10	A	2627	A
10	A	2703	A
10	A	2738	A
10	A	2769	U
10	A	2789	A
10	A	2810	U
11	B	48	A
11	B	49	G
11	B	54	U
12	D	59	A

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

7 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	$\# Z  > 2$
10	OMC	A	1933	10	19,22,23	3.34	8 (42%)	26,31,34	0.77	0
44	IAS	l	119	44	6,7,8	1.08	0	6,8,10	1.42	1 (16%)
33	MA6	a	1546	33	19,26,27	1.05	2 (10%)	18,38,41	4.42	3 (16%)
10	OMG	A	2264	56,10	18,26,27	2.82	6 (33%)	19,38,41	1.47	4 (21%)
10	5MU	A	1952	56,10	19,22,23	7.49	8 (42%)	28,32,35	3.13	9 (32%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	2MG	A	2458	10	18,26,27	2.55	7 (38%)	16,38,41	1.43	4 (25%)
33	MA6	a	1545	33	19,26,27	1.06	2 (10%)	18,38,41	4.43	3 (16%)

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
10	OMC	A	1933	10	-	0/9/27/28	0/2/2/2
44	IAS	l	119	44	-	1/7/7/8	-
33	MA6	a	1546	33	-	3/7/29/30	0/3/3/3
10	OMG	A	2264	56,10	-	0/5/27/28	0/3/3/3
10	5MU	A	1952	56,10	-	0/7/25/26	0/2/2/2
10	2MG	A	2458	10	-	2/5/27/28	0/3/3/3
33	MA6	a	1545	33	-	0/7/29/30	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1952	5MU	C4-C5	21.35	1.80	1.44
10	A	1952	5MU	C6-N1	16.21	1.65	1.38
10	A	1952	5MU	C6-C5	-12.09	1.14	1.34
10	A	1952	5MU	C4-N3	-11.23	1.18	1.38
10	A	2264	OMG	C2-N2	7.13	1.51	1.34
10	A	1933	OMC	C2-N3	6.80	1.50	1.36
10	A	1933	OMC	C6-C5	6.42	1.50	1.35
10	A	1933	OMC	C4-N4	5.45	1.46	1.33
10	A	1952	5MU	O2-C2	-5.36	1.13	1.23
10	A	2458	2MG	C2-N2	5.26	1.45	1.33
10	A	1933	OMC	C4-N3	5.14	1.44	1.34
10	A	2264	OMG	C4-N3	5.05	1.49	1.37
10	A	1933	OMC	C2-N1	4.91	1.50	1.40
10	A	1952	5MU	C2-N3	4.89	1.46	1.38
10	A	2458	2MG	C2-N1	4.86	1.44	1.36
10	A	2264	OMG	C2-N3	4.62	1.44	1.33
10	A	2264	OMG	C6-N1	4.59	1.44	1.37
10	A	1933	OMC	O2-C2	-4.54	1.15	1.23
10	A	2458	2MG	C6-N1	4.20	1.44	1.37
10	A	2458	2MG	C4-N3	3.92	1.46	1.37
10	A	2458	2MG	C5-C6	3.42	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2458	2MG	C5-C4	-3.27	1.34	1.43
10	A	1933	OMC	C6-N1	3.24	1.45	1.38
10	A	2264	OMG	C2-N1	3.20	1.45	1.37
10	A	1952	5MU	C2-N1	3.12	1.43	1.38
10	A	2264	OMG	O6-C6	-2.92	1.17	1.23
10	A	1933	OMC	C5-C4	2.91	1.49	1.42
10	A	1952	5MU	C5M-C5	2.81	1.57	1.50
33	a	1546	MA6	C5-C4	-2.77	1.33	1.40
33	a	1545	MA6	C5-C4	-2.76	1.33	1.40
10	A	2458	2MG	O6-C6	-2.56	1.18	1.23
33	a	1545	MA6	C2-N3	2.27	1.35	1.32
33	a	1546	MA6	C2-N3	2.18	1.35	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1545	MA6	N1-C6-N6	-15.82	100.40	117.06
33	a	1546	MA6	N1-C6-N6	-15.78	100.44	117.06
10	A	1952	5MU	C5-C4-N3	9.16	123.13	115.31
33	a	1545	MA6	C1'-N9-C4	-8.20	112.23	126.64
33	a	1546	MA6	C1'-N9-C4	-7.95	112.67	126.64
10	A	1952	5MU	C5-C6-N1	-7.26	115.87	123.34
10	A	1952	5MU	C4-N3-C2	-6.42	119.04	127.35
33	a	1546	MA6	N3-C2-N1	-5.42	120.21	128.68
33	a	1545	MA6	N3-C2-N1	-5.29	120.41	128.68
10	A	1952	5MU	N3-C2-N1	4.74	121.19	114.89
10	A	1952	5MU	C5M-C5-C6	-4.40	116.97	122.85
10	A	1952	5MU	O4-C4-C5	-3.85	120.44	124.90
10	A	2458	2MG	C5-C6-N1	3.52	120.17	113.95
10	A	2264	OMG	C5-C6-N1	3.40	119.96	113.95
10	A	1952	5MU	C5M-C5-C4	3.30	122.39	118.77
10	A	2264	OMG	C2-N1-C6	-3.20	119.20	125.10
10	A	1952	5MU	C6-C5-C4	3.11	120.63	118.03
10	A	2458	2MG	C8-N7-C5	2.77	108.26	102.99
10	A	1952	5MU	O2-C2-N1	-2.62	119.30	122.79
10	A	2264	OMG	C8-N7-C5	2.45	107.65	102.99
10	A	2264	OMG	O6-C6-C5	-2.34	119.80	124.37
10	A	2458	2MG	CM2-N2-C2	-2.27	118.85	123.86
10	A	2458	2MG	O6-C6-C5	-2.21	120.05	124.37
44	l	119	IAS	OXT-C-CA	2.07	120.43	113.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2458	2MG	C3'-C4'-C5'-O5'
10	A	2458	2MG	O4'-C4'-C5'-O5'
33	a	1546	MA6	O4'-C4'-C5'-O5'
33	a	1546	MA6	C4'-C5'-O5'-P
44	l	119	IAS	CA-CB-CG-OD1
33	a	1546	MA6	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](#)

Of 359 ligands modelled in this entry, 353 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
58	PUT	A	3136	-	5,5,5	0.26	0	4,4,4	0.45	0
58	PUT	a	1670	-	5,5,5	0.23	0	4,4,4	0.47	0
59	SCM	a	1652	-	23,25,25	1.32	4 (17%)	26,39,39	1.39	4 (15%)
58	PUT	a	1669	-	5,5,5	0.24	0	4,4,4	0.51	0
54	ATP	0	602	55	26,33,33	3.41	10 (38%)	31,52,52	2.38	9 (29%)
54	ATP	0	601	55	26,33,33	3.43	10 (38%)	31,52,52	2.39	9 (29%)

