Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 07:26 am GMT

PDB ID	:	6HA8
EMDB ID	:	EMD-0177
Title	:	Cryo-EM structure of the ABCF protein VmlR bound to the Bacillus subtilis ribosome
Authors	:	Crowe-McAuliffe, C.; Graf, M.; Huter, P.; Abdelshahid, M.; Novacek, J.; Wilson, D.N.
Deposited on	:	2018-08-07
Resolution	:	3.50 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

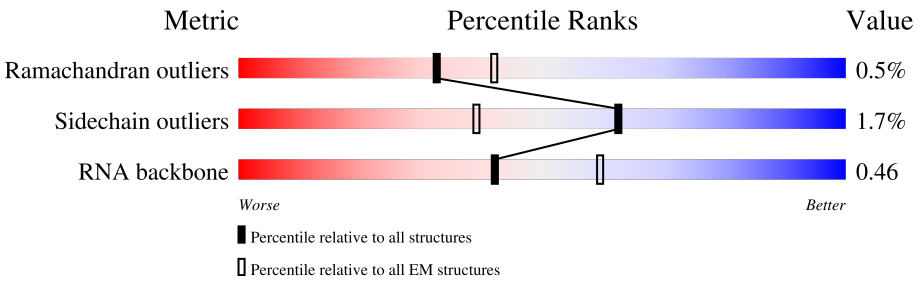
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.50 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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2928	7%, 61%, 31%, 6%
2	B	112	57%, 36%, 7%
3	C	277	5%, 97%
4	D	209	97%
5	E	207	6%, 96%
6	F	179	41%, 92%, 6%
7	G	179	46%, 98%
8	J	145	5%, 95%

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Mol	Chain	Length	Quality of chain
9	K	122	7% 99%
10	L	146	9% 97%
11	M	144	16% 93% 6%
12	N	120	8% 99%
13	O	120	22% 98%
14	P	115	10% 97%
15	Q	119	95%
16	R	102	5% 93%
17	S	113	5% 94%
18	T	95	14% 93% 5%
19	U	103	13% 97%
20	V	548	45% 95%
21	W	94	11% 84% 13%
22	X	62	21% 87% 6% 6%
23	Y	66	15% 98%
24	Z	59	12% 97%
25	0	59	5% 85% 8%
26	1	49	96%
27	2	44	98%
28	3	66	94%
29	4	37	14% 100%
30	6	66	67% 94% 5%
31	7	3	67% 33%
32	8	232	89% 91% 9%
33	a	1554	13% 66% 29%

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Mol	Chain	Length	Quality of chain
34	b	246	86% 82% 6% 11%
35	c	218	53% 94% 6%
36	d	200	77% 93%
37	e	166	31% 97%
38	f	95	71% 95%
39	g	156	39% 94%
40	h	132	55% 95%
41	i	130	45% 92%
42	j	102	61% 92% 7%
43	k	131	51% 85% 13%
44	l	138	57% 93%
45	m	121	60% 85% 11%
46	n	61	56% 93% 5%
47	o	89	60% 92%
48	p	90	64% 92% 6%
49	q	87	68% 92%
50	r	79	58% 76% 5% 19%
51	s	92	52% 84% 15%
52	t	88	52% 91% 6%
53	x	75	41% 56% 32% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	TEL	A	3001	X	-	-	-

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 146404 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2887	61997	27661	11460	19992	2884	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	112	2392	1068	435	778	111	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	272	2083	1296	408	373	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	206	1569	985	289	290	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	205	1561	980	289	290	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	176	1386	882	241	256	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	175	1342	835	248	257	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	142	1123	710	206	202	5	0	0

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	122	920	571	173	172	4	0	0

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	146	1081	671	207	201	2	0	0

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	135	1076	690	205	176	5	0	0

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	N	119	953	583	186	180	4	0	0

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	120	912	564	176	171	1	0	0

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	P	115	944	600	185	158	1	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Q	117	940	591	189	156	4	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	R	101	786	501	139	146	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	109	842	525	164	150	3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	90	725	452	134	136	3	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	101	762	478	142	138	4	0	0

- Molecule 20 is a protein called Nucleotide-binding protein ExpZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	541	4177	2637	737	796	7	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-5	MET	-	initiating methionine	UNP P39115
V	-4	HIS	-	expression tag	UNP P39115
V	-3	HIS	-	expression tag	UNP P39115
V	-2	HIS	-	expression tag	UNP P39115
V	-1	HIS	-	expression tag	UNP P39115
V	0	HIS	-	expression tag	UNP P39115
V	1	HIS	-	expression tag	UNP P39115
V	129	GLN	GLU	engineered mutation	UNP P39115
V	432	GLN	GLU	engineered mutation	UNP P39115
V	486	ALA	-	expression tag	UNP P39115
V	487	ALA	-	expression tag	UNP P39115
V	488	ALA	-	expression tag	UNP P39115
V	489	ALA	-	expression tag	UNP P39115
V	490	ALA	-	expression tag	UNP P39115
V	491	ALA	-	expression tag	UNP P39115
V	492	ALA	-	expression tag	UNP P39115
V	493	ALA	-	expression tag	UNP P39115
V	494	ALA	-	expression tag	UNP P39115
V	495	ALA	-	expression tag	UNP P39115
V	496	ALA	-	expression tag	UNP P39115
V	497	ALA	-	expression tag	UNP P39115
V	498	ALA	-	expression tag	UNP P39115
V	499	ALA	-	expression tag	UNP P39115
V	500	ALA	-	expression tag	UNP P39115
V	501	ALA	-	expression tag	UNP P39115
V	502	ALA	-	expression tag	UNP P39115
V	503	ALA	-	expression tag	UNP P39115
V	504	ALA	-	expression tag	UNP P39115
V	505	ALA	-	expression tag	UNP P39115
V	506	ALA	-	expression tag	UNP P39115
V	507	ALA	-	expression tag	UNP P39115
V	508	ALA	-	expression tag	UNP P39115
V	509	ALA	-	expression tag	UNP P39115
V	510	ALA	-	expression tag	UNP P39115
V	511	ALA	-	expression tag	UNP P39115
V	512	ALA	-	expression tag	UNP P39115
V	513	ALA	-	expression tag	UNP P39115
V	514	ALA	-	expression tag	UNP P39115
V	515	ALA	-	expression tag	UNP P39115
V	516	ALA	-	expression tag	UNP P39115
V	517	ALA	-	expression tag	UNP P39115
V	518	ALA	-	expression tag	UNP P39115
V	519	ALA	-	expression tag	UNP P39115

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Chain	Residue	Modelled	Actual	Comment	Reference
V	520	ALA	-	expression tag	UNP P39115
V	521	ALA	-	expression tag	UNP P39115
V	522	ALA	-	expression tag	UNP P39115
V	523	ALA	-	expression tag	UNP P39115
V	524	ALA	-	expression tag	UNP P39115
V	525	ALA	-	expression tag	UNP P39115
V	526	ALA	-	expression tag	UNP P39115
V	527	ALA	-	expression tag	UNP P39115
V	528	ALA	-	expression tag	UNP P39115
V	529	ALA	-	expression tag	UNP P39115
V	530	ALA	-	expression tag	UNP P39115
V	531	ALA	-	expression tag	UNP P39115
V	532	ALA	-	expression tag	UNP P39115
V	533	ALA	-	expression tag	UNP P39115
V	534	ALA	-	expression tag	UNP P39115
V	535	ALA	-	expression tag	UNP P39115
V	536	ALA	-	expression tag	UNP P39115
V	537	ALA	-	expression tag	UNP P39115
V	538	ALA	-	expression tag	UNP P39115
V	539	ALA	-	expression tag	UNP P39115
V	540	ALA	-	expression tag	UNP P39115
V	541	ALA	-	expression tag	UNP P39115
V	542	ALA	-	expression tag	UNP P39115

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	W	82	630	390	123	117	0	0

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	X	58	444	275	92	75	2	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	65	530	328	102	98	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	58	455	281	89	84	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	0	54	426	262	86	71	7	0	0

- Molecule 26 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	1	48	401	244	80	73	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	2	44	367	222	89	54	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	3	64	512	321	107	82	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	4	37	296	186	60	45	5	0	0

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	6	63	499	312	91	91	5	0	0

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	7	3	60	27	7	23	3	0	0

- Molecule 32 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	8	212	1599	1015	273	306	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
33	a	1533	32891	14667	6034	10657	1533	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	b	218	1757	1119	309	323	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	c	206	1619	1011	304	301	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	d	195	1568	991	291	284	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	e	164	1218	767	225	224	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	f	92	755	476	132	146	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	g	149	1181	740	220	215	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	h	131	1036	655	191	187	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	i	125	966	599	191	175	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	j	95	761	479	139	141	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	k	114	838	516	164	156	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	l	136	1052	653	211	186	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	m	108	868	534	176	158	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	n	60	497	317	98	77	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	o	85	710	436	144	129	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	p	88	695	441	128	124	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	q	84	691	435	128	126	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	r	64	518	332	96	88	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	s	78	633	409	112	110	2	0	0

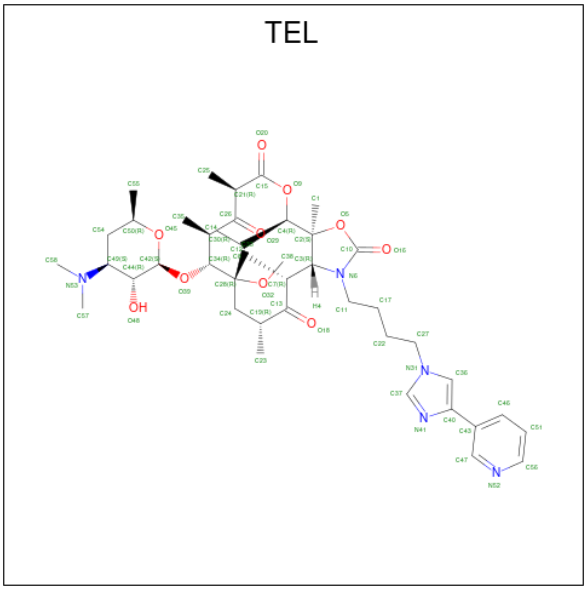
- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	t	83	637	390	130	116	1	0	0

- Molecule 53 is a RNA chain called P-tRNA(Leu).

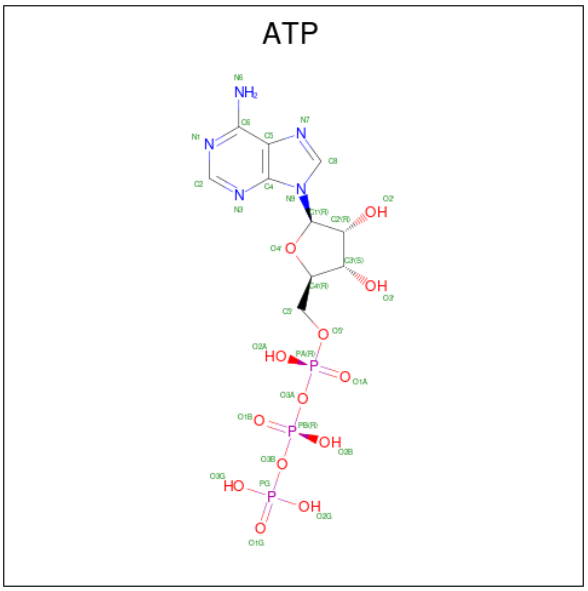
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	x	75	1603	714	284	530	75	0	0

- Molecule 54 is TELITHROMYCIN (three-letter code: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
54	A	1	58	43	5	10	0

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



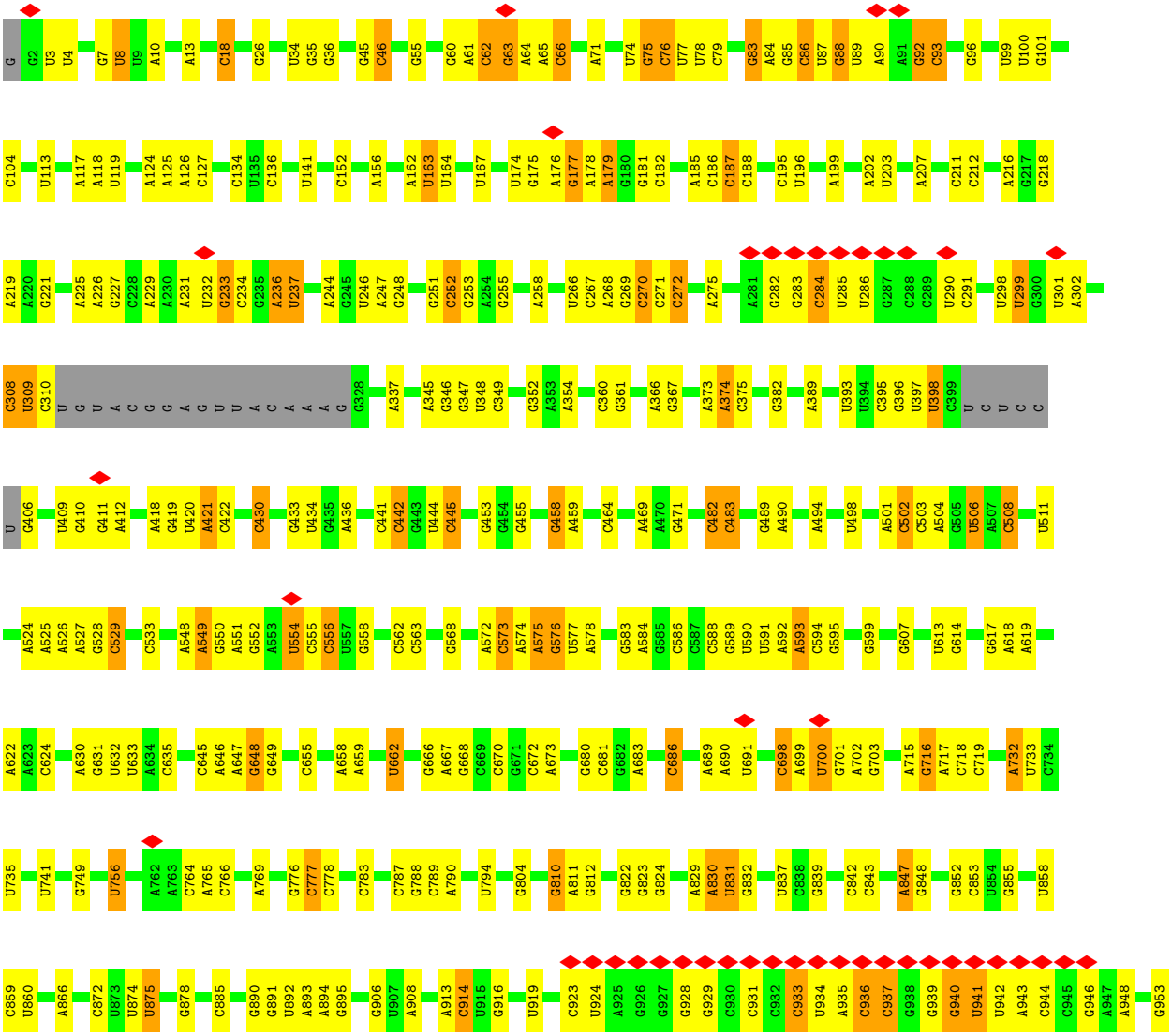
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	V	1	62	20	10	26	6	0
			Total	C	N	O	P	
55	V	1	62	20	10	26	6	0

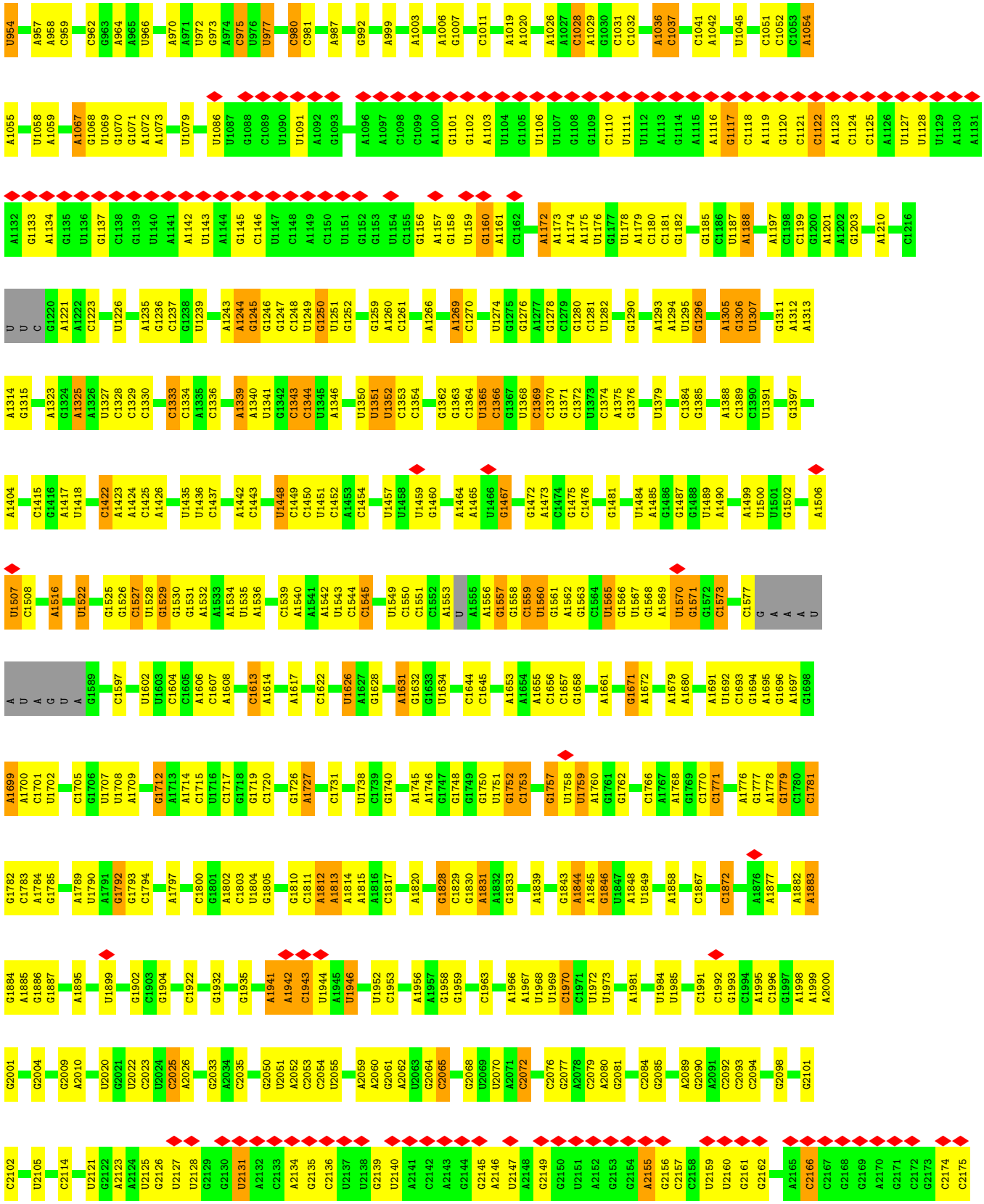
3 Residue-property plots (i)

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

- Molecule 1: 23S rRNA

Chain A: 7% 61% 31% 6%

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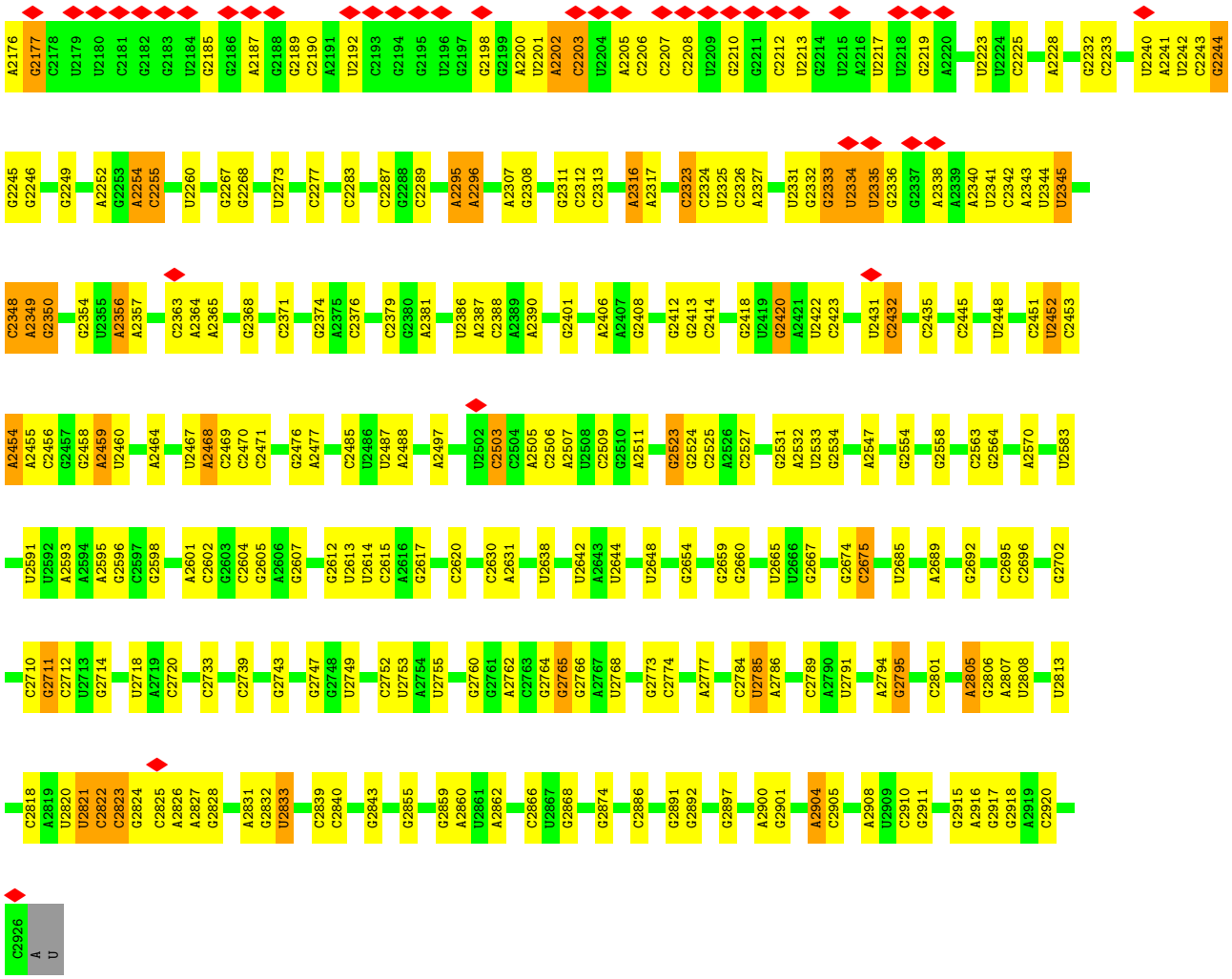

- Molecule 2: 5S rRNA

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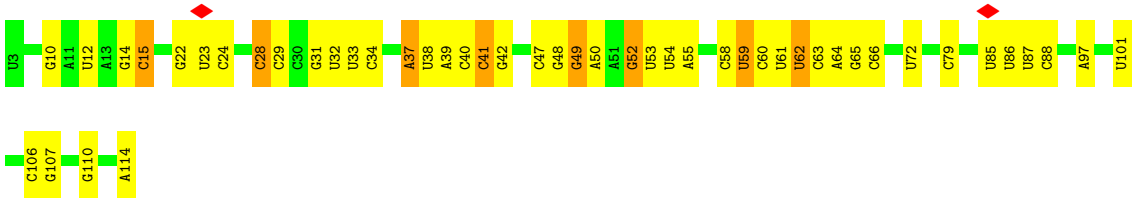

- Molecule 3: 50S ribosomal protein L2

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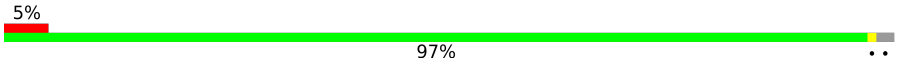
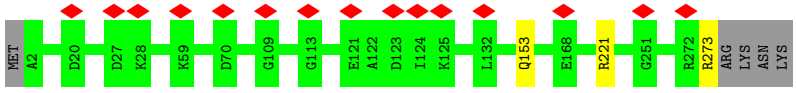
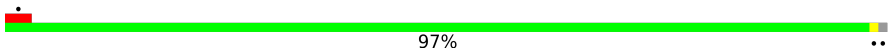
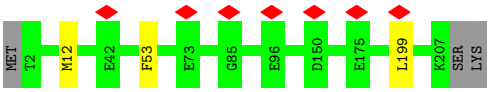




- Molecule 4: 50S ribosomal protein L3

Chain D:





• Molecule 5: 50S ribosomal protein L4

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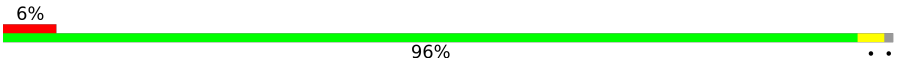
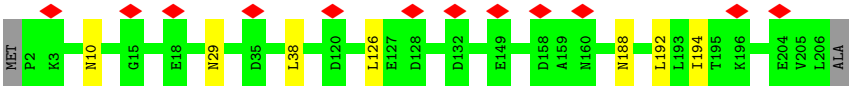
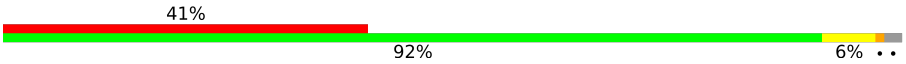
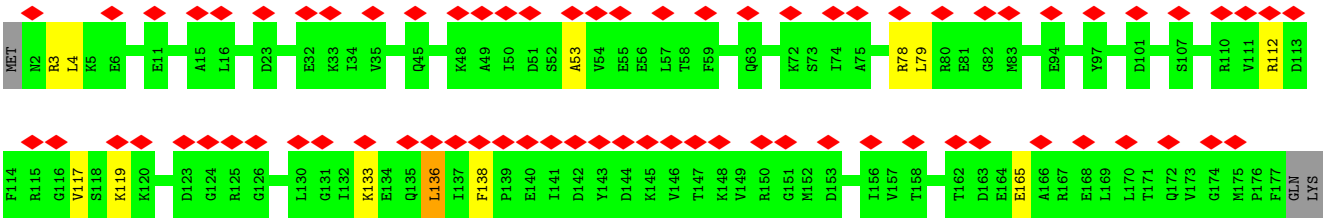




• Molecule 6: 50S ribosomal protein L5

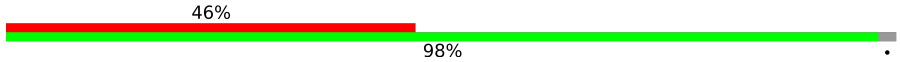
Chain F:

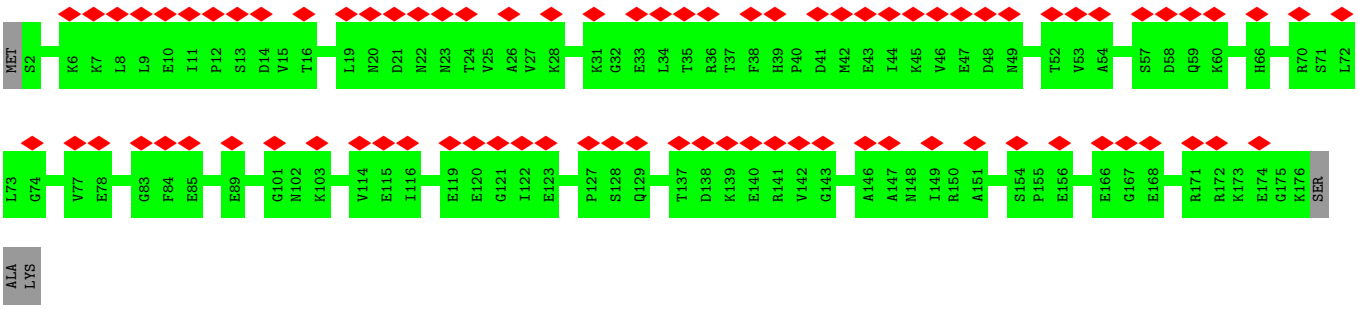




• Molecule 7: 50S ribosomal protein L6

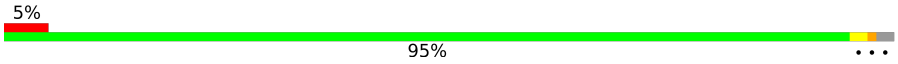
Chain G:

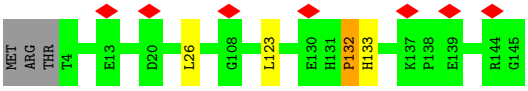




• Molecule 8: 50S ribosomal protein L13

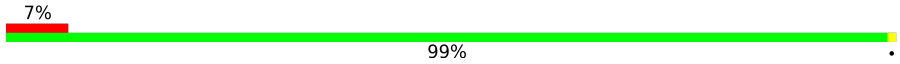
Chain J:

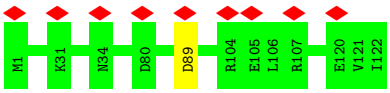




• Molecule 9: 50S ribosomal protein L14

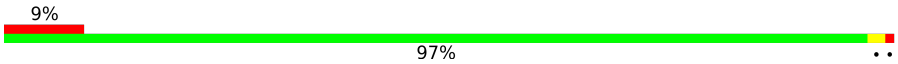
Chain K:

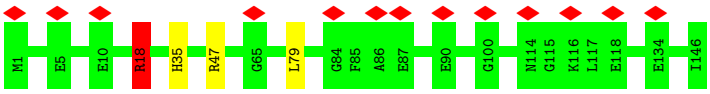




• Molecule 10: 50S ribosomal protein L15

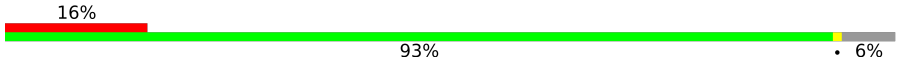
Chain L:

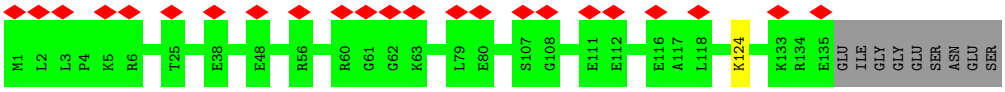




• Molecule 11: 50S ribosomal protein L16

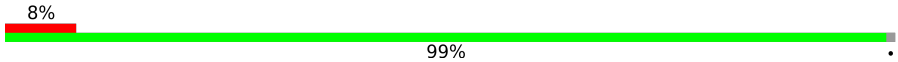
Chain M:

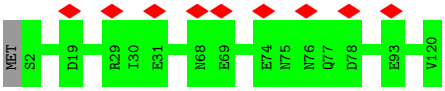




• Molecule 12: 50S ribosomal protein L17

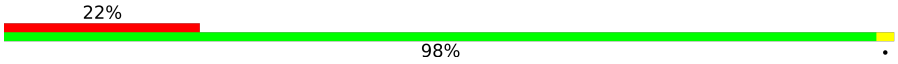
Chain N:

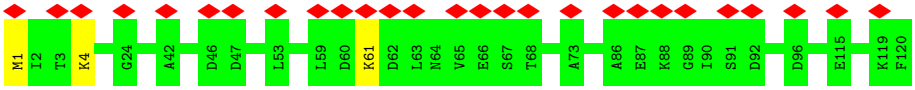




• Molecule 13: 50S ribosomal protein L18

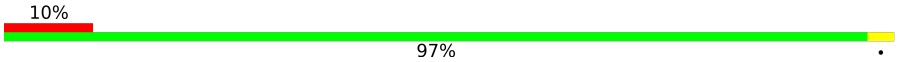
Chain O:





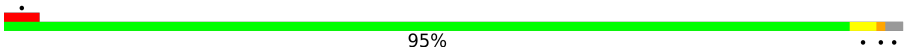
• Molecule 14: 50S ribosomal protein L19

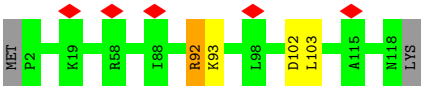
Chain P:



• Molecule 15: 50S ribosomal protein L20

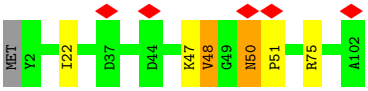
Chain Q:





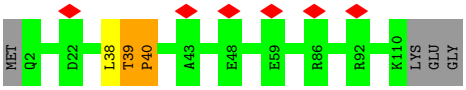
• Molecule 16: 50S ribosomal protein L21

Chain R: 5% 93%



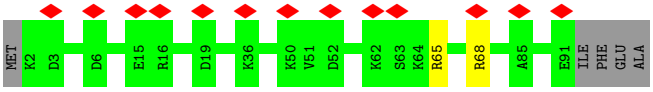
• Molecule 17: 50S ribosomal protein L22

Chain S: 5% 94%



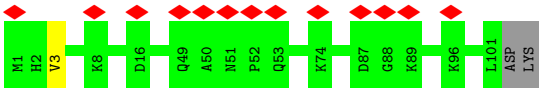
• Molecule 18: 50S ribosomal protein L23

Chain T: 14% 93% 5%



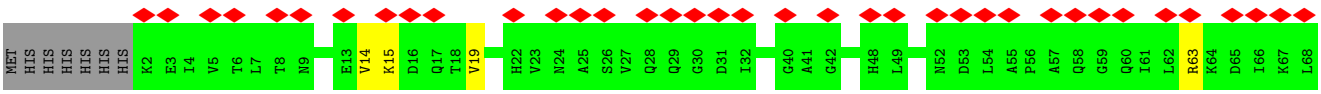
• Molecule 19: 50S ribosomal protein L24

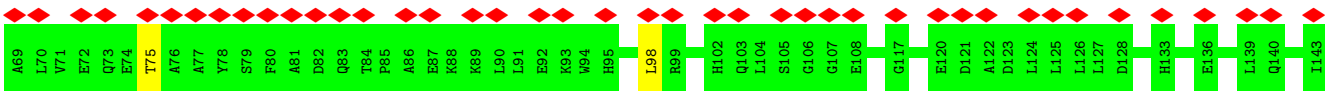
Chain U: 13% 97%

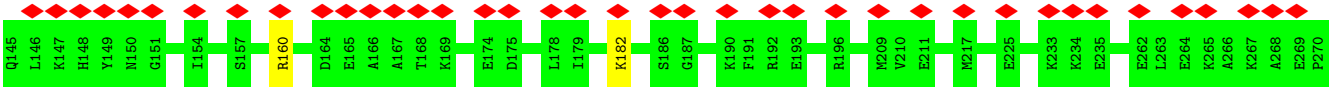


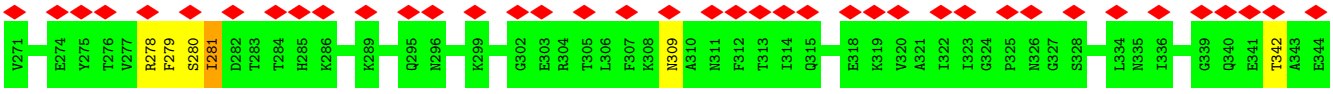
• Molecule 20: Nucleotide-binding protein ExpZ