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
58	PUT	A	3136	-	-	0/3/3/3	-
58	PUT	a	1670	-	-	0/3/3/3	-
59	SCM	a	1652	-	-	0/4/57/57	0/3/3/3
58	PUT	a	1669	-	-	0/3/3/3	-
54	ATP	0	602	55	-	6/18/38/38	0/3/3/3
54	ATP	0	601	55	-	9/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	0	601	ATP	C2'-C3'	-10.55	1.24	1.53
54	0	602	ATP	C2'-C3'	-10.44	1.24	1.53
54	0	601	ATP	O4'-C1'	6.96	1.50	1.41
54	0	602	ATP	O4'-C1'	6.90	1.50	1.41
54	0	602	ATP	O4'-C4'	-6.64	1.30	1.45
54	0	601	ATP	O4'-C4'	-6.48	1.30	1.45
54	0	601	ATP	C3'-C4'	5.61	1.67	1.53
54	0	602	ATP	C3'-C4'	5.45	1.66	1.53
54	0	602	ATP	C2'-C1'	4.51	1.60	1.53
54	0	601	ATP	C2'-C1'	4.48	1.60	1.53
54	0	601	ATP	O2'-C2'	3.28	1.50	1.43
54	0	602	ATP	O2'-C2'	3.26	1.50	1.43
54	0	601	ATP	C6-N6	3.24	1.45	1.34
54	0	602	ATP	C6-N6	3.24	1.45	1.34
54	0	602	ATP	C5-C4	-2.78	1.33	1.40
54	0	601	ATP	C5-C4	-2.74	1.33	1.40
59	a	1652	SCM	O1B-C7	-2.55	1.40	1.44
59	a	1652	SCM	C12-C7	2.49	1.57	1.52
59	a	1652	SCM	C10-N10	-2.39	1.43	1.47
59	a	1652	SCM	O2B-C12	-2.28	1.40	1.44
54	0	601	ATP	O3'-C3'	2.14	1.48	1.43
54	0	601	ATP	C2-N3	2.14	1.35	1.32
54	0	602	ATP	C2-N3	2.12	1.35	1.32
54	0	602	ATP	O3'-C3'	2.09	1.47	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	0	601	ATP	C5-C6-N6	6.69	130.51	120.35
54	0	602	ATP	C5-C6-N6	6.67	130.49	120.35
54	0	602	ATP	C1'-N9-C4	6.04	137.25	126.64
54	0	601	ATP	C1'-N9-C4	5.94	137.08	126.64
54	0	602	ATP	N3-C2-N1	-5.50	120.07	128.68

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	0	601	ATP	N3-C2-N1	-5.47	120.12	128.68
54	0	602	ATP	N6-C6-N1	-4.61	109.01	118.57
54	0	601	ATP	N6-C6-N1	-4.61	109.01	118.57
59	a	1652	SCM	C1M-N10-C10	-3.24	109.66	114.38
54	0	602	ATP	O4'-C1'-C2'	-3.04	102.48	106.93
54	0	601	ATP	C3'-C2'-C1'	2.87	105.30	100.98
54	0	601	ATP	C2'-C3'-C4'	2.69	107.87	102.64
54	0	602	ATP	C3'-C2'-C1'	2.67	105.00	100.98
54	0	601	ATP	PA-O3A-PB	-2.64	123.78	132.83
54	0	601	ATP	PB-O3B-PG	-2.50	124.24	132.83
54	0	602	ATP	C2'-C3'-C4'	2.47	107.44	102.64
54	0	602	ATP	PB-O3B-PG	-2.39	124.61	132.83
59	a	1652	SCM	C11-C12-C7	-2.34	106.32	111.66
59	a	1652	SCM	O2B-C6-O1	-2.30	104.22	107.01
54	0	601	ATP	O4'-C1'-C2'	-2.25	103.64	106.93
59	a	1652	SCM	O11-C11-C12	-2.18	104.17	109.94
54	0	602	ATP	PA-O3A-PB	-2.05	125.80	132.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

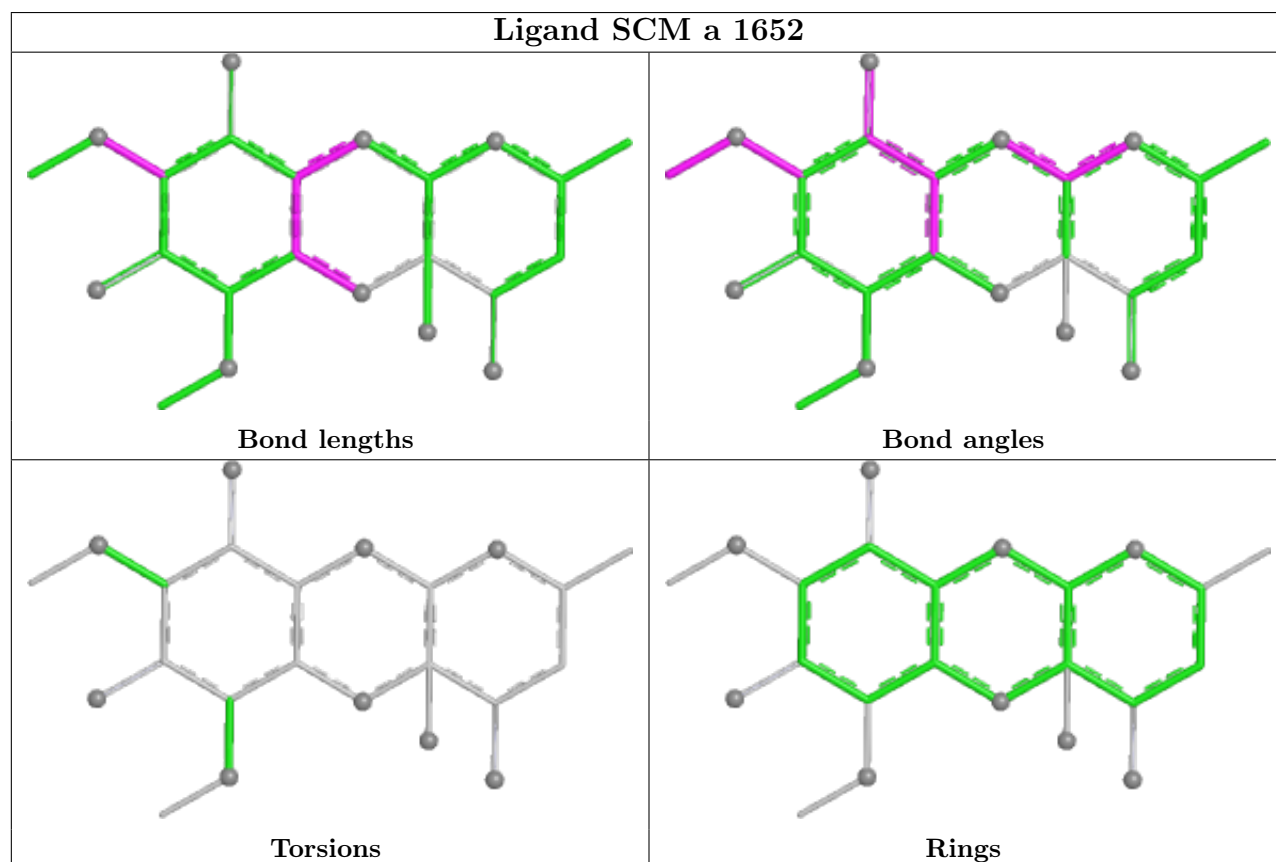
Mol	Chain	Res	Type	Atoms
54	0	601	ATP	PB-O3B-PG-O2G
54	0	601	ATP	C5'-O5'-PA-O1A
54	0	601	ATP	C5'-O5'-PA-O2A
54	0	601	ATP	C5'-O5'-PA-O3A
54	0	601	ATP	O4'-C4'-C5'-O5'
54	0	602	ATP	C5'-O5'-PA-O3A
54	0	601	ATP	C3'-C4'-C5'-O5'
54	0	602	ATP	O4'-C4'-C5'-O5'
54	0	602	ATP	C5'-O5'-PA-O1A
54	0	602	ATP	C5'-O5'-PA-O2A
54	0	601	ATP	PG-O3B-PB-O2B
54	0	602	ATP	PA-O3A-PB-O2B
54	0	602	ATP	C3'-C4'-C5'-O5'
54	0	601	ATP	PB-O3B-PG-O1G
54	0	601	ATP	PG-O3B-PB-O1B

There are no ring outliers.