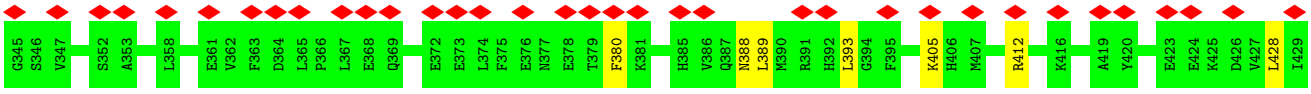
Chain V: 45% 95%

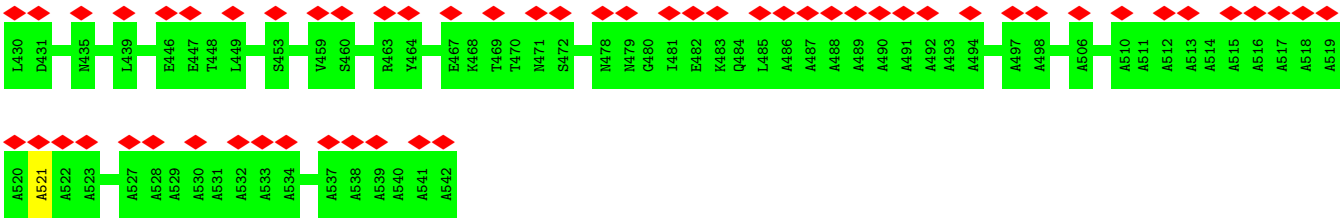






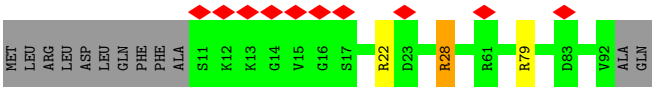






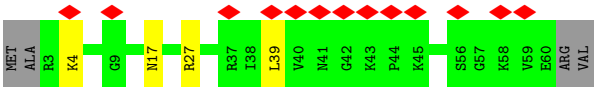
- Molecule 21: 50S ribosomal protein L27

Chain W:



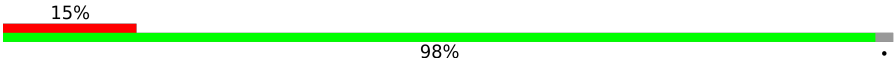
- Molecule 22: 50S ribosomal protein L28

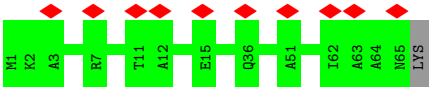
Chain X:



- Molecule 23: 50S ribosomal protein L29

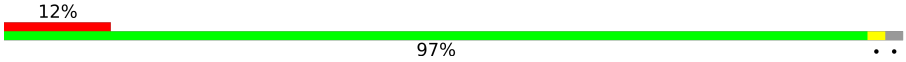
Chain Y:

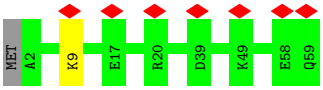




- Molecule 24: 50S ribosomal protein L30

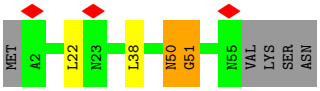
Chain Z:





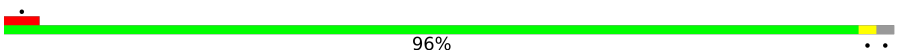
- Molecule 25: 50S ribosomal protein L32

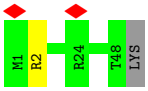
Chain 0:



- Molecule 26: 50S ribosomal protein L33 1

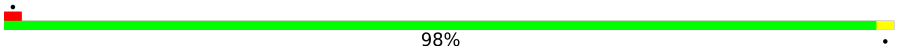
Chain 1:

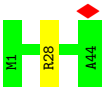




• Molecule 27: 50S ribosomal protein L34

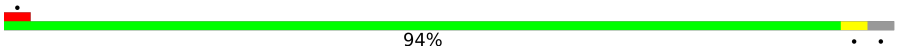
Chain 2:

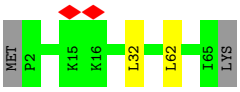




• Molecule 28: 50S ribosomal protein L35

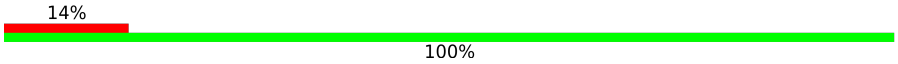
Chain 3:

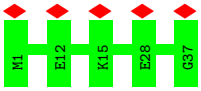




• Molecule 29: 50S ribosomal protein L36

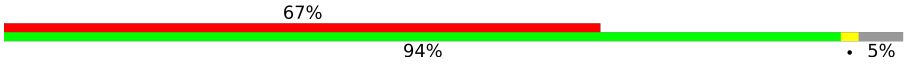
Chain 4:

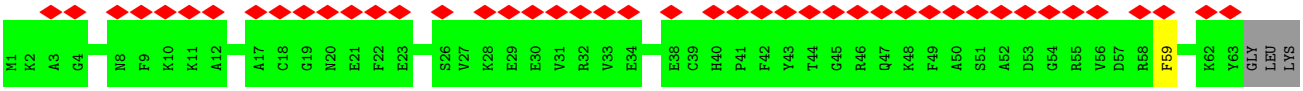




• Molecule 30: 50S ribosomal protein L31

Chain 6:



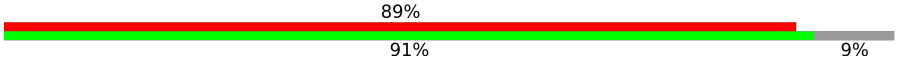


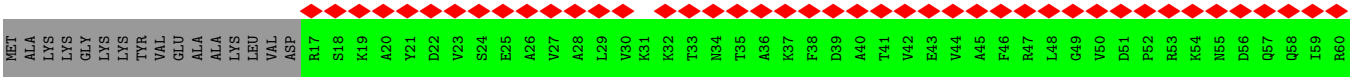
• Molecule 31: mRNA

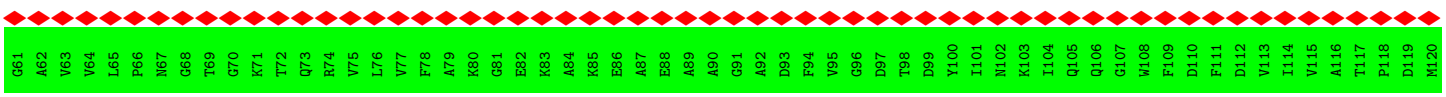
Chain 7:

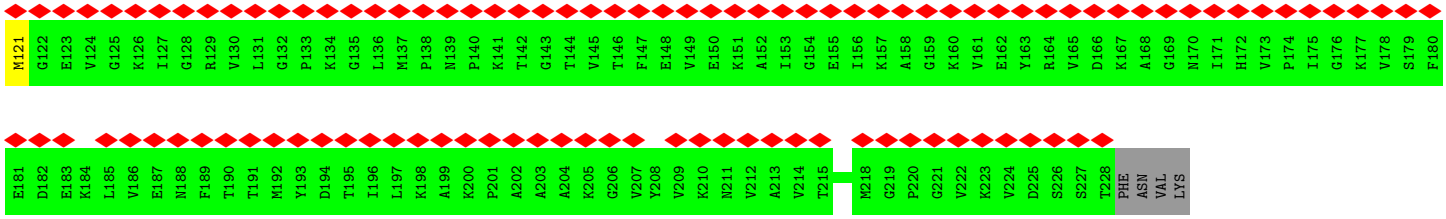
• Molecule 32: 50S ribosomal protein L1

Chain 8:



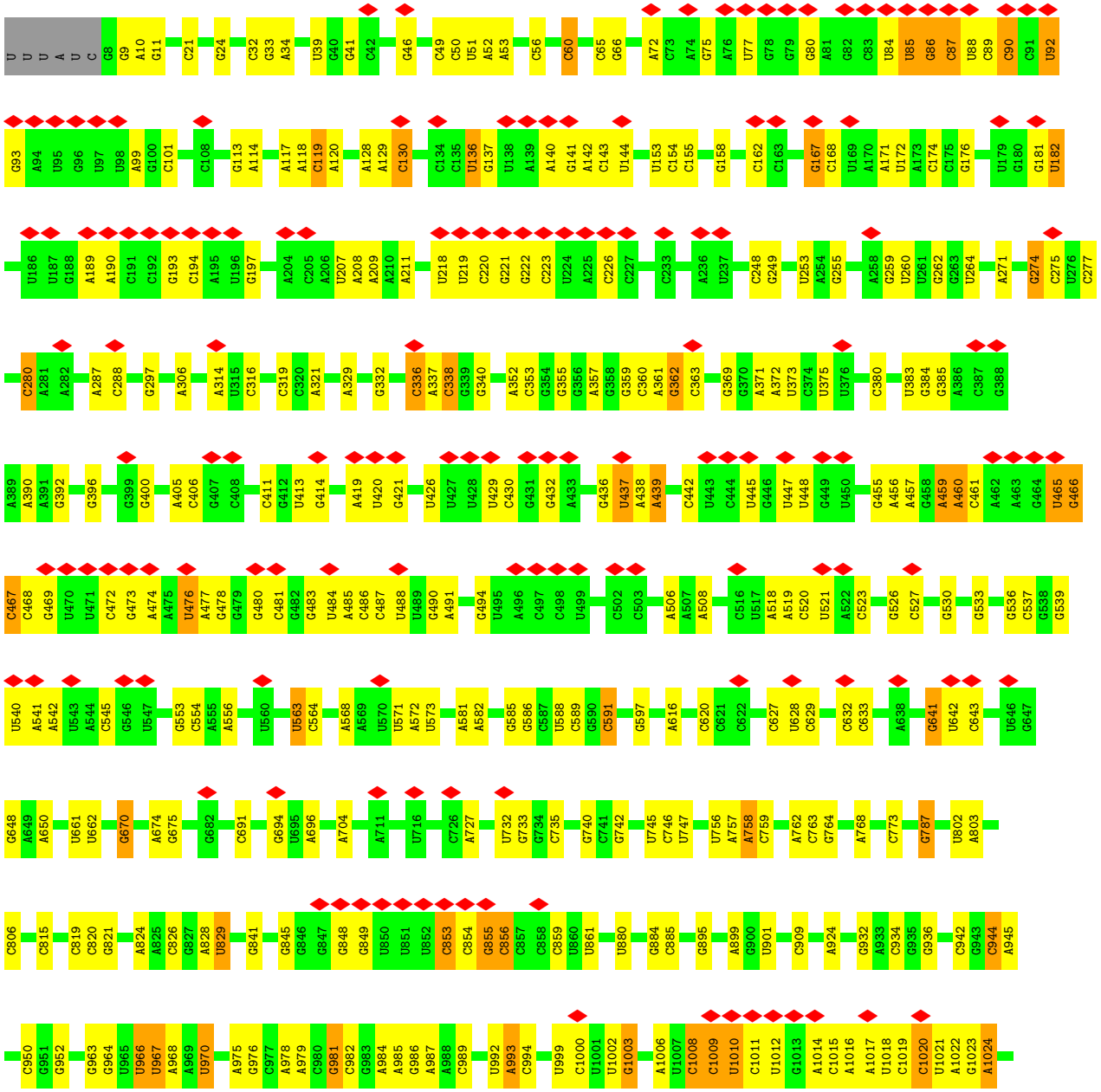


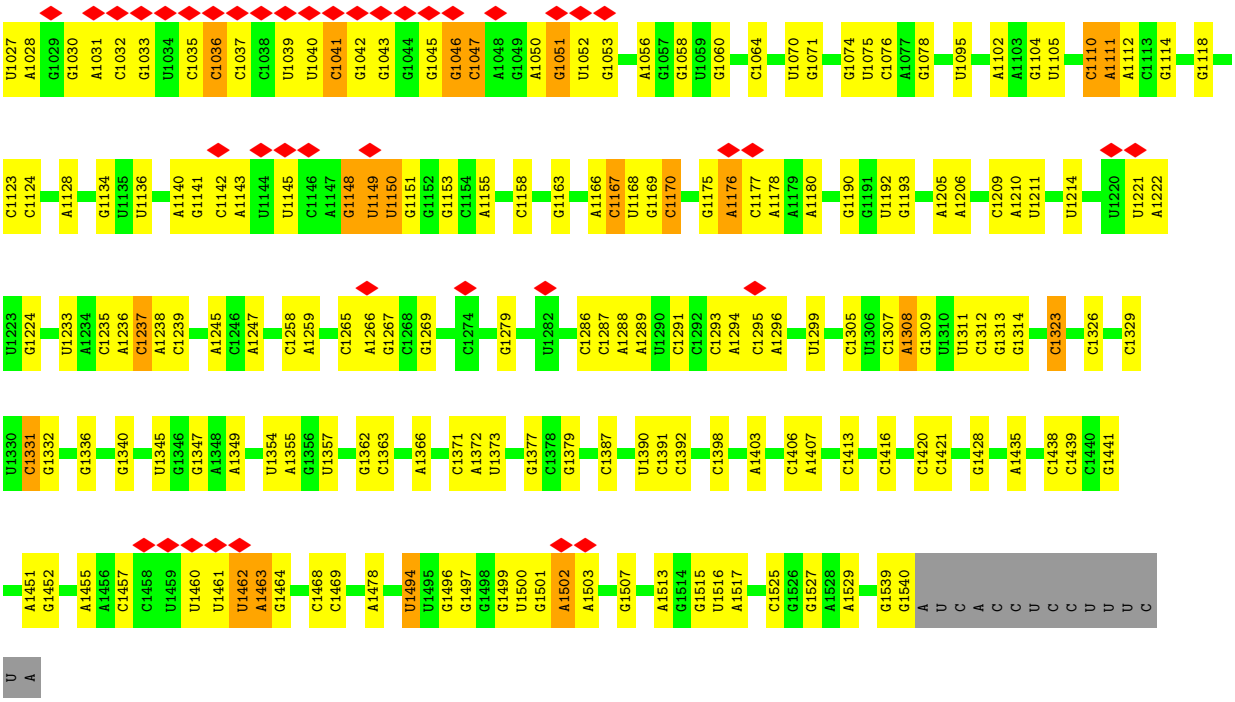




• Molecule 33: 16S rRNA

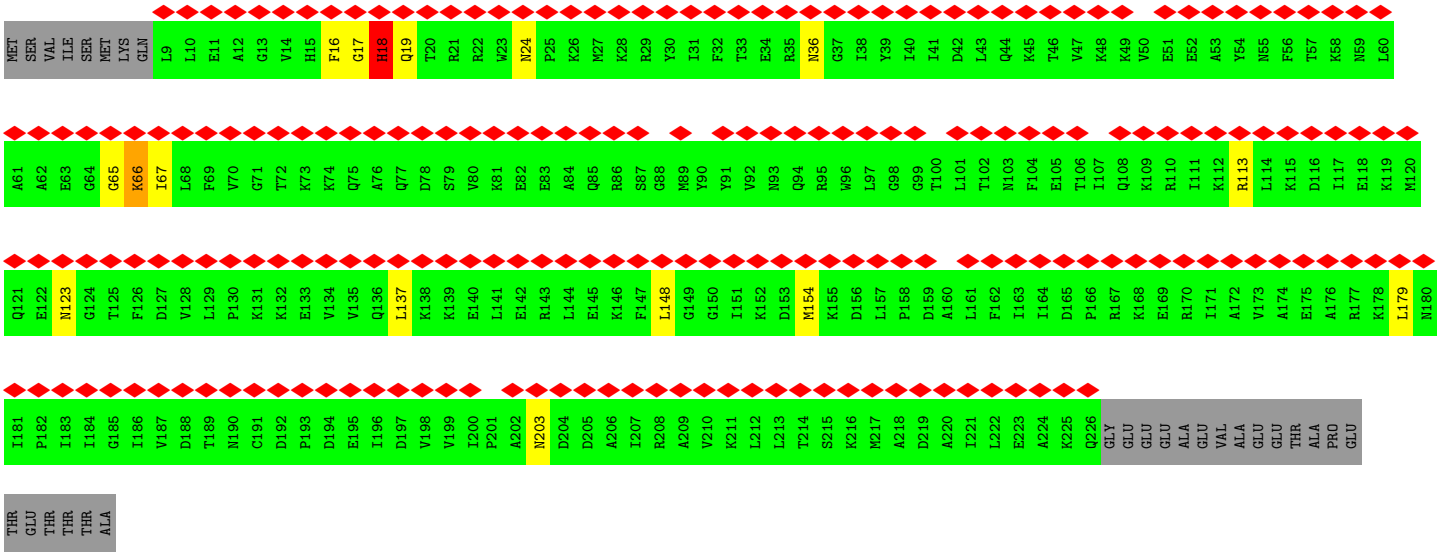
Chain a:





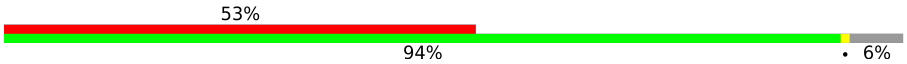
- Molecule 34: 30S ribosomal protein S2

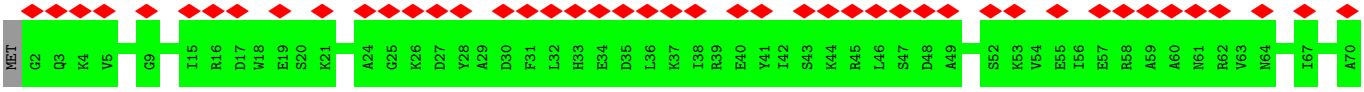
Chain b:

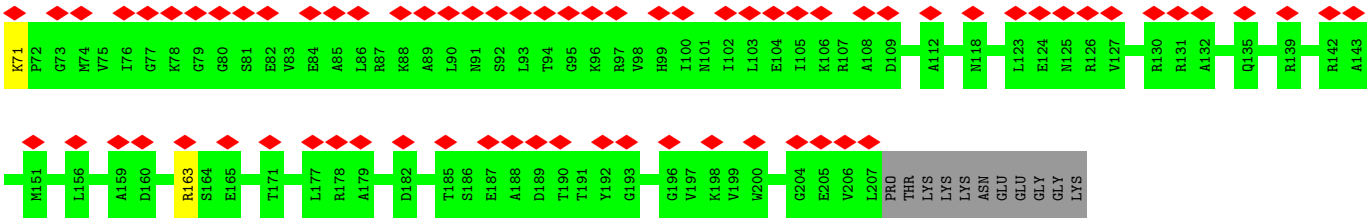


- Molecule 35: 30S ribosomal protein S3

Chain c:

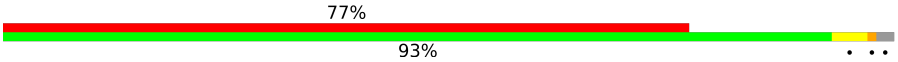


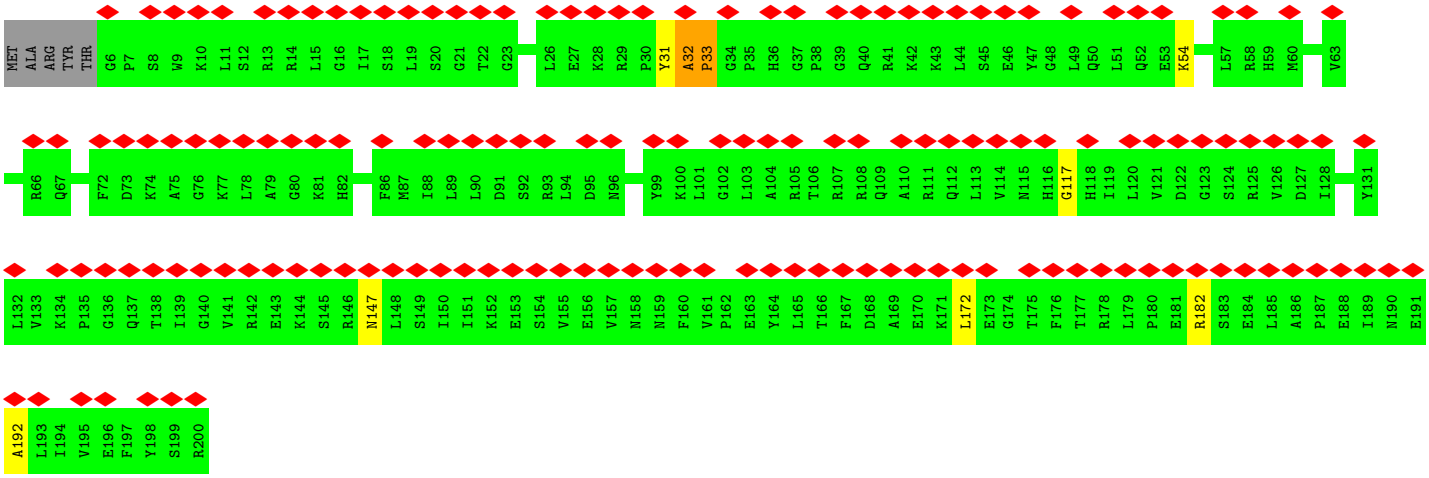




• Molecule 36: 30S ribosomal protein S4

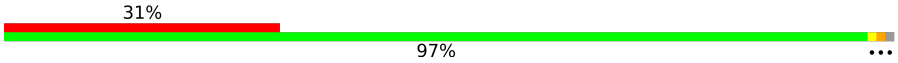
Chain d:

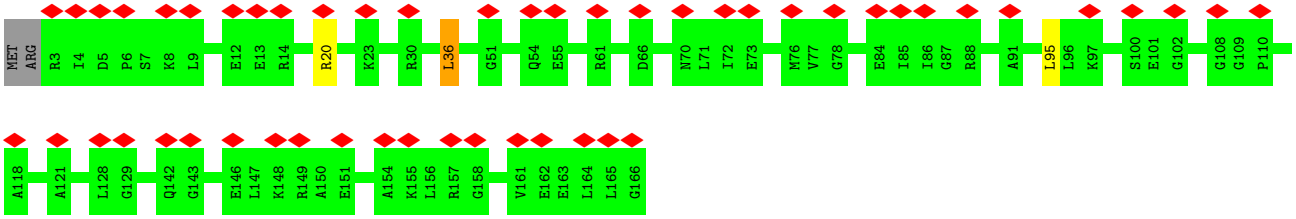




• Molecule 37: 30S ribosomal protein S5

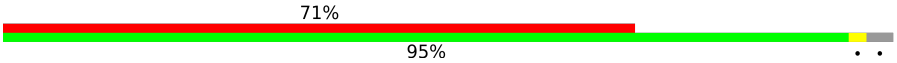
Chain e:





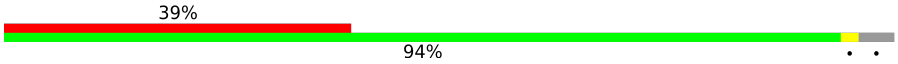
• Molecule 38: 30S ribosomal protein S6

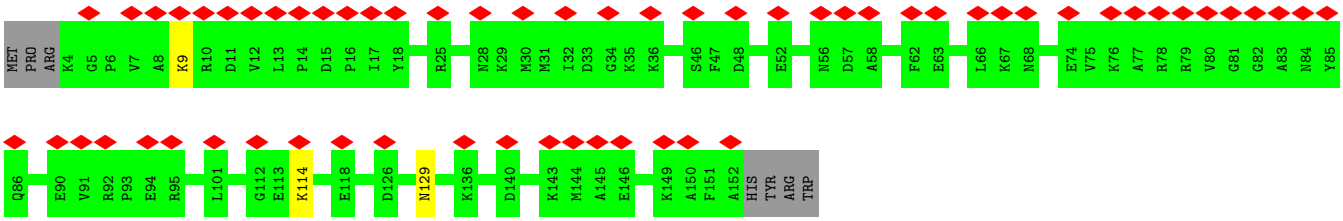
Chain f:



• Molecule 39: 30S ribosomal protein S7

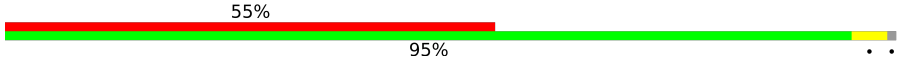
Chain g:

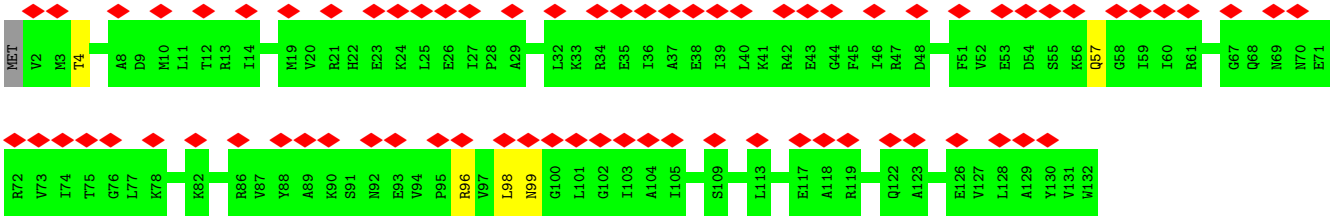




- Molecule 40: 30S ribosomal protein S8

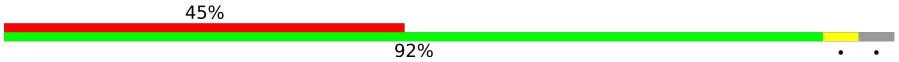
Chain h:

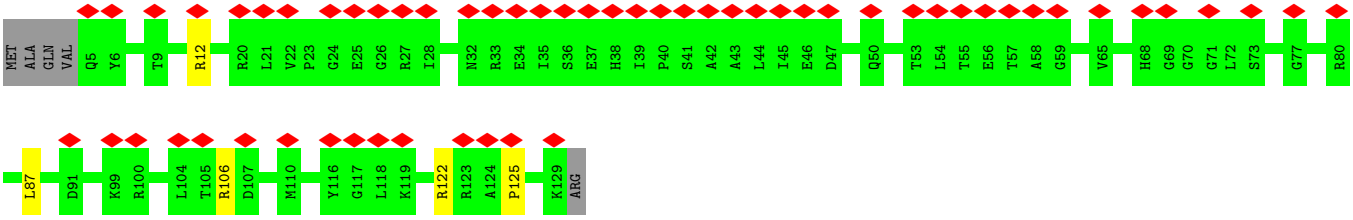




- Molecule 41: 30S ribosomal protein S9

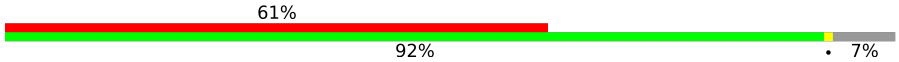
Chain i:

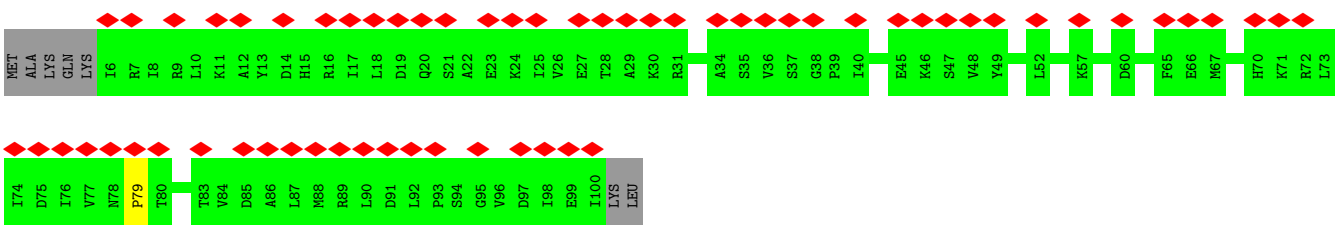




- Molecule 42: 30S ribosomal protein S10

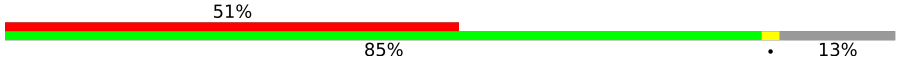
Chain j:

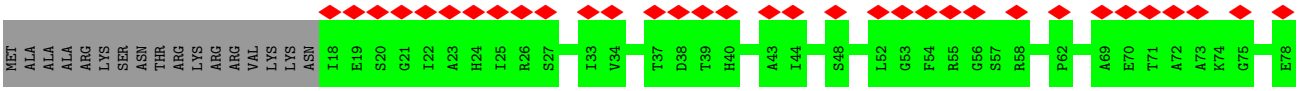




- Molecule 43: 30S ribosomal protein S11

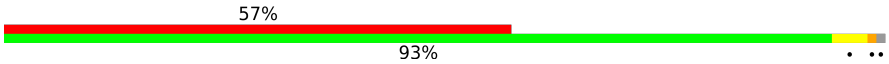
Chain k:

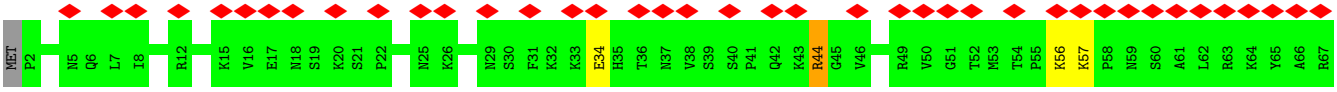


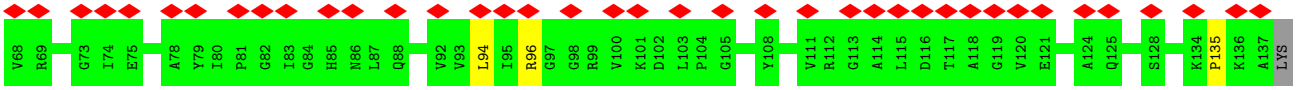


- Molecule 44: 30S ribosomal protein S12

Chain l:

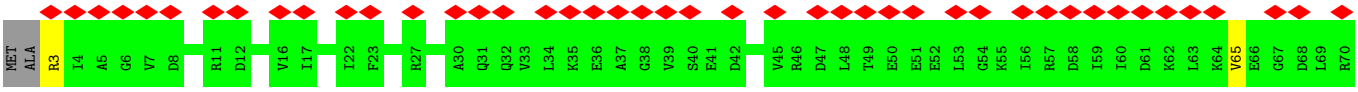


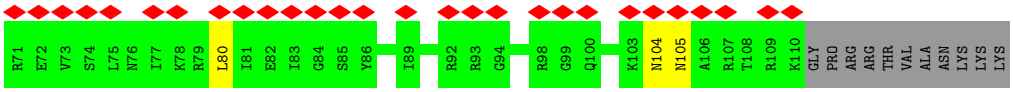




- Molecule 45: 30S ribosomal protein S13

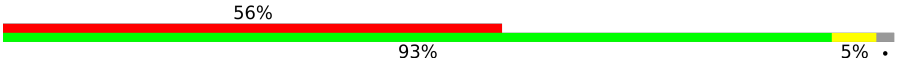
Chain m:

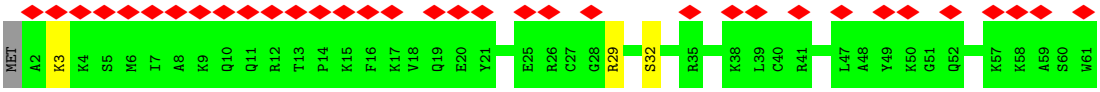




- Molecule 46: 30S ribosomal protein S14

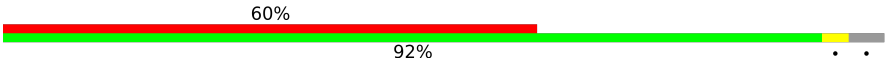
Chain n:

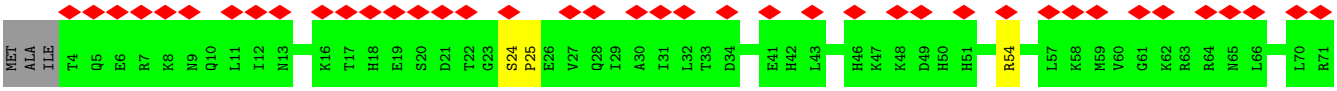


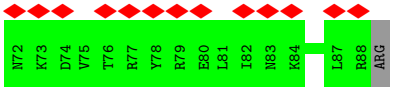


- Molecule 47: 30S ribosomal protein S15

Chain o:

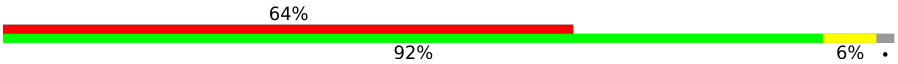


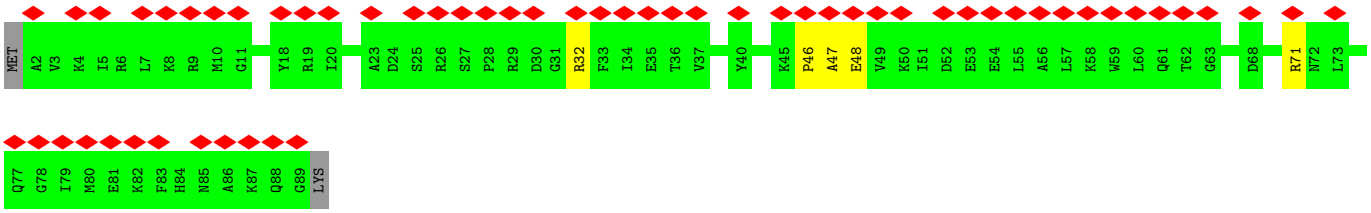




- Molecule 48: 30S ribosomal protein S16

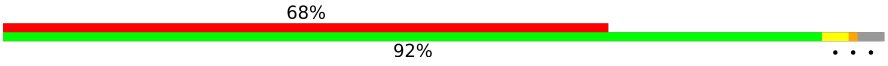
Chain p:

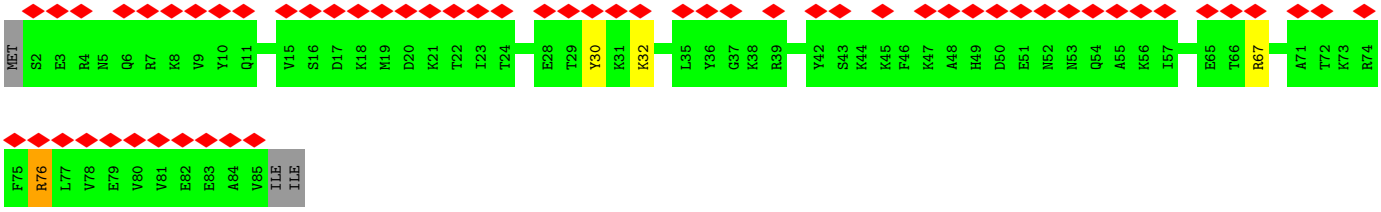




• Molecule 49: 30S ribosomal protein S17

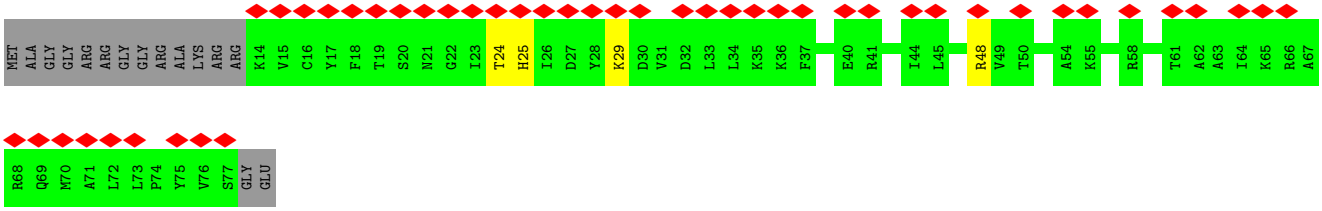
Chain q:





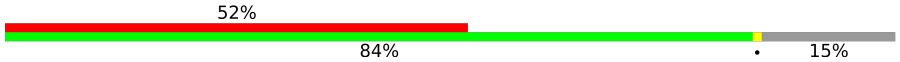
• Molecule 50: 30S ribosomal protein S18

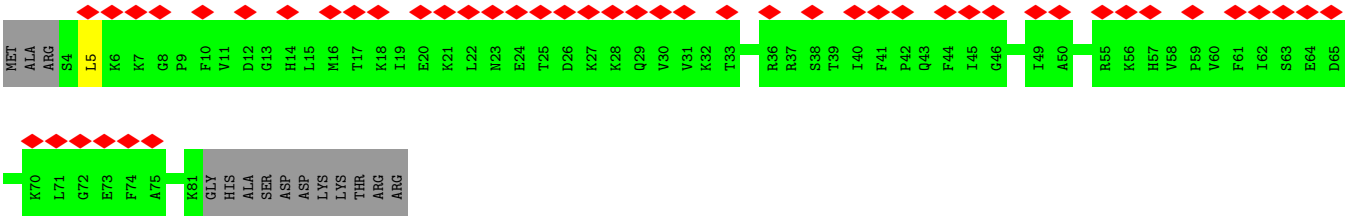
Chain r:



• Molecule 51: 30S ribosomal protein S19

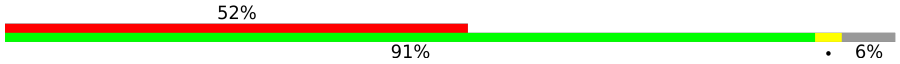
Chain s:

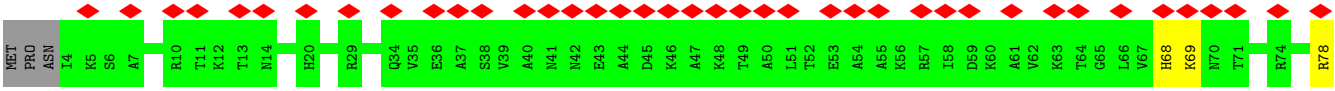


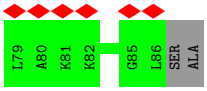


• Molecule 52: 30S ribosomal protein S20

Chain t:

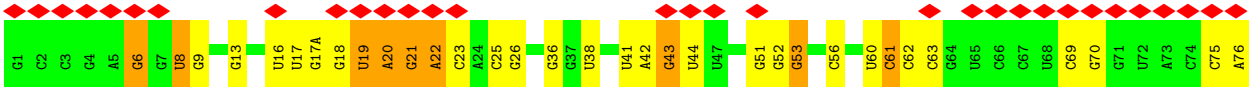






- Molecule 53: P-tRNA(Leu)

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	28972	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 ($e^-/Å^2$)	1.425	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.634	Depositor
Minimum map value	-0.379	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TEL, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.05	17/69438 (0.0%)	1.31	711/108311 (0.7%)
2	B	0.79	0/2675	1.34	36/4170 (0.9%)
3	C	0.59	0/2120	0.76	0/2845
4	D	0.61	0/1591	0.75	1/2132 (0.0%)
5	E	0.54	0/1580	0.74	2/2132 (0.1%)
6	F	0.44	0/1405	0.83	4/1887 (0.2%)
7	G	0.40	0/1360	0.70	0/1832
8	J	0.57	0/1146	0.78	0/1542
9	K	0.60	0/927	0.79	1/1245 (0.1%)
10	L	0.53	0/1093	0.77	2/1457 (0.1%)
11	M	0.55	0/1099	0.76	0/1468
12	N	0.54	0/960	0.74	0/1284
13	O	0.45	0/921	0.77	0/1236
14	P	0.55	0/957	0.77	0/1279
15	Q	0.62	0/952	0.81	2/1266 (0.2%)
16	R	0.62	0/797	0.87	4/1070 (0.4%)
17	S	0.54	0/851	0.78	2/1146 (0.2%)
18	T	0.52	0/731	0.71	0/974
19	U	0.51	1/772 (0.1%)	0.75	0/1032
20	V	0.41	0/4247	0.72	3/5736 (0.1%)
21	W	0.62	0/638	0.94	2/847 (0.2%)
22	X	0.46	0/448	0.77	1/596 (0.2%)
23	Y	0.44	0/531	0.70	0/707
24	Z	0.47	0/457	0.79	0/613
25	0	0.61	0/433	0.81	0/574
26	1	0.57	0/406	0.76	1/540 (0.2%)
27	2	0.58	0/370	0.78	0/483
28	3	0.55	0/519	0.70	0/680
29	4	0.47	0/299	0.66	0/393
30	6	0.42	0/509	0.72	0/678
31	7	0.61	0/65	1.36	2/98 (2.0%)
32	8	0.32	0/1624	0.66	0/2192

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	a	0.63	1/36826 (0.0%)	1.23	291/57450 (0.5%)
34	b	0.35	0/1782	0.71	3/2392 (0.1%)
35	c	0.38	0/1641	0.67	0/2208
36	d	0.36	0/1598	0.72	0/2147
37	e	0.39	0/1230	0.75	1/1655 (0.1%)
38	f	0.32	0/766	0.61	0/1031
39	g	0.38	0/1196	0.75	0/1604
40	h	0.36	0/1048	0.75	0/1407
41	i	0.38	0/979	0.76	2/1315 (0.2%)
42	j	0.38	0/773	0.70	0/1044
43	k	0.35	0/852	0.70	1/1153 (0.1%)
44	l	0.37	0/1069	0.79	3/1435 (0.2%)
45	m	0.36	0/873	0.76	1/1166 (0.1%)
46	n	0.41	0/507	0.82	1/672 (0.1%)
47	o	0.33	0/718	0.62	0/960
48	p	0.39	0/708	0.73	0/950
49	q	0.40	0/699	0.79	1/933 (0.1%)
50	r	0.33	0/526	0.67	0/705
51	s	0.35	0/649	0.69	0/872
52	t	0.36	0/639	0.65	0/852
53	x	0.65	0/1790	1.52	28/2787 (1.0%)
All	All	0.81	19/158790 (0.0%)	1.17	1106/237183 (0.5%)

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
3	C	0	1
4	D	0	1
6	F	0	3
8	J	0	1
10	L	0	2
13	O	0	1
15	Q	0	1
16	R	0	2
17	S	0	1
20	V	0	11
25	0	0	2
30	6	0	1
34	b	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	d	0	5
37	e	0	1
38	f	0	1
39	g	0	2
40	h	0	1
44	l	0	2
45	m	0	3
47	o	0	1
49	q	0	1
50	r	0	2
All	All	0	51

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	631	G	N9-C4	-7.63	1.31	1.38
1	A	830	A	N9-C4	-6.90	1.33	1.37
1	A	1067	A	N9-C4	-6.87	1.33	1.37
1	A	574	A	N9-C4	-6.32	1.34	1.37
1	A	631	G	C2-N3	-5.92	1.28	1.32
1	A	776	G	C8-N7	-5.80	1.27	1.30
1	A	1812	A	N9-C4	-5.80	1.34	1.37
1	A	700	U	C1'-N1	5.70	1.57	1.48
1	A	1188	A	N9-C4	-5.57	1.34	1.37
1	A	847	A	N9-C4	-5.52	1.34	1.37
19	U	3	VAL	CB-CG1	-5.48	1.41	1.52
1	A	1820	A	N9-C4	-5.47	1.34	1.37
1	A	776	G	N7-C5	-5.47	1.35	1.39
33	a	993	A	N9-C4	5.43	1.41	1.37
1	A	572	A	N9-C4	-5.38	1.34	1.37
1	A	589	G	N9-C4	-5.37	1.33	1.38
1	A	1054	A	N9-C4	-5.18	1.34	1.37
1	A	374	A	N9-C4	-5.00	1.34	1.37
1	A	589	G	N3-C4	-5.00	1.31	1.35