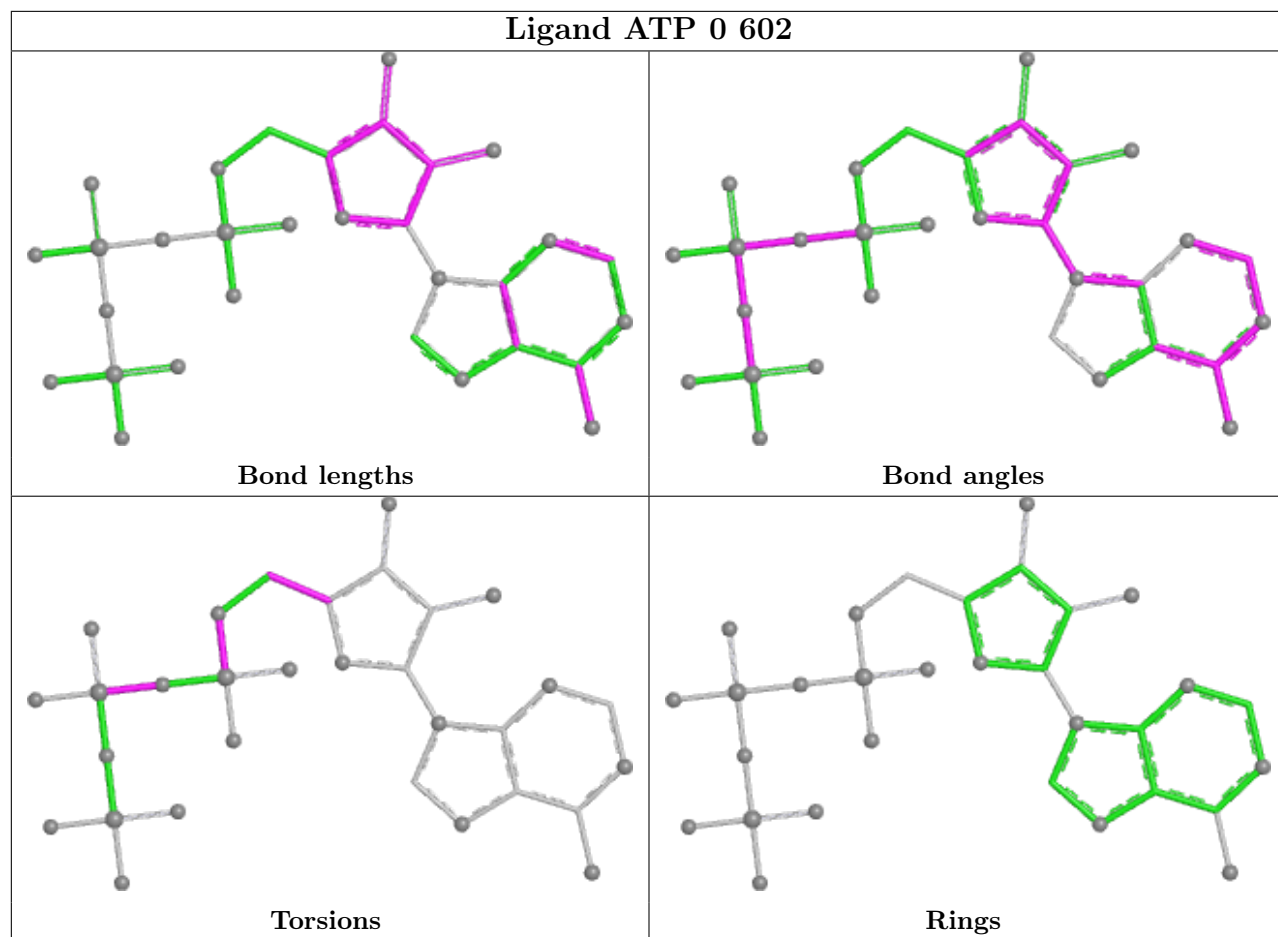
No monomer is involved in short contacts.

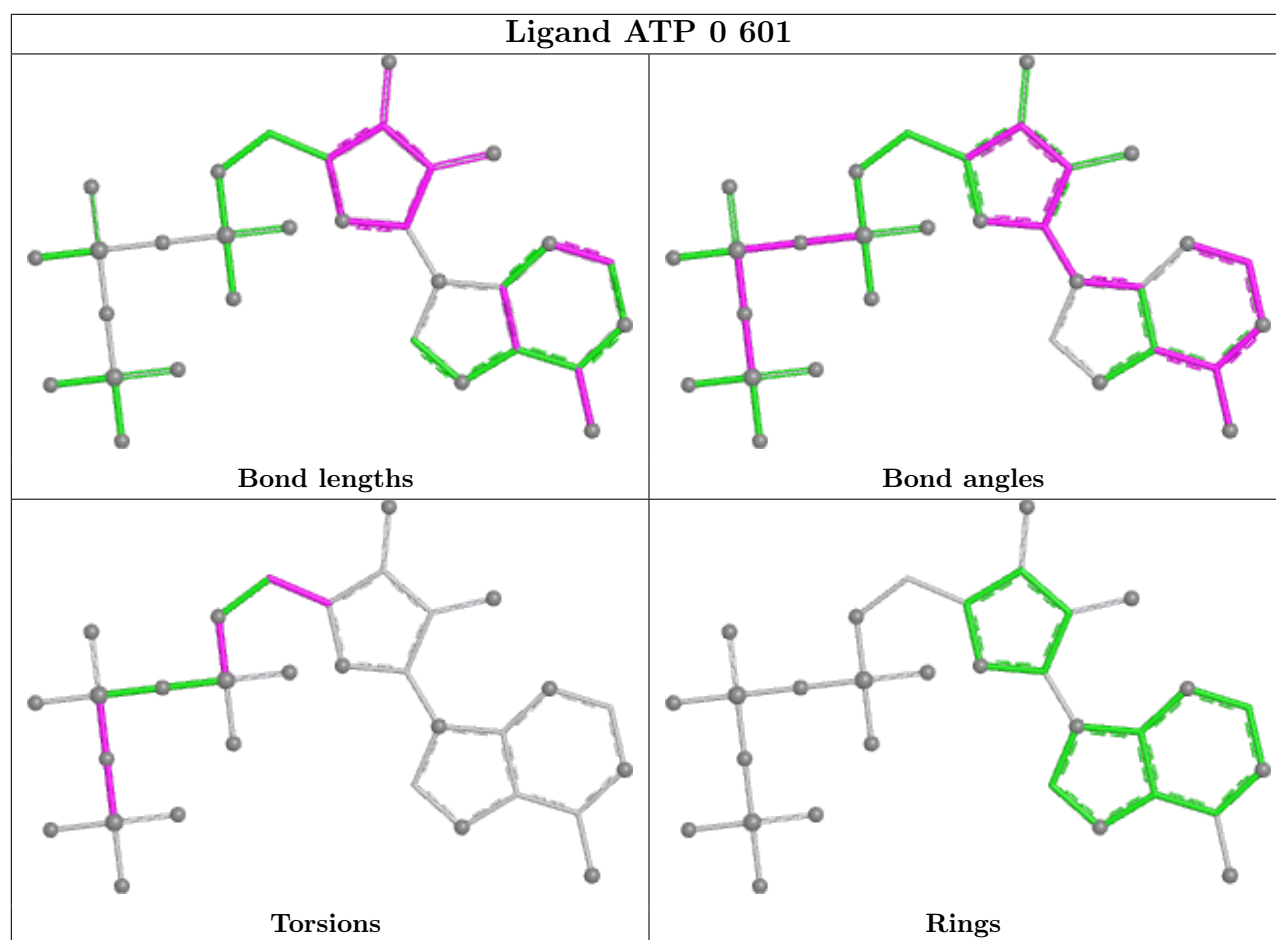
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.



## Ligand ATP 0 602





## 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.



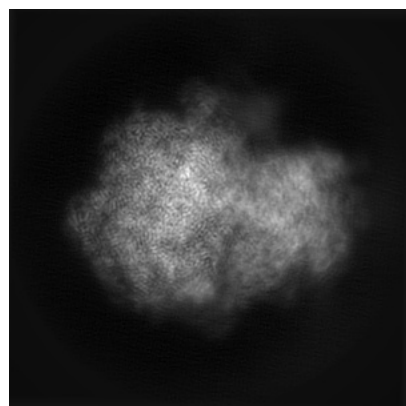
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13241. These allow visual inspection of the internal detail of the map and identification of artifacts.