All (1106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	1502	A	C8-N9-C4	-14.51	100.00	105.80
53	x	6	G	O5'-P-OP2	-14.04	93.07	105.70
1	A	756	U	N3-C2-O2	-12.07	113.75	122.20
1	A	2054	C	C5-C6-N1	12.06	127.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2243	C	N1-C2-O2	11.98	126.09	118.90
1	A	2334	U	C5-C4-O4	-11.91	118.75	125.90
1	A	2334	U	O4'-C1'-N1	11.30	117.24	108.20
33	a	1502	A	N7-C8-N9	11.27	119.43	113.80
1	A	2334	U	C2-N1-C1'	11.01	130.92	117.70
53	x	8	U	O5'-P-OP1	10.86	123.73	110.70
1	A	398	U	N3-C2-O2	-10.81	114.63	122.20
1	A	2025	C	N3-C2-O2	-10.76	114.37	121.90
1	A	1943	C	N1-C2-O2	10.51	125.21	118.90
1	A	2243	C	N3-C2-O2	-10.51	114.54	121.90
2	B	24	C	N1-C2-O2	10.51	125.21	118.90
1	A	92	G	C8-N9-C4	10.44	110.58	106.40
1	A	589	G	N3-C4-N9	-10.43	119.74	126.00
1	A	631	G	N3-C4-C5	10.38	133.79	128.60
1	A	2157	C	N1-C2-O2	10.38	125.13	118.90
1	A	631	G	N3-C4-N9	-10.30	119.82	126.00
1	A	483	C	C5-C6-N1	10.07	126.04	121.00
1	A	769	A	N1-C6-N6	-10.07	112.56	118.60
1	A	1527	C	C2-N1-C1'	10.07	129.87	118.80
1	A	2335	U	N3-C2-O2	-9.96	115.23	122.20
33	a	1009	C	C2-N1-C1'	9.92	129.72	118.80
1	A	2695	C	N1-C2-O2	9.74	124.74	118.90
1	A	2334	U	C6-N1-C1'	-9.58	107.78	121.20
33	a	1176	A	O5'-P-OP1	-9.46	97.19	105.70
1	A	1366	C	C5-C6-N1	9.40	125.70	121.00
1	A	631	G	C4-N9-C1'	-9.31	114.40	126.50
1	A	2822	C	C2-N1-C1'	9.25	128.98	118.80
33	a	1009	C	N1-C2-O2	9.21	124.43	118.90
33	a	1076	C	N1-C2-O2	9.07	124.34	118.90
33	a	1046	G	O5'-P-OP1	-9.06	97.54	105.70
1	A	2025	C	N1-C2-O2	9.05	124.33	118.90
2	B	62	U	C2-N1-C1'	9.04	128.54	117.70
1	A	1476	C	C5-C6-N1	9.03	125.51	121.00
1	A	1353	C	C2-N1-C1'	9.01	128.71	118.80
1	A	442	C	C6-N1-C2	-8.99	116.70	120.30
33	a	60	C	C6-N1-C2	-8.92	116.73	120.30
1	A	2350	G	N3-C4-C5	-8.86	124.17	128.60
53	x	19	U	O5'-P-OP2	-8.84	97.75	105.70
33	a	1502	A	C5'-C4'-O4'	-8.71	98.65	109.10
1	A	2334	U	N3-C4-O4	8.70	125.49	119.40
33	a	1076	C	C2-N1-C1'	8.68	128.34	118.80
33	a	1331	C	C2-N1-C1'	8.66	128.33	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2695	C	N3-C2-O2	-8.65	115.84	121.90
33	a	101	C	N1-C2-O2	8.63	124.08	118.90
1	A	442	C	C5-C6-N1	8.62	125.31	121.00
1	A	1943	C	N3-C2-O2	-8.61	115.87	121.90
1	A	272	C	N1-C2-O2	8.54	124.02	118.90
2	B	24	C	C2-N1-C1'	8.51	128.16	118.80
1	A	1872	C	C6-N1-C2	-8.51	116.90	120.30
33	a	101	C	N3-C2-O2	-8.47	115.97	121.90
33	a	989	C	N1-C2-O2	8.46	123.98	118.90
1	A	2918	G	C4-N9-C1'	8.45	137.49	126.50
21	W	28	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	A	75	G	O4'-C1'-N9	8.40	114.92	108.20
1	A	769	A	N1-C2-N3	-8.38	125.11	129.30
1	A	1872	C	C5-C6-N1	8.36	125.18	121.00
1	A	631	G	C8-N9-C1'	8.34	137.84	127.00
1	A	588	C	N1-C2-O2	8.32	123.89	118.90
1	A	1133	G	O4'-C1'-N9	8.27	114.82	108.20
1	A	442	C	O5'-P-OP1	8.26	120.62	110.70
1	A	1707	U	N3-C2-O2	-8.26	116.42	122.20
1	A	1985	U	N3-C2-O2	-8.21	116.45	122.20
1	A	2054	C	C6-N1-C2	-8.19	117.02	120.30
1	A	1343	C	C2-N1-C1'	8.19	127.81	118.80
1	A	1527	C	N1-C2-O2	8.18	123.81	118.90
1	A	508	C	C2-N1-C1'	8.16	127.78	118.80
1	A	442	C	O5'-P-OP2	-8.16	98.36	105.70
53	x	42	A	P-O3'-C3'	8.16	129.49	119.70
1	A	2335	U	C6-N1-C2	-8.16	116.11	121.00
1	A	398	U	N1-C2-O2	8.14	128.50	122.80
33	a	1170	C	C6-N1-C2	-8.13	117.05	120.30
1	A	397	U	N1-C2-O2	8.09	128.46	122.80
33	a	1076	C	C6-N1-C2	-8.09	117.06	120.30
33	a	620	C	N1-C2-O2	8.08	123.75	118.90
1	A	1343	C	C6-N1-C2	-8.07	117.07	120.30
1	A	2105	U	C2-N1-C1'	8.05	127.36	117.70
1	A	1352	U	C2-N1-C1'	8.03	127.33	117.70
1	A	648	G	O4'-C1'-N9	8.02	114.61	108.20
1	A	483	C	C6-N1-C2	-8.01	117.09	120.30
1	A	756	U	N1-C2-O2	8.01	128.41	122.80
1	A	2350	G	C4-N9-C1'	8.00	136.90	126.50
1	A	719	C	C5-C6-N1	8.00	125.00	121.00
1	A	589	G	C8-N9-C1'	8.00	137.40	127.00
1	A	1527	C	C5-C6-N1	7.94	124.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	1331	C	N1-C2-O2	7.92	123.65	118.90
1	A	1067	A	C5-N7-C8	-7.92	99.94	103.90
53	x	20	A	P-O3'-C3'	7.91	129.19	119.70
1	A	1476	C	C6-N1-C2	-7.91	117.14	120.30
1	A	2105	U	N1-C2-O2	7.90	128.33	122.80
1	A	573	C	N1-C2-O2	7.88	123.63	118.90
1	A	2296	A	O5'-P-OP1	-7.88	98.61	105.70
1	A	589	G	N9-C4-C5	7.86	108.54	105.40
1	A	1571	G	O5'-P-OP2	-7.86	98.63	105.70
33	a	1439	C	N3-C2-O2	-7.84	116.41	121.90
33	a	1305	C	N3-C2-O2	-7.83	116.42	121.90
1	A	1036	A	C8-N9-C4	-7.83	102.67	105.80
33	a	136	U	N3-C2-O2	-7.80	116.74	122.20
1	A	397	U	N3-C2-O2	-7.80	116.74	122.20
1	A	645	C	C6-N1-C2	-7.80	117.18	120.30
1	A	2768	U	N3-C2-O2	-7.76	116.77	122.20
1	A	2114	C	C2-N1-C1'	7.75	127.33	118.80
33	a	1037	C	N1-C2-O2	7.75	123.55	118.90
1	A	672	C	C6-N1-C2	-7.75	117.20	120.30
1	A	1872	C	C2-N1-C1'	7.74	127.32	118.80
1	A	2485	C	C5-C6-N1	7.74	124.87	121.00
1	A	831	U	N3-C2-O2	-7.73	116.79	122.20
1	A	2388	C	O5'-P-OP2	-7.73	98.75	105.70
33	a	993	A	C2-N3-C4	7.71	114.46	110.60
1	A	2255	C	N1-C2-O2	7.69	123.51	118.90
1	A	1028	C	N1-C2-O2	7.68	123.51	118.90
33	a	143	C	N3-C2-O2	-7.68	116.52	121.90
1	A	1343	C	C5-C6-N1	7.68	124.84	121.00
1	A	272	C	N3-C2-O2	-7.67	116.53	121.90
53	x	21	G	C4-N9-C1'	7.67	136.47	126.50
1	A	1771	C	N1-C2-O2	7.66	123.50	118.90
2	B	24	C	N3-C2-O2	-7.66	116.54	121.90
1	A	1985	U	N1-C2-O2	7.66	128.16	122.80
2	B	79	C	N1-C2-O2	7.65	123.49	118.90
1	A	1374	C	N1-C2-O2	7.65	123.49	118.90
1	A	2356	A	N7-C8-N9	7.62	117.61	113.80
1	A	92	G	N7-C8-N9	-7.62	109.29	113.10
1	A	1963	C	C6-N1-C2	-7.62	117.25	120.30
33	a	60	C	C5-C6-N1	7.61	124.81	121.00
33	a	1009	C	N3-C2-O2	-7.61	116.57	121.90
1	A	2157	C	N3-C2-O2	-7.60	116.58	121.90
1	A	1817	C	C2-N1-C1'	7.58	127.14	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2072	C	N1-C2-O2	7.57	123.44	118.90
33	a	620	C	N3-C2-O2	-7.57	116.60	121.90
33	a	1047	C	C6-N1-C2	-7.56	117.28	120.30
1	A	1831	A	N7-C8-N9	7.55	117.57	113.80
1	A	508	C	N1-C2-O2	7.54	123.42	118.90
2	B	15	C	C5-C6-N1	7.54	124.77	121.00
1	A	1122	C	N1-C2-O2	7.53	123.42	118.90
1	A	589	G	C4-N9-C1'	-7.51	116.74	126.50
33	a	1149	U	C2-N1-C1'	7.48	126.68	117.70
33	a	465	U	N1-C2-O2	7.48	128.03	122.80
1	A	554	U	OP2-P-O3'	7.47	121.64	105.20
2	B	59	U	C2-N1-C1'	7.46	126.66	117.70
33	a	853	C	N1-C2-O2	7.46	123.38	118.90
1	A	1656	C	N1-C2-O2	7.46	123.37	118.90
33	a	1009	C	C6-N1-C1'	-7.45	111.86	120.80
1	A	1366	C	C6-N1-C2	-7.45	117.32	120.30
1	A	2822	C	C5-C6-N1	7.43	124.71	121.00
1	A	1476	C	C2-N1-C1'	7.41	126.95	118.80
1	A	2371	C	C6-N1-C2	-7.41	117.34	120.30
33	a	60	C	C2-N1-C1'	7.40	126.94	118.80
33	a	989	C	N3-C2-O2	-7.40	116.72	121.90
33	a	746	C	C6-N1-C2	-7.40	117.34	120.30
1	A	681	C	C6-N1-C2	-7.39	117.34	120.30
1	A	2334	U	C5-C6-N1	7.39	126.39	122.70
1	A	1067	A	N7-C8-N9	7.38	117.49	113.80
33	a	1331	C	N3-C2-O2	-7.36	116.75	121.90
1	A	2131	U	C2-N1-C1'	7.36	126.53	117.70
53	x	19	U	O5'-P-OP1	7.35	119.52	110.70
33	a	759	C	C6-N1-C2	-7.35	117.36	120.30
33	a	1076	C	N3-C2-O2	-7.35	116.75	121.90
33	a	1438	C	N3-C2-O2	-7.34	116.76	121.90
6	F	136	LEU	CB-CG-CD1	-7.33	98.55	111.00
33	a	113	G	O5'-P-OP1	-7.31	99.12	105.70
1	A	1942	A	O4'-C1'-N9	7.29	114.03	108.20
1	A	1450	C	C2-N1-C1'	7.29	126.82	118.80
1	A	1817	C	N1-C2-O2	7.28	123.27	118.90
1	A	593	A	C2-N3-C4	7.27	114.24	110.60
1	A	2335	U	C2-N1-C1'	7.27	126.43	117.70
1	A	508	C	C6-N1-C2	-7.27	117.39	120.30
33	a	92	U	P-O3'-C3'	7.27	128.42	119.70
33	a	136	U	N1-C2-O2	7.26	127.88	122.80
1	A	1527	C	OP1-P-O3'	7.26	121.17	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2356	A	C8-N9-C4	-7.26	102.90	105.80
1	A	1942	A	N7-C8-N9	-7.26	110.17	113.80
33	a	168	C	N1-C2-O2	7.26	123.25	118.90
1	A	1415	C	N1-C2-O2	7.25	123.25	118.90
43	k	80	GLY	N-CA-C	7.25	131.24	113.10
1	A	576	G	OP2-P-O3'	7.25	121.15	105.20
1	A	1701	C	C6-N1-C2	-7.24	117.40	120.30
2	B	59	U	N1-C2-O2	7.24	127.87	122.80
33	a	465	U	C2-N1-C1'	7.24	126.39	117.70
33	a	1439	C	N1-C2-O2	7.24	123.24	118.90
1	A	2025	C	C2-N1-C1'	7.24	126.76	118.80
1	A	284	C	N3-C2-O2	-7.23	116.84	121.90
1	A	1327	U	N1-C2-O2	7.23	127.86	122.80
33	a	1076	C	C5-C6-N1	7.23	124.61	121.00
1	A	1848	A	O5'-P-OP2	-7.22	99.20	105.70
1	A	2350	G	C2-N3-C4	7.21	115.50	111.90
1	A	1527	C	C6-N1-C2	-7.21	117.42	120.30
33	a	362	G	O5'-P-OP1	-7.20	99.22	105.70
33	a	1070	U	C5-C6-N1	7.19	126.30	122.70
1	A	2386	U	O5'-P-OP1	-7.19	99.23	105.70
33	a	1175	G	OP1-P-O3'	-7.17	89.42	105.20
1	A	8	U	C2-N1-C1'	7.17	126.30	117.70
1	A	1941	A	N7-C8-N9	7.16	117.38	113.80
20	V	393	LEU	CA-CB-CG	7.15	131.74	115.30
1	A	2485	C	C6-N1-C2	-7.13	117.45	120.30
1	A	2323	C	C2-N1-C1'	7.13	126.64	118.80
2	B	41	C	C5-C6-N1	7.13	124.56	121.00
53	x	62	C	P-O3'-C3'	7.13	128.25	119.70
10	L	79	LEU	CA-CB-CG	7.12	131.68	115.30
1	A	2918	G	C8-N9-C1'	-7.12	117.75	127.00
1	A	1369	C	C2-N1-C1'	7.11	126.62	118.80
1	A	2345	U	C5-C6-N1	7.11	126.26	122.70
53	x	22	A	P-O3'-C3'	7.10	128.22	119.70
1	A	831	U	N1-C2-O2	7.08	127.76	122.80
1	A	1244	A	OP1-P-O3'	7.08	120.77	105.20
33	a	1421	C	C6-N1-C2	-7.07	117.47	120.30
1	A	1244	A	O4'-C1'-N9	7.07	113.86	108.20
33	a	143	C	N1-C2-O2	7.05	123.13	118.90
1	A	1817	C	C6-N1-C2	-7.05	117.48	120.30
1	A	2094	C	C6-N1-C2	-7.04	117.48	120.30
33	a	271	A	C8-N9-C4	-7.04	102.98	105.80
2	B	28	C	N1-C2-O2	7.04	123.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2054	C	C2-N1-C1'	7.03	126.53	118.80
1	A	2105	U	N3-C2-O2	-7.03	117.28	122.20
1	A	284	C	C6-N1-C2	-7.02	117.49	120.30
1	A	2131	U	C5-C6-N1	7.01	126.21	122.70
1	A	1831	A	C8-N9-C4	-7.01	103.00	105.80
2	B	24	C	C6-N1-C2	-6.98	117.51	120.30
33	a	1287	C	N1-C2-O2	6.98	123.09	118.90
46	n	3	LYS	CD-CE-NZ	-6.98	95.65	111.70
53	x	69	C	C5-C6-N1	6.97	124.49	121.00
1	A	422	C	C2-N1-C1'	6.97	126.47	118.80
1	A	1366	C	C2-N1-C1'	6.96	126.46	118.80
1	A	1559	C	N3-C2-O2	-6.96	117.03	121.90
1	A	1817	C	C5-C6-N1	6.95	124.48	121.00
33	a	143	C	C6-N1-C2	-6.95	117.52	120.30
33	a	486	C	C2-N1-C1'	6.95	126.44	118.80
1	A	1527	C	C6-N1-C1'	-6.94	112.47	120.80
33	a	1463	A	O5'-P-OP2	-6.94	99.46	105.70
1	A	2648	U	N3-C2-O2	-6.93	117.35	122.20
2	B	29	C	C2-N1-C1'	6.93	126.42	118.80
1	A	1028	C	C2-N1-C1'	6.93	126.42	118.80
16	R	48	VAL	CG1-CB-CG2	6.92	121.98	110.90
1	A	2795	G	N3-C4-C5	-6.92	125.14	128.60
33	a	280	C	N1-C2-O2	6.91	123.04	118.90
33	a	1305	C	N1-C2-O2	6.91	123.04	118.90
1	A	2035	C	C6-N1-C2	-6.90	117.54	120.30
33	a	1391	C	N1-C2-O2	6.89	123.04	118.90
1	A	422	C	C5-C6-N1	6.89	124.45	121.00
2	B	24	C	C5-C6-N1	6.89	124.44	121.00
33	a	465	U	N3-C2-O2	-6.88	117.38	122.20
1	A	1545	C	C2-N1-C1'	6.88	126.36	118.80
1	A	8	U	C5-C6-N1	6.87	126.14	122.70
1	A	2822	C	C6-N1-C2	-6.86	117.56	120.30
1	A	1803	C	C6-N1-C2	-6.86	117.56	120.30
1	A	1942	A	C6-C5-N7	6.86	137.10	132.30
1	A	2157	C	C2-N1-C1'	6.86	126.34	118.80
1	A	2503	C	C6-N1-C2	-6.84	117.56	120.30
1	A	2255	C	N3-C2-O2	-6.83	117.12	121.90
2	B	15	C	C2-N1-C1'	6.83	126.31	118.80
1	A	1122	C	C6-N1-C2	-6.82	117.57	120.30
1	A	442	C	C2-N3-C4	6.81	123.30	119.90
33	a	1036	C	C5-C6-N1	6.81	124.40	121.00
33	a	1010	U	N3-C2-O2	-6.80	117.44	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1942	A	C8-N9-C4	6.80	108.52	105.80
1	A	924	U	C5-C6-N1	6.79	126.10	122.70
1	A	914	C	C6-N1-C2	-6.78	117.59	120.30
1	A	2471	C	C6-N1-C2	-6.77	117.59	120.30
49	q	76	ARG	NE-CZ-NH2	-6.75	116.92	120.30
33	a	853	C	N3-C2-O2	-6.73	117.19	121.90
1	A	769	A	C5-C6-N6	6.73	129.08	123.70
44	l	44	ARG	CA-CB-CG	6.73	128.20	113.40
1	A	2223	U	N3-C2-O2	-6.72	117.50	122.20
1	A	2350	G	N3-C4-N9	6.71	130.03	126.00
1	A	2432	C	C6-N1-C2	-6.70	117.62	120.30
1	A	92	G	N9-C4-C5	-6.70	102.72	105.40
1	A	631	G	N3-C2-N2	-6.69	115.22	119.90
1	A	1941	A	C4-N9-C1'	6.68	138.32	126.30
1	A	508	C	C5-C6-N1	6.67	124.33	121.00
1	A	633	U	C5-C6-N1	6.67	126.03	122.70
1	A	1247	G	O4'-C1'-N9	6.67	113.53	108.20
1	A	1328	C	N1-C2-O2	6.67	122.90	118.90
21	W	28	ARG	CB-CG-CD	6.66	128.93	111.60
1	A	445	C	C5-C6-N1	6.66	124.33	121.00
1	A	1963	C	N3-C2-O2	-6.65	117.24	121.90
1	A	830	A	C5-N7-C8	-6.65	100.58	103.90
1	A	1559	C	N1-C2-O2	6.64	122.88	118.90
1	A	2092	C	N1-C2-O2	6.64	122.88	118.90
1	A	670	C	C5-C6-N1	6.62	124.31	121.00
1	A	1352	U	N3-C2-O2	-6.62	117.57	122.20
2	B	28	C	N3-C2-O2	-6.61	117.27	121.90
1	A	2316	A	P-O3'-C3'	6.61	127.63	119.70
1	A	2102	C	C6-N1-C2	-6.60	117.66	120.30
53	x	53	G	N9-C4-C5	-6.60	102.76	105.40
53	x	69	C	C2-N1-C1'	6.60	126.06	118.80
33	a	1176	A	O5'-C5'-C4'	6.59	124.22	111.70
1	A	1327	U	N3-C2-O2	-6.58	117.59	122.20
1	A	1028	C	N3-C2-O2	-6.58	117.29	121.90
53	x	53	G	C8-N9-C1'	-6.58	118.45	127.00
1	A	1757	G	O4'-C1'-N9	6.57	113.46	108.20
1	A	1570	U	OP2-P-O3'	6.56	119.64	105.20
33	a	1037	C	N3-C2-O2	-6.56	117.31	121.90
1	A	2833	U	N3-C2-O2	-6.56	117.61	122.20
1	A	1339	A	P-O3'-C3'	6.55	127.56	119.70
1	A	430	C	N3-C2-O2	-6.55	117.32	121.90
1	A	554	U	P-O3'-C3'	6.54	127.55	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1712	G	C4-N9-C1'	6.54	135.00	126.50
1	A	933	C	P-O3'-C3'	6.54	127.54	119.70
6	F	136	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	662	U	C5-C6-N1	6.53	125.96	122.70
33	a	39	U	N3-C2-O2	-6.51	117.64	122.20
1	A	2202	A	O4'-C1'-N9	6.50	113.40	108.20
1	A	573	C	C2-N1-C1'	6.50	125.95	118.80
1	A	2752	C	C6-N1-C2	-6.49	117.70	120.30
33	a	1525	C	C5-C6-N1	6.48	124.24	121.00
1	A	62	C	P-O3'-C3'	6.48	127.48	119.70
1	A	1036	A	N7-C8-N9	6.48	117.04	113.80
33	a	1468	C	O5'-P-OP1	-6.48	99.87	105.70
1	A	2295	A	OP2-P-O3'	6.47	119.45	105.20
1	A	1828	G	P-O3'-C3'	6.46	127.46	119.70
1	A	2675	C	C5-C6-N1	6.46	124.23	121.00
33	a	993	A	N3-C4-N9	6.46	132.57	127.40
33	a	1438	C	N1-C2-O2	6.46	122.78	118.90
1	A	2094	C	C5-C6-N1	6.46	124.23	121.00
33	a	459	A	P-O3'-C3'	6.46	127.45	119.70
1	A	1792	G	O5'-P-OP2	-6.45	99.89	105.70
1	A	1237	C	N3-C2-O2	-6.45	117.38	121.90
1	A	1527	C	N3-C2-O2	-6.45	117.39	121.90
1	A	719	C	C6-N1-C2	-6.44	117.72	120.30
1	A	1804	U	N3-C2-O2	-6.44	117.69	122.20
1	A	2371	C	C5-C6-N1	6.43	124.22	121.00
1	A	2765	G	N3-C4-N9	6.43	129.86	126.00
1	A	2254	A	P-O3'-C3'	6.43	127.42	119.70
1	A	2774	C	C2-N1-C1'	6.43	125.87	118.80
1	A	778	C	N1-C2-O2	6.42	122.75	118.90
2	B	61	U	C2-N1-C1'	6.42	125.41	117.70
33	a	1111	A	P-O3'-C3'	6.42	127.40	119.70
33	a	372	A	OP1-P-O3'	6.41	119.30	105.20
15	Q	103	LEU	CA-CB-CG	6.41	130.03	115.30
1	A	2243	C	C2-N1-C1'	6.40	125.84	118.80
1	A	2911	G	N7-C8-N9	6.39	116.30	113.10
1	A	1731	C	N1-C2-O2	6.39	122.74	118.90
1	A	2768	U	N1-C2-O2	6.38	127.27	122.80
33	a	1158	C	C6-N1-C2	-6.38	117.75	120.30
33	a	271	A	N7-C8-N9	6.38	116.99	113.80
1	A	482	C	O4'-C1'-N1	6.37	113.29	108.20
33	a	1149	U	N1-C2-O2	6.36	127.25	122.80
1	A	445	C	C6-N1-C2	-6.36	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2503	C	N3-C2-O2	-6.36	117.45	121.90
1	A	875	U	C2-N1-C1'	6.36	125.33	117.70
31	7	25	C	N1-C2-O2	6.35	122.71	118.90
1	A	1771	C	C2-N1-C1'	6.35	125.78	118.80
1	A	502	C	O5'-P-OP2	-6.34	100.00	105.70
1	A	635	C	C6-N1-C2	-6.34	117.76	120.30
1	A	589	G	C6-C5-N7	6.33	134.20	130.40
1	A	2739	C	C6-N1-C2	-6.33	117.77	120.30
1	A	716	G	C4-N9-C1'	6.33	134.73	126.50
2	B	15	C	C6-N1-C2	-6.33	117.77	120.30
1	A	2350	G	C8-N9-C4	-6.33	103.87	106.40
1	A	2665	U	N3-C2-O2	-6.33	117.77	122.20
1	A	735	U	C5-C4-O4	-6.32	122.11	125.90
1	A	1771	C	C6-N1-C2	-6.32	117.77	120.30
33	a	264	U	C5-C6-N1	6.32	125.86	122.70
1	A	1476	C	N1-C2-O2	6.32	122.69	118.90
1	A	716	G	C8-N9-C1'	-6.31	118.80	127.00
1	A	2695	C	C2-N1-C1'	6.31	125.74	118.80
33	a	747	U	C5-C6-N1	6.31	125.85	122.70
33	a	1460	U	N1-C2-O2	6.29	127.20	122.80
1	A	1450	C	N1-C2-O2	6.29	122.67	118.90
2	B	62	U	C6-N1-C1'	-6.29	112.39	121.20
22	X	39	LEU	CA-CB-CG	6.29	129.76	115.30
1	A	1353	C	N1-C2-O2	6.29	122.67	118.90
33	a	1438	C	C6-N1-C2	-6.28	117.79	120.30
1	A	299	U	N3-C2-O2	-6.28	117.80	122.20
53	x	69	C	C6-N1-C2	-6.28	117.79	120.30
1	A	1296	G	C4-N9-C1'	6.28	134.66	126.50
1	A	2223	U	N1-C2-O2	6.28	127.19	122.80
33	a	467	C	C6-N1-C2	-6.28	117.79	120.30
33	a	537	C	C2-N1-C1'	6.27	125.69	118.80
1	A	588	C	C2-N1-C1'	6.26	125.69	118.80
1	A	1450	C	C6-N1-C2	-6.26	117.80	120.30
1	A	397	U	C2-N1-C1'	6.26	125.21	117.70
1	A	776	G	C4-N9-C1'	6.25	134.63	126.50
33	a	92	U	OP1-P-O3'	6.25	118.95	105.20
1	A	2157	C	C5-C6-N1	6.25	124.12	121.00
2	B	59	U	N3-C2-O2	-6.25	117.83	122.20
33	a	1391	C	C2-N1-C1'	6.24	125.67	118.80
1	A	2822	C	C6-N1-C1'	-6.24	113.31	120.80
33	a	119	C	O5'-P-OP1	-6.24	100.08	105.70
1	A	1712	G	N9-C1'-C2'	6.24	122.11	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	460	A	C2-N3-C4	6.24	113.72	110.60
1	A	2422	U	N1-C2-O2	6.23	127.16	122.80
1	A	589	G	N3-C4-C5	6.23	131.71	128.60
1	A	152	C	C6-N1-C2	-6.23	117.81	120.30
1	A	1352	U	N1-C2-O2	6.23	127.16	122.80
1	A	233	G	O4'-C1'-N9	6.22	113.18	108.20
1	A	1712	G	C8-N9-C1'	-6.22	118.91	127.00
33	a	476	U	C2-N1-C1'	6.22	125.17	117.70
1	A	2207	C	C6-N1-C2	-6.22	117.81	120.30
33	a	1036	C	C6-N1-C2	-6.22	117.81	120.30
1	A	1353	C	C6-N1-C1'	-6.21	113.34	120.80
1	A	2092	C	C2-N1-C1'	6.21	125.64	118.80
1	A	1448	U	N3-C2-O2	-6.21	117.85	122.20
33	a	970	U	C2-N1-C1'	6.21	125.15	117.70
33	a	1210	A	OP2-P-O3'	6.21	118.85	105.20
1	A	975	C	C2-N1-C1'	6.20	125.62	118.80
33	a	1148	G	P-O3'-C3'	6.20	127.14	119.70
33	a	21	C	C6-N1-C2	-6.20	117.82	120.30
33	a	763	C	C2-N1-C1'	6.19	125.61	118.80
1	A	76	C	OP1-P-OP2	-6.18	110.33	119.60
1	A	2805	A	P-O3'-C3'	6.18	127.12	119.70
33	a	1041	C	OP2-P-O3'	6.17	118.78	105.20
1	A	2035	C	C5-C6-N1	6.17	124.09	121.00
1	A	789	C	C6-N1-C2	-6.17	117.83	120.30
33	a	758	A	N7-C8-N9	6.17	116.89	113.80
33	a	1008	C	C2-N1-C1'	6.17	125.59	118.80
2	B	62	U	N1-C2-O2	6.17	127.12	122.80
1	A	1567	U	OP1-P-O3'	6.17	118.76	105.20
1	A	1831	A	O4'-C1'-N9	6.17	113.13	108.20
33	a	1170	C	N3-C2-O2	-6.17	117.58	121.90
1	A	2467	U	OP2-P-O3'	6.16	118.76	105.20
1	A	1671	G	C8-N9-C4	-6.16	103.94	106.40
33	a	319	C	C6-N1-C2	-6.16	117.84	120.30
17	S	38	LEU	C-N-CA	6.15	137.07	121.70
1	A	1634	U	N1-C2-O2	6.14	127.10	122.80
33	a	1210	A	P-O3'-C3'	6.14	127.07	119.70
1	A	1656	C	N3-C2-O2	-6.14	117.60	121.90
1	A	872	C	C6-N1-C2	-6.14	117.84	120.30
1	A	1702	U	O5'-P-OP1	-6.13	100.18	105.70
1	A	1631	A	N7-C8-N9	6.13	116.86	113.80
1	A	2065	C	C5-C6-N1	6.12	124.06	121.00
33	a	336	C	N1-C2-O2	6.12	122.57	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2092	C	C6-N1-C2	-6.12	117.85	120.30
1	A	1527	C	P-O3'-C3'	6.11	127.03	119.70
33	a	942	C	C6-N1-C2	-6.11	117.86	120.30
1	A	1545	C	C5-C6-N1	6.11	124.06	121.00
1	A	2350	G	C8-N9-C1'	-6.11	119.06	127.00
1	A	977	U	C5-C6-N1	6.11	125.75	122.70
1	A	810	G	OP1-P-O3'	6.10	118.63	105.20
1	A	1707	U	N1-C2-O2	6.10	127.07	122.80
1	A	885	C	N1-C2-O2	6.10	122.56	118.90
1	A	2791	U	C5-C6-N1	6.10	125.75	122.70
1	A	2055	U	C5-C6-N1	6.10	125.75	122.70
53	x	53	G	C4-C5-N7	6.10	113.24	110.80
1	A	1045	U	N3-C2-O2	-6.09	117.94	122.20
1	A	62	C	OP2-P-O3'	6.08	118.58	105.20
1	A	885	C	C6-N1-C2	-6.07	117.87	120.30
1	A	936	C	C2-N1-C1'	6.07	125.48	118.80
1	A	2685	U	C2-N1-C1'	6.07	124.98	117.70
33	a	591	C	N1-C2-O2	6.07	122.54	118.90
53	x	21	G	N3-C4-C5	-6.07	125.57	128.60
1	A	972	U	C5-C6-N1	6.06	125.73	122.70
1	A	980	C	C5-C6-N1	6.06	124.03	121.00
9	K	89	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	1067	A	C8-N9-C4	-6.05	103.38	105.80
1	A	2423	C	N1-C2-O2	6.05	122.53	118.90
33	a	1331	C	C6-N1-C2	-6.05	117.88	120.30
33	a	1020	C	C6-N1-C2	-6.05	117.88	120.30
33	a	1110	C	C6-N1-C2	-6.05	117.88	120.30
33	a	468	C	C6-N1-C2	-6.05	117.88	120.30
2	B	59	U	C5-C6-N1	6.04	125.72	122.70
33	a	87	C	N1-C2-O2	6.04	122.52	118.90
1	A	1122	C	N3-C2-O2	-6.03	117.68	121.90
1	A	1307	U	N1-C2-O2	6.03	127.02	122.80
1	A	1771	C	C5-C6-N1	6.03	124.02	121.00
33	a	1457	C	C2-N1-C1'	6.03	125.44	118.80
1	A	2620	C	C6-N1-C2	-6.03	117.89	120.30
33	a	86	G	N7-C8-N9	6.03	116.12	113.10
33	a	85	U	C2-N1-C1'	6.03	124.94	117.70
33	a	1439	C	C6-N1-C2	-6.03	117.89	120.30
33	a	167	G	C6-C5-N7	-6.03	126.78	130.40
1	A	2023	C	C6-N1-C2	-6.02	117.89	120.30
53	x	53	G	C4-N9-C1'	6.02	134.33	126.50
53	x	21	G	N3-C4-N9	6.01	129.61	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2189	G	C8-N9-C1'	-6.01	119.19	127.00
33	a	1391	C	C6-N1-C2	-6.00	117.90	120.30
33	a	413	U	C5-C6-N1	6.00	125.70	122.70
33	a	171	A	C8-N9-C4	-6.00	103.40	105.80
53	x	38	U	N3-C2-O2	-5.99	118.00	122.20
53	x	53	G	C6-C5-N7	-5.99	126.80	130.40
1	A	2503	C	N1-C2-O2	5.99	122.49	118.90
33	a	1463	A	P-O3'-C3'	5.99	126.89	119.70
33	a	1390	U	N1-C2-O2	5.99	126.99	122.80
1	A	1067	A	C2-N3-C4	-5.99	107.61	110.60
1	A	442	C	N1-C2-O2	5.98	122.49	118.90
1	A	2795	G	N3-C4-N9	5.98	129.59	126.00
33	a	856	C	C6-N1-C2	-5.98	117.91	120.30
53	x	21	G	C8-N9-C1'	-5.97	119.24	127.00
1	A	1305	A	P-O3'-C3'	5.97	126.86	119.70
1	A	1339	A	OP2-P-O3'	5.97	118.33	105.20
33	a	537	C	N1-C2-O2	5.97	122.48	118.90
1	A	1353	C	C5-C6-N1	5.96	123.98	121.00
1	A	2749	U	N3-C2-O2	-5.96	118.03	122.20
33	a	632	C	C5-C6-N1	5.96	123.98	121.00
1	A	1237	C	N1-C2-O2	5.95	122.47	118.90
33	a	101	C	C6-N1-C2	-5.95	117.92	120.30
1	A	1450	C	N3-C2-O2	-5.95	117.73	121.90
20	V	389	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	46	C	O5'-P-OP2	-5.95	100.35	105.70
33	a	476	U	N1-C2-O2	5.94	126.96	122.80
1	A	1397	G	OP2-P-O3'	5.94	118.27	105.20
1	A	1631	A	C8-N9-C4	-5.94	103.42	105.80
1	A	2452	U	OP2-P-O3'	5.94	118.27	105.20
1	A	2454	A	OP2-P-O3'	5.94	118.26	105.20
1	A	2114	C	C5-C6-N1	5.93	123.97	121.00
1	A	2604	C	C6-N1-C2	-5.93	117.93	120.30
33	a	1441	G	O5'-P-OP1	-5.93	100.36	105.70
33	a	993	A	N3-C4-C5	-5.92	122.65	126.80
1	A	2155	A	P-O3'-C3'	5.92	126.80	119.70
33	a	1024	A	O5'-P-OP2	-5.91	100.39	105.70
1	A	1353	C	C6-N1-C2	-5.90	117.94	120.30
33	a	537	C	C6-N1-C2	-5.90	117.94	120.30
53	x	38	U	N1-C2-O2	5.90	126.93	122.80
1	A	186	C	O5'-P-OP1	-5.90	100.39	105.70
1	A	1307	U	N3-C2-O2	-5.89	118.07	122.20
1	A	1781	C	C5-C6-N1	5.89	123.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2712	C	N1-C2-O2	5.89	122.44	118.90
1	A	783	C	C5-C6-N1	5.88	123.94	121.00
1	A	936	C	N1-C2-O2	5.88	122.43	118.90
33	a	136	U	C2-N1-C1'	5.88	124.75	117.70
33	a	168	C	N3-C2-O2	-5.87	117.79	121.90
1	A	1963	C	N1-C2-O2	5.87	122.42	118.90
1	A	2749	U	N1-C2-O2	5.87	126.91	122.80
33	a	1237	C	N1-C2-O2	5.87	122.42	118.90
1	A	588	C	N3-C2-O2	-5.87	117.79	121.90
1	A	1507	U	OP2-P-O3'	5.87	118.11	105.20
1	A	430	C	N1-C2-O2	5.87	122.42	118.90
1	A	2092	C	N3-C2-O2	-5.86	117.80	121.90
1	A	1883	A	C8-N9-C4	-5.86	103.46	105.80
1	A	1631	A	P-O3'-C3'	5.86	126.73	119.70
1	A	2388	C	C6-N1-C2	-5.86	117.96	120.30
33	a	411	C	C6-N1-C2	-5.86	117.96	120.30
33	a	1331	C	C6-N1-C1'	-5.85	113.78	120.80
1	A	2833	U	N1-C2-O2	5.85	126.89	122.80
1	A	2459	A	O4'-C1'-N9	5.85	112.88	108.20
1	A	1626	U	N3-C2-O2	-5.84	118.11	122.20
1	A	2685	U	N3-C2-O2	-5.84	118.11	122.20
2	B	58	C	C6-N1-C2	-5.84	117.96	120.30
1	A	573	C	N3-C2-O2	-5.84	117.81	121.90
5	E	38	LEU	CB-CG-CD1	-5.84	101.08	111.00
1	A	2605	G	C4-N9-C1'	5.84	134.09	126.50
1	A	2665	U	N1-C2-O2	5.84	126.89	122.80
1	A	940	G	N7-C8-N9	5.83	116.02	113.10
33	a	591	C	N3-C2-O2	-5.83	117.82	121.90
1	A	1454	C	N3-C2-O2	-5.83	117.82	121.90
1	A	406	G	N3-C4-N9	-5.83	122.50	126.00
1	A	1560	U	C2-N1-C1'	5.83	124.69	117.70
1	A	975	C	C5-C6-N1	5.82	123.91	121.00
1	A	309	U	OP1-P-O3'	5.82	118.00	105.20
1	A	954	U	C5-C6-N1	5.82	125.61	122.70
33	a	260	U	N3-C2-O2	-5.82	118.13	122.20
33	a	1363	C	C6-N1-C2	-5.82	117.97	120.30
1	A	1942	A	C4-C5-C6	-5.82	114.09	117.00
1	A	1981	A	N7-C8-N9	5.81	116.71	113.80
1	A	2911	G	C8-N9-C4	-5.81	104.08	106.40
1	A	113	U	C2-N1-C1'	5.81	124.67	117.70
1	A	2054	C	C4-C5-C6	-5.80	114.50	117.40
1	A	1800	C	C6-N1-C2	-5.80	117.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	523	C	C5-C6-N1	5.80	123.90	121.00
1	A	980	C	N1-C2-O2	5.80	122.38	118.90
33	a	1416	C	N1-C2-O2	5.80	122.38	118.90
1	A	810	G	C4-N9-C1'	5.80	134.04	126.50
1	A	2114	C	C6-N1-C2	-5.80	117.98	120.30
1	A	2685	U	C5-C6-N1	5.79	125.60	122.70
1	A	2840	C	C6-N1-C2	-5.79	117.98	120.30
1	A	2813	U	C5-C6-N1	5.79	125.59	122.70
33	a	1150	U	C2-N1-C1'	5.78	124.64	117.70
10	L	18	ARG	CA-CB-CG	5.78	126.12	113.40
33	a	130	C	C5-C6-N1	5.78	123.89	121.00
33	a	1305	C	C6-N1-C2	-5.78	117.99	120.30
1	A	2665	U	C2-N1-C1'	5.77	124.63	117.70
1	A	885	C	N3-C2-O2	-5.77	117.86	121.90
1	A	2591	U	N3-C2-O2	-5.77	118.16	122.20
1	A	2295	A	P-O3'-C3'	5.76	126.62	119.70
33	a	280	C	N3-C2-O2	-5.76	117.86	121.90
1	A	2072	C	C5-C6-N1	5.76	123.88	121.00
33	a	859	C	N3-C2-O2	-5.76	117.87	121.90
1	A	860	U	N3-C2-O2	-5.75	118.17	122.20
33	a	1391	C	C5-C6-N1	5.75	123.88	121.00
1	A	1781	C	C6-N1-C2	-5.75	118.00	120.30
1	A	2105	U	C6-N1-C1'	-5.75	113.15	121.20
1	A	2192	U	N1-C2-O2	5.75	126.83	122.80
1	A	2785	U	O4'-C1'-N1	5.75	112.80	108.20
33	a	448	U	N1-C2-O2	5.75	126.83	122.80
1	A	1156	G	C8-N9-C4	-5.75	104.10	106.40
1	A	1351	U	P-O3'-C3'	5.75	126.60	119.70
1	A	631	G	N1-C2-N2	5.75	121.37	116.20
33	a	970	U	N1-C2-O2	5.75	126.82	122.80
1	A	1770	C	C6-N1-C2	-5.74	118.00	120.30
1	A	576	G	P-O3'-C3'	5.74	126.59	119.70
44	l	44	ARG	N-CA-CB	5.74	120.93	110.60
1	A	1941	A	C8-N9-C1'	-5.74	117.37	127.70
1	A	1942	A	C4-N9-C1'	-5.74	115.97	126.30
1	A	2445	C	C5-C6-N1	5.74	123.87	121.00
33	a	467	C	C2-N1-C1'	5.73	125.11	118.80
33	a	746	C	C5-C6-N1	5.73	123.87	121.00
1	A	211	C	C5-C6-N1	5.73	123.86	121.00
1	A	508	C	N3-C2-O2	-5.73	117.89	121.90
33	a	86	G	C8-N9-C4	-5.72	104.11	106.40
1	A	2605	G	C8-N9-C1'	-5.72	119.56	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	1416	C	N3-C2-O2	-5.72	117.90	121.90
1	A	1883	A	N7-C8-N9	5.71	116.66	113.80
33	a	1421	C	C5-C6-N1	5.71	123.85	121.00
53	x	61	C	C5-C6-N1	5.71	123.85	121.00
1	A	2203	C	N1-C2-O2	5.71	122.32	118.90
1	A	2733	C	C6-N1-C2	-5.71	118.02	120.30
2	B	79	C	N3-C2-O2	-5.70	117.91	121.90