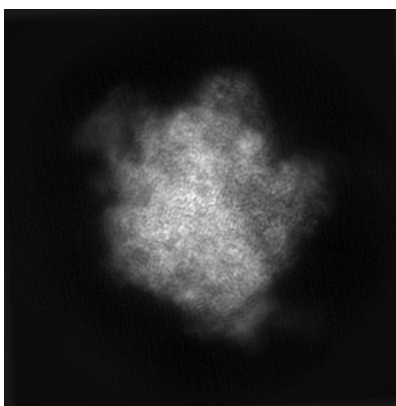
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

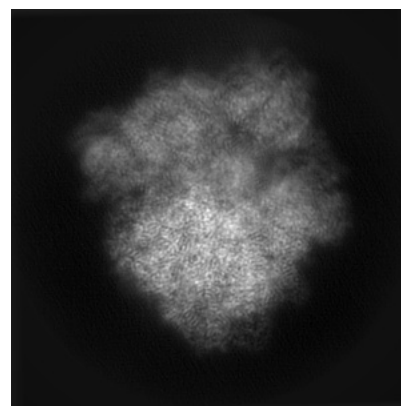
#### 6.1.1 Primary map



X

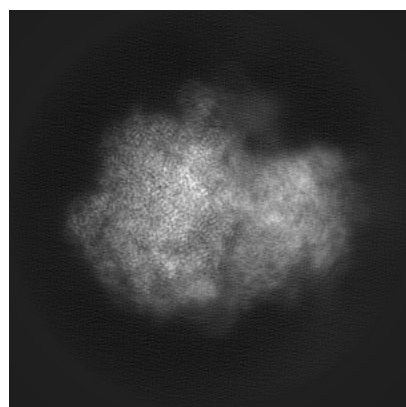


Y

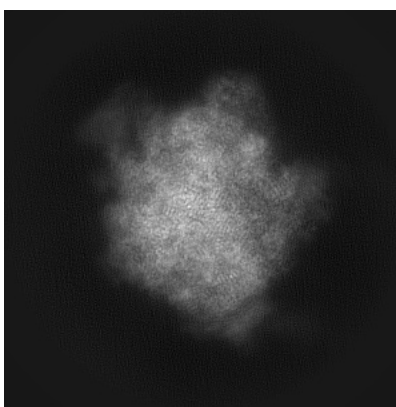


Z

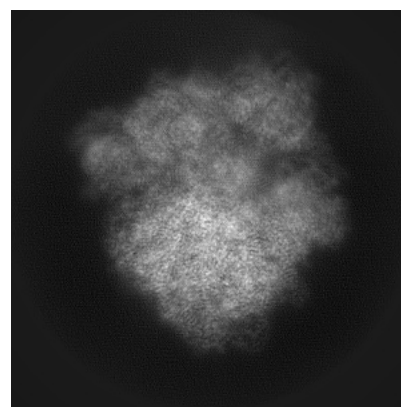
#### 6.1.2 Raw map



X



Y

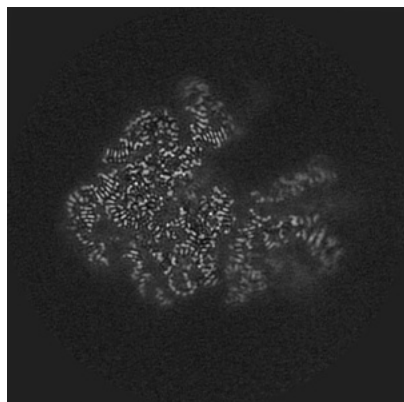


Z

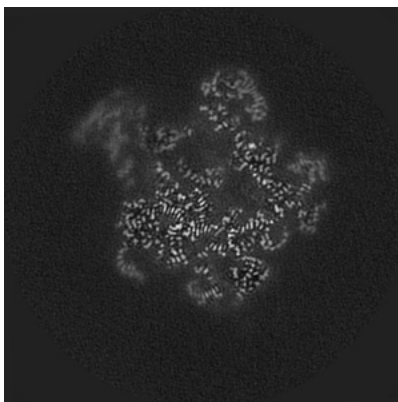
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

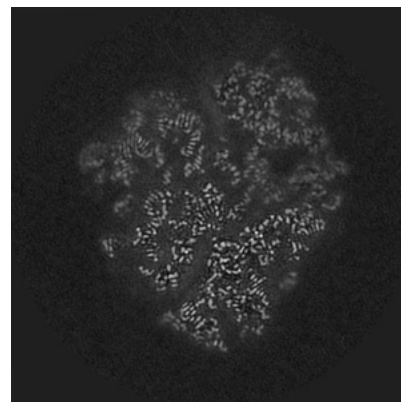
### 6.2.1 Primary map



X Index: 210

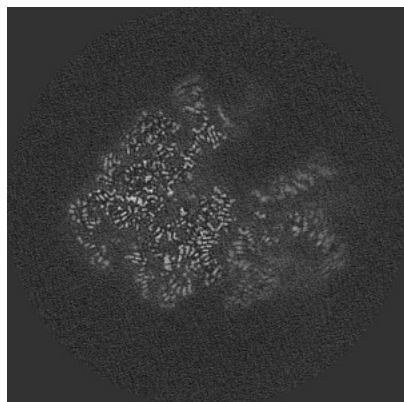


Y Index: 210

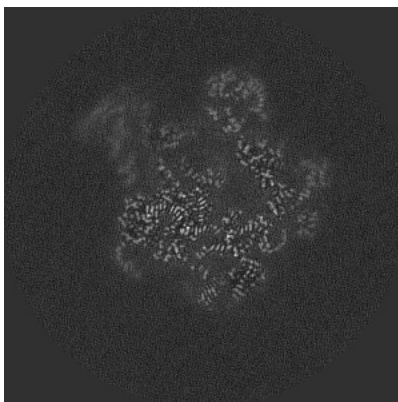


Z Index: 210

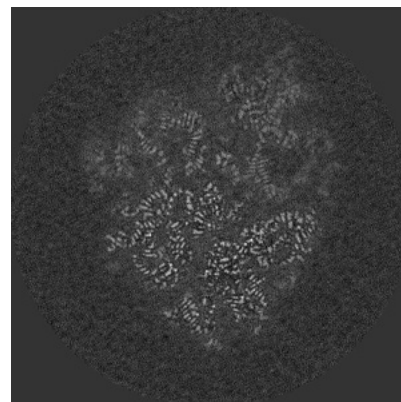
### 6.2.2 Raw map



X Index: 210



Y Index: 210

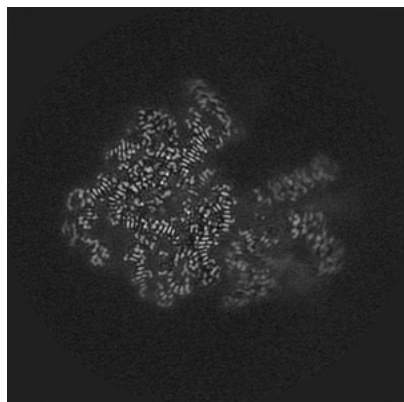


Z Index: 210

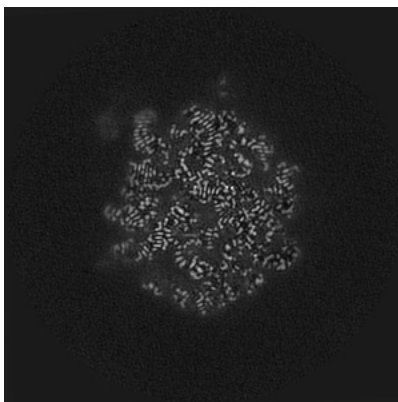
The images above show central slices of the map in three orthogonal directions.

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

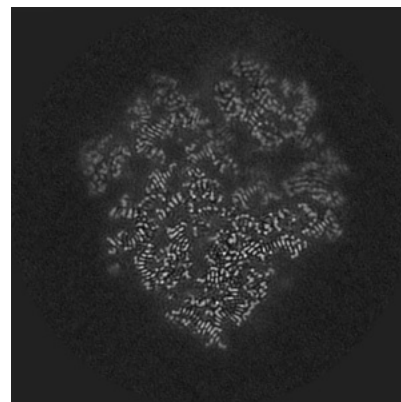
### 6.3.1 Primary map



X Index: 206

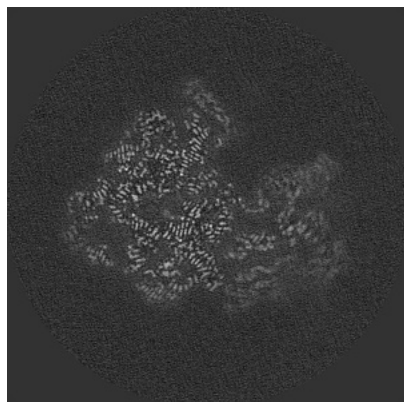


Y Index: 170

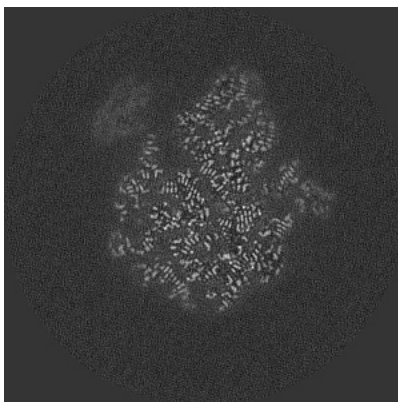


Z Index: 217

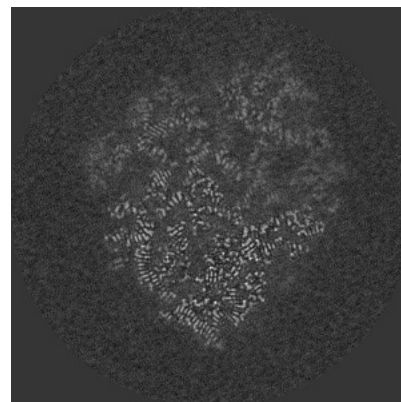
### 6.3.2 Raw map



X Index: 202



Y Index: 186

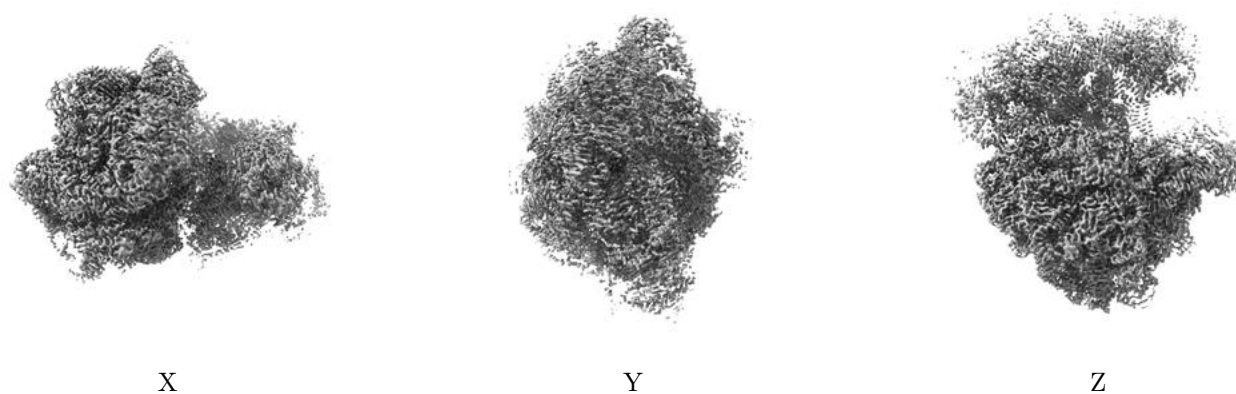


Z Index: 215

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

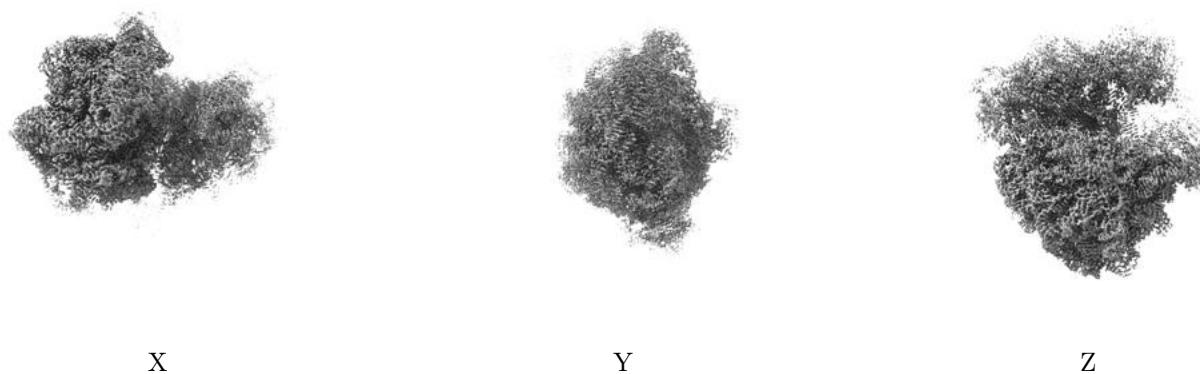
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

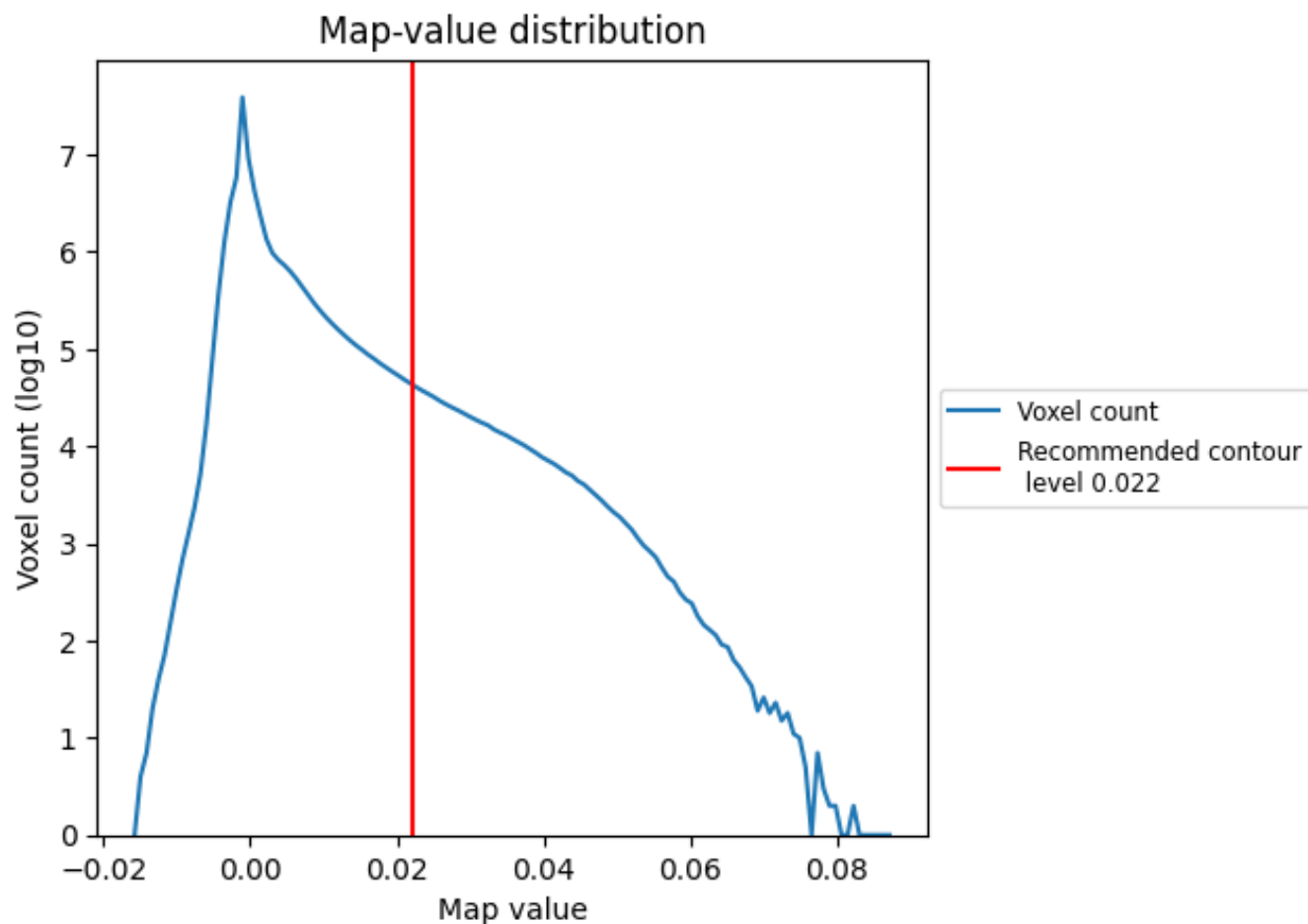
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

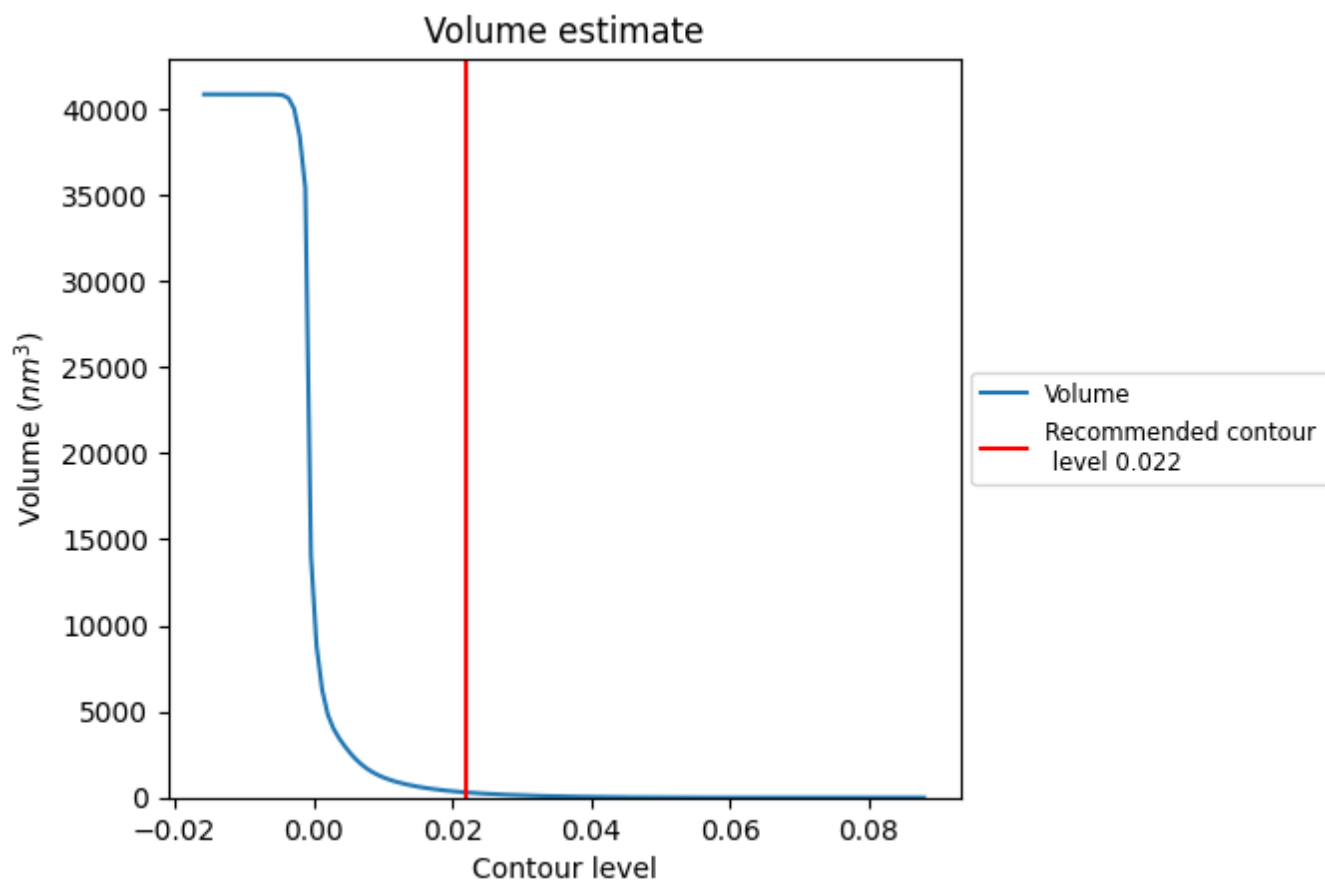
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

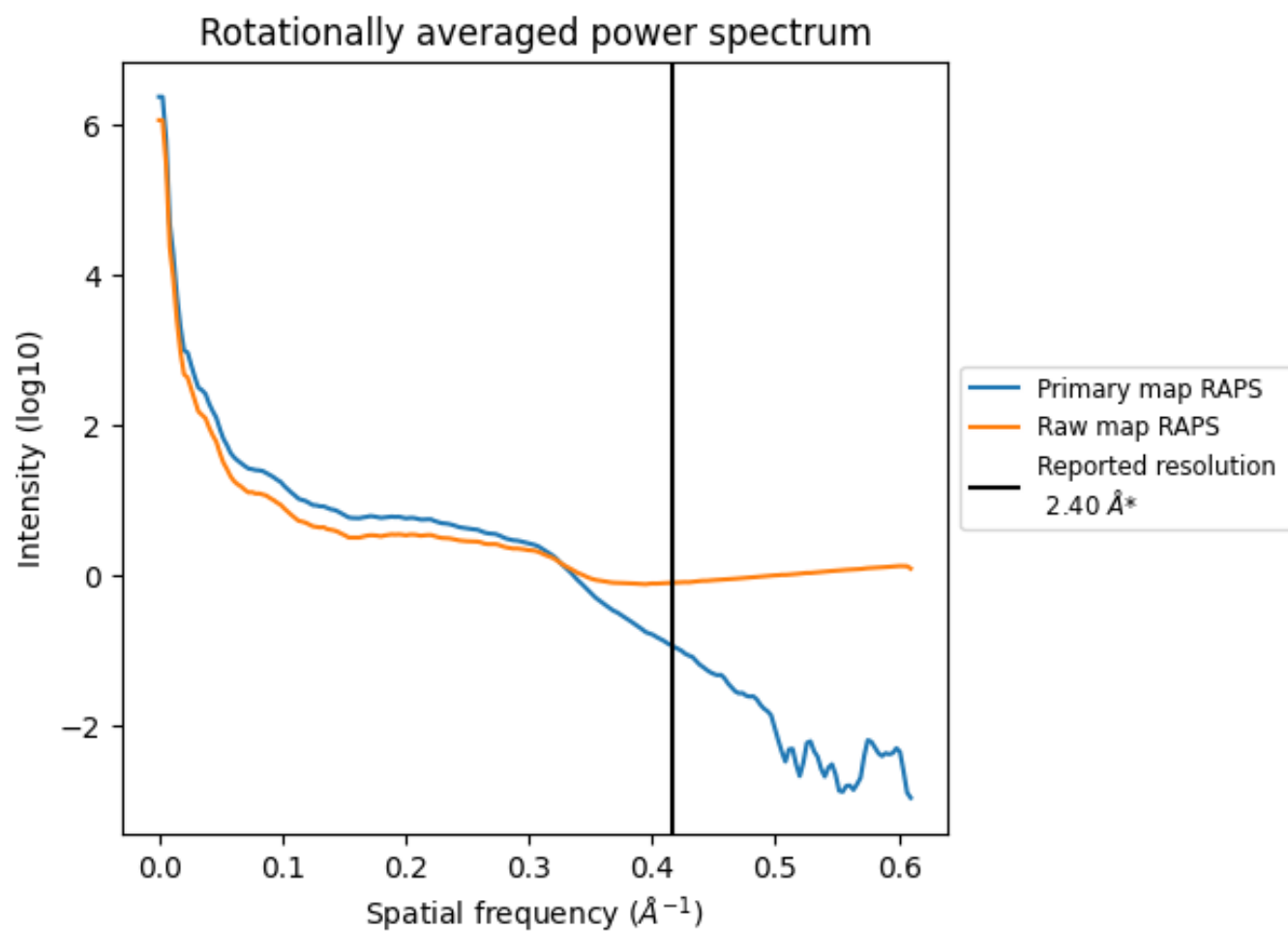


The volume at the recommended contour level is 299 nm<sup>3</sup>; this corresponds to an approximate mass of 270 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

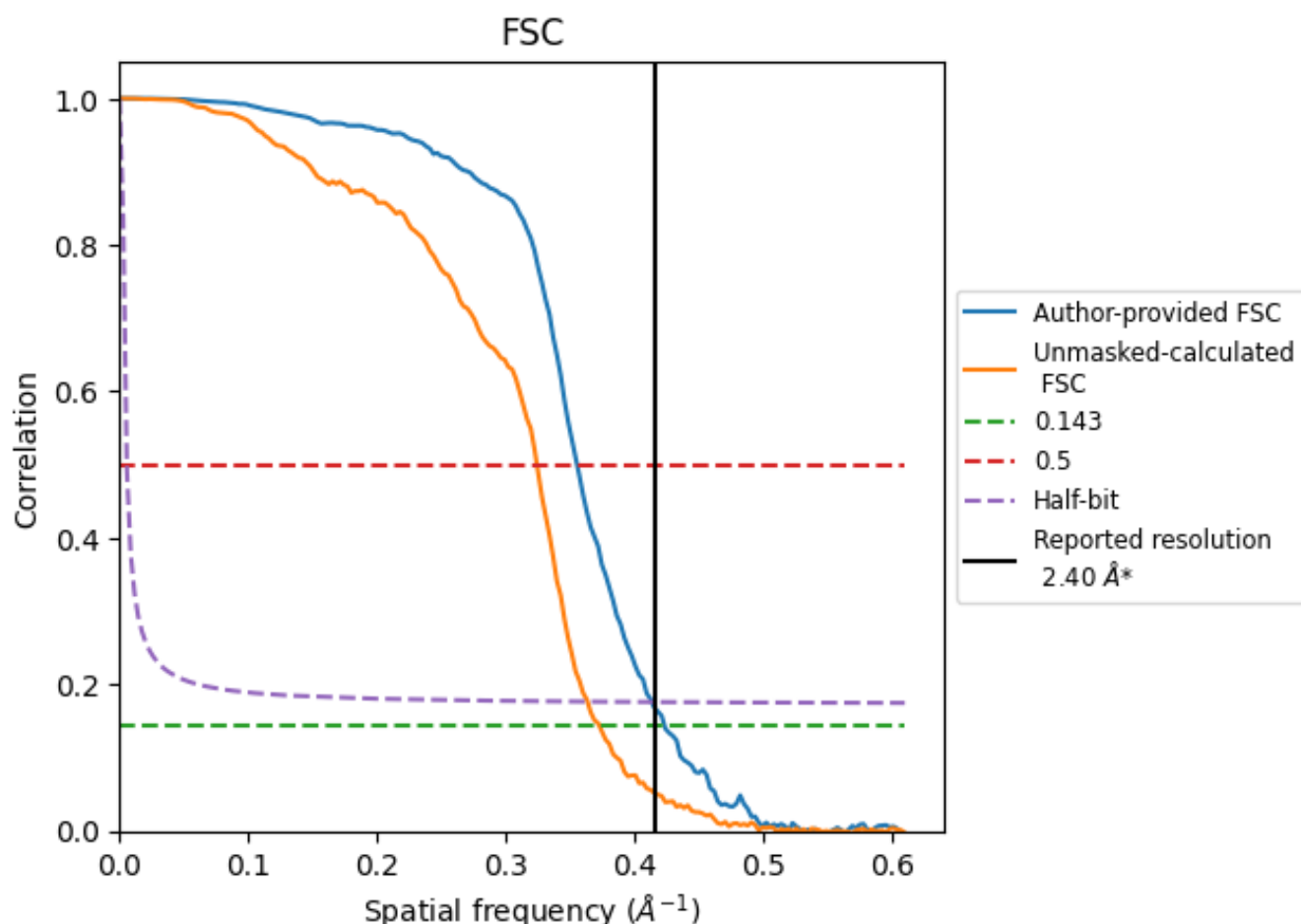


\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 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 0.417 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

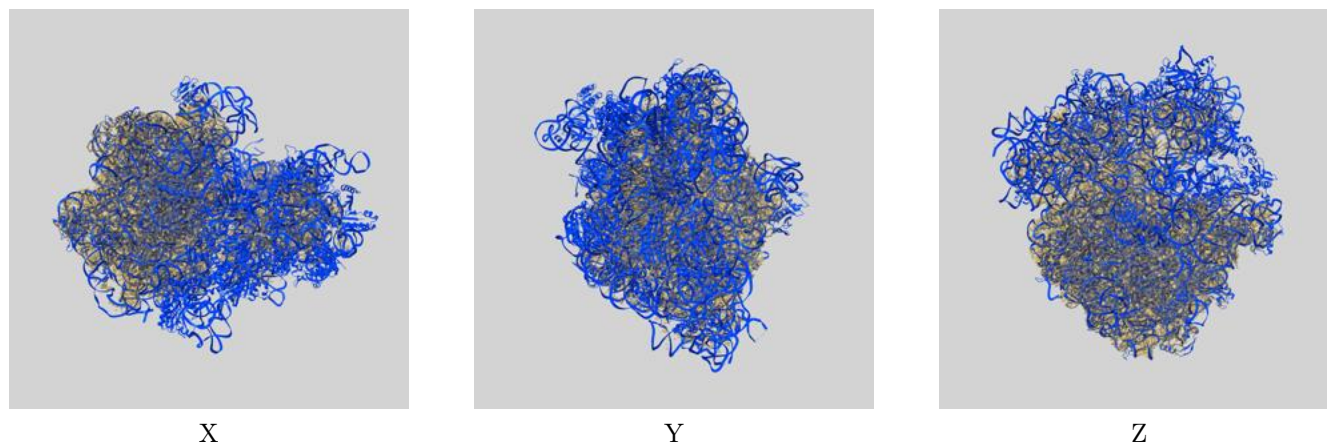
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.36	2.81	2.42
Unmasked-calculated*	2.68	3.08	2.75

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.68 differs from the reported value 2.4 by more than 10 %

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

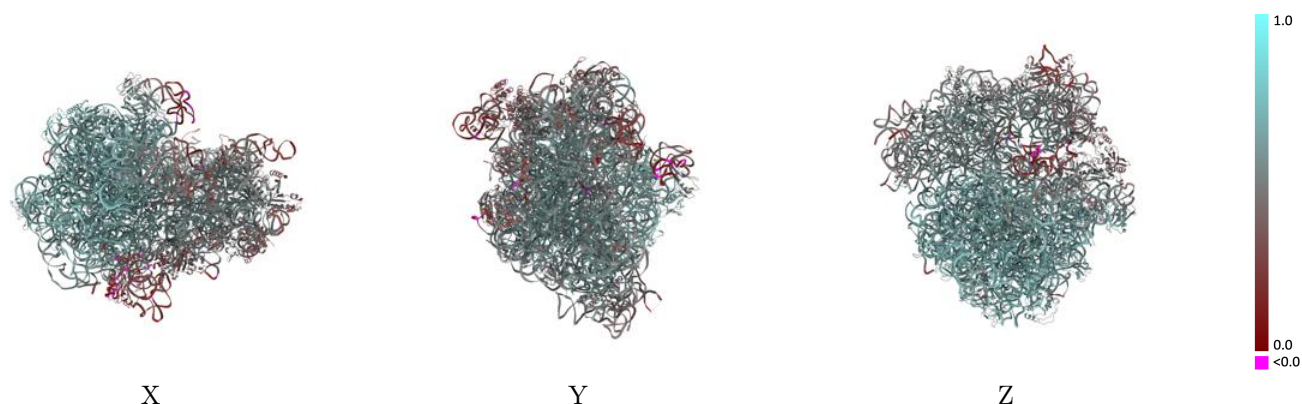
This section contains information regarding the fit between EMDB map EMD-13241 and PDB model 7P7Q. Per-residue inclusion information can be found in section [3](#) on page [19](#).

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



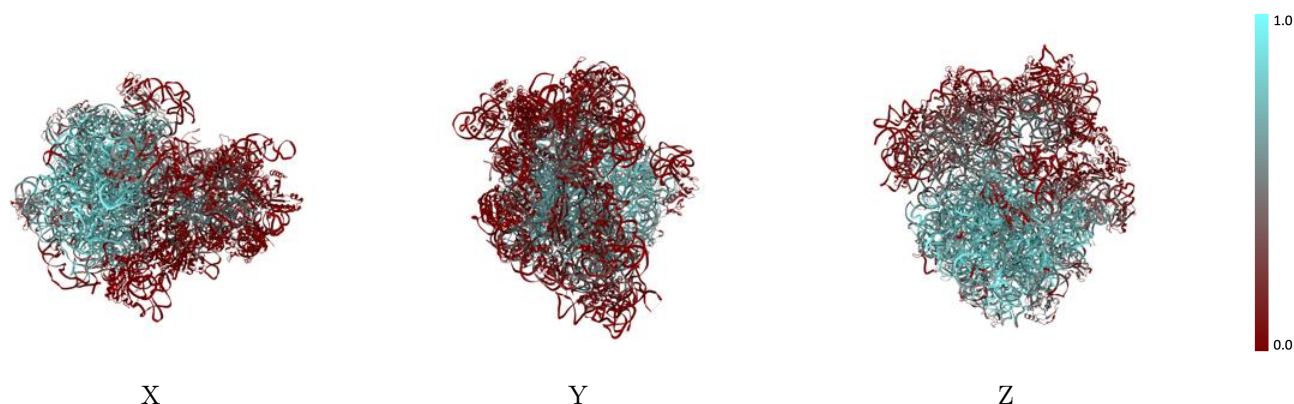
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



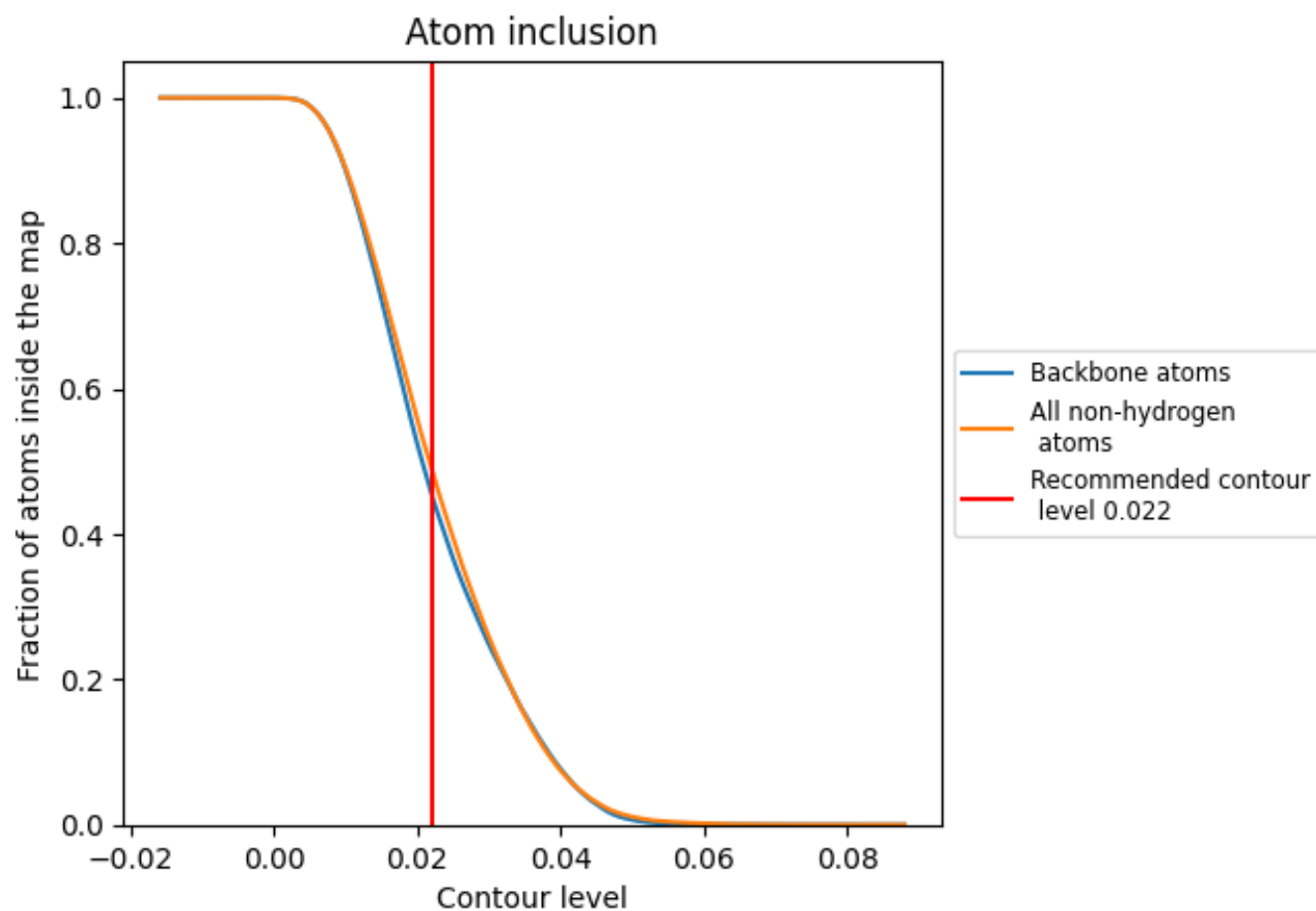
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ







































The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4899	 0.5720
0	 0.0384	 0.4770
1	 0.3674	 0.5990
2	 0.5261	 0.6230
3	 0.0016	 0.3570
4	 0.6910	 0.6710
5	 0.5899	 0.6370
6	 0.8063	 0.6860
7	 0.7680	 0.6850
8	 0.6318	 0.6420
A	 0.7448	 0.6240
B	 0.4032	 0.5520
D	 0.2851	 0.5650
F	 0.0000	 0.2680
G	 0.6829	 0.6630
H	 0.6587	 0.6590
I	 0.5731	 0.6460
J	 0.0293	 0.4530
K	 0.1205	 0.5360
M	 0.6111	 0.6540
N	 0.6002	 0.6460
O	 0.5621	 0.6420
P	 0.5979	 0.6420
Q	 0.6362	 0.6430
R	 0.2922	 0.5660
S	 0.5975	 0.6390
T	 0.7062	 0.6690
U	 0.5525	 0.6500
V	 0.6448	 0.6570
W	 0.5118	 0.6250
X	 0.2917	 0.5840
Y	 0.6808	 0.6650
Z	 0.4292	 0.6300
a	 0.3322	 0.5260
b	 0.1719	 0.2870



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Chain	Atom inclusion	Q-score
c	 0.0035	 0.4040
d	 0.0903	 0.4840
e	 0.0282	 0.4970
f	 0.0965	 0.5200
g	 0.0169	 0.4680
h	 0.0220	 0.4670
i	 0.0502	 0.5220
j	 0.0496	 0.4560
k	 0.0731	 0.4530
l	 0.0286	 0.4080
m	 0.1189	 0.5150
n	 0.0196	 0.4330
o	 0.1702	 0.5350
p	 0.1246	 0.5270
q	 0.0637	 0.5010
r	 0.0639	 0.5100
s	 0.0344	 0.4230
t	 0.0000	 0.3990
u	 0.1005	 0.4900