33	a	856	C	C5-C6-N1	5.70	123.85	121.00
1	A	86	C	O4'-C1'-N1	5.69	112.75	108.20
1	A	2126	G	C4-N9-C1'	5.69	133.90	126.50
1	A	842	C	C5-C6-N1	5.69	123.84	121.00
1	A	252	C	OP2-P-O3'	5.68	117.71	105.20
1	A	2765	G	C4-C5-N7	5.68	113.07	110.80
2	B	28	C	C6-N1-C2	-5.68	118.03	120.30
33	a	1398	C	C5-C6-N1	5.68	123.84	121.00
33	a	1502	A	N3-C4-C5	-5.68	122.82	126.80
1	A	966	U	N1-C2-O2	5.68	126.78	122.80
1	A	1415	C	N3-C2-O2	-5.68	117.92	121.90
1	A	924	U	C6-N1-C2	-5.67	117.59	121.00
1	A	212	C	N1-C2-O2	5.67	122.30	118.90
1	A	1339	A	O4'-C1'-N9	-5.67	103.66	108.20
1	A	308	C	C2-N1-C1'	5.67	125.04	118.80
33	a	675	G	O5'-P-OP2	-5.67	100.60	105.70
1	A	1052	C	C6-N1-C2	-5.66	118.03	120.30
1	A	2335	U	N1-C2-O2	5.66	126.76	122.80
33	a	86	G	C6-C5-N7	-5.66	127.00	130.40
1	A	2349	A	C2-N3-C4	5.66	113.43	110.60
1	A	246	U	N1-C2-O2	5.66	126.76	122.80
1	A	716	G	C4-C5-N7	5.66	113.06	110.80
33	a	1045	G	P-O3'-C3'	-5.66	112.91	119.70
1	A	549	A	OP2-P-O3'	5.65	117.64	105.20
1	A	1137	G	C4-N9-C1'	5.65	133.85	126.50
1	A	1631	A	OP1-P-O3'	5.65	117.63	105.20
1	A	1369	C	C6-N1-C2	-5.65	118.04	120.30
1	A	574	A	C5-N7-C8	-5.65	101.08	103.90
1	A	1634	U	N3-C2-O2	-5.64	118.25	122.20
1	A	221	G	N3-C2-N2	-5.64	115.95	119.90
1	A	284	C	C2-N1-C1'	5.64	125.00	118.80
33	a	1237	C	N3-C2-O2	-5.64	117.95	121.90
1	A	1122	C	C5-C6-N1	5.63	123.82	121.00
1	A	1329	C	C5-C6-N1	5.63	123.82	121.00
1	A	586	C	N3-C2-O2	-5.63	117.96	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1771	C	N3-C2-O2	-5.63	117.96	121.90
1	A	2711	G	O5'-P-OP2	-5.63	100.64	105.70
1	A	4	U	C5-C6-N1	5.62	125.51	122.70
1	A	914	C	N3-C2-O2	-5.62	117.96	121.90
1	A	1507	U	P-O3'-C3'	5.62	126.45	119.70
1	A	2801	C	N3-C2-O2	-5.62	117.97	121.90
33	a	1003	G	N3-C4-N9	5.62	129.37	126.00
53	x	21	G	N7-C8-N9	5.62	115.91	113.10
1	A	506	U	N1-C2-O2	5.61	126.73	122.80
1	A	2791	U	C2-N1-C1'	5.61	124.43	117.70
1	A	977	U	C6-N1-C2	-5.61	117.64	121.00
1	A	1333	C	C2-N1-C1'	5.60	124.96	118.80
1	A	104	C	N3-C2-O2	-5.60	117.98	121.90
1	A	2904	A	OP2-P-O3'	5.60	117.52	105.20
33	a	641	G	C8-N9-C4	-5.60	104.16	106.40
1	A	776	G	C8-N9-C1'	-5.59	119.73	127.00
1	A	1613	C	C6-N1-C2	-5.59	118.06	120.30
1	A	2422	U	N3-C2-O2	-5.59	118.29	122.20
1	A	422	C	C6-N1-C2	-5.59	118.06	120.30
1	A	2189	G	C4-N9-C1'	5.59	133.77	126.50
1	A	2225	C	N1-C2-O2	5.59	122.25	118.90
1	A	686	C	C5-C6-N1	5.59	123.79	121.00
41	i	122	ARG	CB-CG-CD	5.59	126.13	111.60
1	A	895	G	N3-C4-C5	-5.58	125.81	128.60
1	A	966	U	N3-C2-O2	-5.58	118.29	122.20
33	a	735	C	C6-N1-C2	-5.58	118.07	120.30
33	a	1032	C	P-O3'-C3'	5.58	126.40	119.70
1	A	556	C	N1-C2-O2	5.58	122.25	118.90
1	A	1942	A	N1-C6-N6	-5.58	115.25	118.60
33	a	274	G	O4'-C1'-N9	-5.58	103.74	108.20
1	A	1695	A	C8-N9-C4	5.58	108.03	105.80
33	a	56	C	N1-C2-O2	5.58	122.25	118.90
1	A	1365	U	N1-C1'-C2'	-5.57	105.87	112.00
33	a	472	C	C6-N1-C2	-5.57	118.07	120.30
33	a	1460	U	N3-C2-O2	-5.57	118.30	122.20
1	A	88	G	P-O3'-C3'	5.57	126.38	119.70
33	a	829	U	OP2-P-O3'	5.57	117.45	105.20
1	A	63	G	OP1-P-OP2	-5.57	111.25	119.60
1	A	1753	C	C6-N1-C2	-5.57	118.07	120.30
1	A	1296	G	C8-N9-C1'	-5.56	119.77	127.00
33	a	465	U	C5-C6-N1	5.56	125.48	122.70
1	A	1374	C	N3-C2-O2	-5.56	118.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	236	A	C3'-C2'-C1'	5.56	105.94	101.50
1	A	464	C	C5-C6-N1	5.56	123.78	121.00
33	a	130	C	N1-C2-O2	5.55	122.23	118.90
33	a	167	G	C4-N9-C1'	5.55	133.72	126.50
1	A	1622	C	C5-C6-N1	5.55	123.78	121.00
1	A	2840	C	C5-C6-N1	5.55	123.77	121.00
1	A	1953	C	C2-N1-C1'	5.54	124.90	118.80
1	A	681	C	C5-C6-N1	5.54	123.77	121.00
1	A	2177	G	C8-N9-C4	-5.54	104.18	106.40
33	a	60	C	N1-C2-O2	5.54	122.23	118.90
33	a	1032	C	C6-N1-C2	-5.54	118.08	120.30
33	a	901	U	N1-C2-O2	5.54	126.68	122.80
33	a	182	U	N1-C2-O2	5.54	126.68	122.80
33	a	1167	C	C2-N1-C1'	5.54	124.89	118.80
53	x	43	G	N1-C6-O6	-5.54	116.58	119.90
1	A	2323	C	C5-C6-N1	5.53	123.77	121.00
33	a	481	C	C6-N1-C2	-5.53	118.09	120.30
1	A	2821	U	N3-C2-O2	-5.53	118.33	122.20
33	a	1123	C	C6-N1-C2	-5.53	118.09	120.30
1	A	308	C	C6-N1-C2	-5.53	118.09	120.30
1	A	483	C	C2-N1-C1'	5.53	124.88	118.80
1	A	533	C	C6-N1-C2	-5.53	118.09	120.30
33	a	1041	C	P-O3'-C3'	5.53	126.33	119.70
1	A	1369	C	N1-C2-O2	5.53	122.22	118.90
20	V	428	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	1567	U	P-O3'-C3'	5.52	126.32	119.70
5	E	126	LEU	CB-CG-CD1	-5.52	101.62	111.00
33	a	1016	A	P-O3'-C3'	5.52	126.32	119.70
2	B	72	U	N3-C2-O2	-5.51	118.34	122.20
33	a	143	C	C2-N1-C1'	5.51	124.87	118.80
1	A	66	C	N1-C2-O2	5.51	122.21	118.90
1	A	1352	U	C6-N1-C1'	-5.51	113.48	121.20
1	A	1545	C	C6-N1-C2	-5.51	118.09	120.30
1	A	1328	C	N3-C2-O2	-5.51	118.04	121.90
1	A	1522	U	N1-C2-O2	5.51	126.66	122.80
1	A	211	C	C6-N1-C2	-5.51	118.10	120.30
1	A	1245	G	OP1-P-OP2	-5.51	111.34	119.60
1	A	1052	C	C5-C6-N1	5.51	123.75	121.00
1	A	187	C	O4'-C1'-N1	5.50	112.60	108.20
1	A	2255	C	C6-N1-C2	-5.50	118.10	120.30
1	A	1476	C	N3-C2-O2	-5.50	118.05	121.90
1	A	1379	U	N3-C2-O2	-5.50	118.35	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1946	U	C5-C6-N1	5.50	125.45	122.70
34	b	18	HIS	C-N-CA	5.50	135.44	121.70
1	A	1813	A	P-O3'-C3'	5.50	126.30	119.70
1	A	1577	C	N1-C2-O2	5.49	122.19	118.90
1	A	2025	C	C6-N1-C2	-5.49	118.11	120.30
1	A	2155	A	OP2-P-O3'	5.49	117.27	105.20
1	A	1573	C	N1-C2-O2	5.48	122.19	118.90
33	a	248	C	O4'-C1'-N1	5.48	112.58	108.20
1	A	940	G	C8-N9-C4	-5.47	104.21	106.40
1	A	843	C	N1-C2-O2	5.47	122.18	118.90
1	A	2273	U	N3-C4-O4	5.47	123.23	119.40
53	x	6	G	O5'-P-OP1	5.47	117.26	110.70
33	a	1398	C	C2-N1-C1'	5.47	124.81	118.80
1	A	252	C	P-O3'-C3'	5.46	126.26	119.70
1	A	1325	A	C4-C5-C6	-5.46	114.27	117.00
33	a	989	C	C6-N1-C2	-5.46	118.11	120.30
1	A	2203	C	C5-C6-N1	5.46	123.73	121.00
2	B	61	U	N1-C2-O2	5.46	126.62	122.80
33	a	1287	C	N3-C2-O2	-5.46	118.08	121.90
1	A	2423	C	N3-C2-O2	-5.46	118.08	121.90
1	A	2345	U	C2-N1-C1'	5.46	124.25	117.70
1	A	2795	G	C8-N9-C4	-5.46	104.22	106.40
33	a	670	G	N3-C4-N9	5.46	129.28	126.00
1	A	1306	G	O5'-P-OP1	-5.46	100.79	105.70
1	A	1943	C	C6-N1-C2	-5.46	118.12	120.30
2	B	24	C	C6-N1-C1'	-5.45	114.26	120.80
1	A	2685	U	N1-C2-O2	5.45	126.61	122.80
1	A	1485	A	O4'-C1'-N9	5.45	112.56	108.20
1	A	2765	G	C6-C5-N7	-5.45	127.13	130.40
33	a	1051	G	N3-C4-N9	5.44	129.26	126.00
33	a	1323	C	C6-N1-C2	-5.44	118.12	120.30
1	A	1817	C	N3-C2-O2	-5.44	118.09	121.90
33	a	1438	C	C2-N1-C1'	5.44	124.78	118.80
1	A	270	C	C6-N1-C2	-5.43	118.13	120.30
1	A	1269	A	P-O3'-C3'	5.43	126.22	119.70
1	A	789	C	C5-C6-N1	5.43	123.72	121.00
16	R	75	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	2283	C	N1-C2-O2	5.42	122.15	118.90
15	Q	92	ARG	CA-CB-CG	5.42	125.33	113.40
1	A	614	G	N3-C4-C5	-5.42	125.89	128.60
1	A	1803	C	N3-C2-O2	-5.42	118.11	121.90
1	A	2487	U	N1-C2-O2	5.42	126.59	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2915	G	C5-C6-O6	-5.42	125.35	128.60
33	a	633	C	C6-N1-C2	-5.42	118.13	120.30
33	a	1123	C	N1-C2-O2	5.42	122.15	118.90
31	7	25	C	N3-C2-O2	-5.41	118.11	121.90
33	a	994	C	C6-N1-C2	-5.41	118.14	120.30
1	A	2289	C	C6-N1-C2	-5.41	118.14	120.30
1	A	1327	U	C2-N1-C1'	5.41	124.19	117.70
1	A	2825	C	N1-C2-O2	5.41	122.14	118.90
33	a	1123	C	C5-C6-N1	5.40	123.70	121.00
1	A	1872	C	N1-C2-O2	5.40	122.14	118.90
1	A	1137	G	C8-N9-C1'	-5.40	119.98	127.00
1	A	1981	A	C5-N7-C8	-5.40	101.20	103.90
33	a	1018	U	C5-C6-N1	5.40	125.40	122.70
1	A	648	G	N9-C4-C5	-5.40	103.24	105.40
33	a	970	U	N3-C2-O2	-5.40	118.42	122.20
1	A	2904	A	P-O3'-C3'	5.39	126.17	119.70
1	A	2333	G	C4-N9-C1'	5.39	133.51	126.50
33	a	563	U	C5-C6-N1	5.39	125.39	122.70
1	A	1844	A	OP1-P-O3'	5.38	117.05	105.20
33	a	1308	A	C4-N9-C1'	5.38	135.99	126.30
33	a	437	U	OP1-P-O3'	5.38	117.04	105.20
1	A	1274	U	N1-C2-O2	5.38	126.57	122.80
1	A	2823	C	O5'-P-OP2	-5.38	100.86	105.70
33	a	691	C	C5-C6-N1	5.38	123.69	121.00
33	a	1391	C	N3-C2-O2	-5.38	118.14	121.90
1	A	1172	A	P-O3'-C3'	5.38	126.15	119.70
1	A	2910	C	C6-N1-C2	-5.38	118.15	120.30
1	A	1516	A	C8-N9-C4	-5.37	103.65	105.80
1	A	2326	C	C5-C6-N1	5.37	123.69	121.00
1	A	575	A	OP2-P-O3'	5.37	117.01	105.20
1	A	1011	C	C5-C6-N1	5.37	123.69	121.00
1	A	2159	U	C5-C6-N1	5.37	125.38	122.70
1	A	2920	C	C6-N1-C2	-5.37	118.15	120.30
1	A	284	C	N1-C2-O2	5.36	122.12	118.90
33	a	787	G	N7-C8-N9	5.36	115.78	113.10
34	b	137	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	1351	U	OP2-P-O3'	5.36	116.99	105.20
1	A	941	U	C2-N1-C1'	5.36	124.13	117.70
1	A	1484	U	N3-C2-O2	-5.36	118.45	122.20
33	a	1525	C	C6-N1-C2	-5.36	118.16	120.30
1	A	1714	A	C4-N9-C1'	5.35	135.93	126.30
1	A	2296	A	OP1-P-OP2	-5.35	111.57	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	848	G	P-O3'-C3'	5.35	126.12	119.70
33	a	950	C	C6-N1-C2	-5.35	118.16	120.30
33	a	90	C	C6-N1-C2	-5.35	118.16	120.30
33	a	1308	A	C2-N3-C4	5.35	113.28	110.60
1	A	562	C	C5-C6-N1	5.35	123.67	121.00
1	A	1559	C	C6-N1-C2	-5.35	118.16	120.30
33	a	787	G	C8-N9-C4	-5.35	104.26	106.40
1	A	2432	C	N3-C2-O2	-5.34	118.16	121.90
1	A	1343	C	N1-C2-O2	5.34	122.11	118.90
1	A	1454	C	N1-C2-O2	5.34	122.11	118.90
16	R	22	ILE	CG1-CB-CG2	-5.34	99.65	111.40
33	a	1070	U	C6-N1-C2	-5.34	117.80	121.00
1	A	2503	C	C2-N1-C1'	5.34	124.67	118.80
16	R	75	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	1334	C	C6-N1-C2	-5.34	118.17	120.30
1	A	670	C	C6-N1-C2	-5.33	118.17	120.30
1	A	1350	U	N3-C2-O2	-5.33	118.47	122.20
33	a	486	C	C6-N1-C1'	-5.33	114.40	120.80
1	A	1344	C	C6-N1-C2	-5.33	118.17	120.30
1	A	1614	A	N7-C8-N9	5.33	116.47	113.80
1	A	2093	C	C6-N1-C2	-5.33	118.17	120.30
33	a	1170	C	O4'-C1'-N1	5.33	112.46	108.20
1	A	778	C	N3-C2-O2	-5.33	118.17	121.90
1	A	1577	C	C6-N1-C2	-5.33	118.17	120.30
1	A	1941	A	C5-N7-C8	-5.33	101.24	103.90
1	A	2092	C	C5-C6-N1	5.33	123.67	121.00
1	A	1846	G	C8-N9-C4	-5.33	104.27	106.40
1	A	113	U	N1-C2-O2	5.32	126.53	122.80
1	A	1813	A	OP2-P-O3'	5.32	116.90	105.20
1	A	2157	C	C6-N1-C2	-5.32	118.17	120.30
1	A	645	C	C5-C6-N1	5.32	123.66	121.00
33	a	1076	C	C6-N1-C1'	-5.32	114.42	120.80
1	A	980	C	C6-N1-C2	-5.31	118.17	120.30
1	A	1336	C	N3-C2-O2	-5.31	118.18	121.90
1	A	1953	C	C5-C6-N1	5.31	123.66	121.00
1	A	777	C	C5-C6-N1	5.31	123.66	121.00
1	A	716	G	C6-C5-N7	-5.31	127.22	130.40
1	A	2287	C	OP2-P-O3'	5.31	116.87	105.20
1	A	2356	A	C3'-C2'-C1'	5.31	105.74	101.50
45	m	80	LEU	CA-CB-CG	5.31	127.50	115.30
1	A	1752	G	N3-C4-N9	5.30	129.18	126.00
1	A	2244	G	O4'-C1'-N9	5.30	112.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	14	G	N3-C4-N9	5.30	129.18	126.00
1	A	2273	U	C5-C6-N1	5.30	125.35	122.70
1	A	937	C	C6-N1-C2	-5.30	118.18	120.30
1	A	2795	G	C2-N3-C4	5.30	114.55	111.90
1	A	2323	C	C6-N1-C2	-5.29	118.18	120.30
33	a	226	C	C6-N1-C2	-5.29	118.18	120.30
1	A	894	A	C5-N7-C8	-5.29	101.25	103.90
33	a	155	C	C2-N1-C1'	5.29	124.62	118.80
34	b	17	GLY	N-CA-C	5.29	126.33	113.10
33	a	1149	U	C6-N1-C1'	-5.29	113.80	121.20
1	A	1705	C	C5-C6-N1	5.29	123.64	121.00
1	A	563	C	C6-N1-C2	-5.28	118.19	120.30
1	A	574	A	C2-N3-C4	-5.28	107.96	110.60
1	A	2348	C	C2-N1-C1'	5.28	124.61	118.80
2	B	58	C	C5-C6-N1	5.28	123.64	121.00
33	a	469	G	N7-C8-N9	5.28	115.74	113.10
1	A	163	U	P-O3'-C3'	5.28	126.03	119.70
1	A	2283	C	N3-C2-O2	-5.28	118.21	121.90
1	A	2820	U	C2-N1-C1'	5.28	124.03	117.70
1	A	271	C	C6-N1-C2	-5.28	118.19	120.30
1	A	421	A	N7-C8-N9	5.28	116.44	113.80
33	a	819	C	C2-N1-C1'	5.28	124.60	118.80
1	A	2765	G	C4-N9-C1'	5.27	133.35	126.50
1	A	556	C	C2-N1-C1'	5.27	124.60	118.80
1	A	1699	A	O4'-C1'-N9	5.27	112.42	108.20
1	A	2065	C	C6-N1-C2	-5.27	118.19	120.30
33	a	1175	G	OP2-P-O3'	5.27	116.79	105.20
1	A	2189	G	N9-C4-C5	-5.27	103.29	105.40
33	a	1357	U	C2-N1-C1'	5.27	124.02	117.70
53	x	21	G	C8-N9-C4	-5.27	104.29	106.40
2	B	37	A	P-O3'-C3'	5.26	126.02	119.70
1	A	1379	U	N1-C2-O2	5.26	126.48	122.80
1	A	2131	U	C6-N1-C2	-5.26	117.84	121.00
1	A	1942	A	C5-N7-C8	5.26	106.53	103.90
1	A	2190	C	C6-N1-C2	-5.26	118.20	120.30
1	A	1467	G	C6-C5-N7	-5.26	127.25	130.40
1	A	1604	C	N3-C2-O2	-5.26	118.22	121.90
33	a	523	C	C6-N1-C2	-5.26	118.20	120.30
33	a	1494	U	C5-C6-N1	5.26	125.33	122.70
1	A	732	A	P-O3'-C3'	5.25	126.01	119.70
1	A	445	C	N1-C2-O2	5.25	122.05	118.90
1	A	2093	C	C5-C6-N1	5.25	123.63	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	e	36	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	1448	U	OP1-P-O3'	5.25	116.75	105.20
33	a	171	A	N7-C8-N9	5.25	116.43	113.80
33	a	1460	U	C2-N1-C1'	5.25	124.00	117.70
33	a	384	G	C4-N9-C1'	5.25	133.32	126.50
1	A	1753	C	C5-C6-N1	5.25	123.62	121.00
1	A	1374	C	C2-N1-C1'	5.25	124.57	118.80
33	a	1149	U	C5-C6-N1	5.25	125.32	122.70
33	a	155	C	N1-C2-O2	5.24	122.05	118.90
33	a	1357	U	N3-C2-O2	-5.24	118.53	122.20
2	B	52	G	C8-N9-C4	-5.24	104.30	106.40
33	a	455	G	P-O3'-C3'	5.24	125.99	119.70
1	A	2166	C	N1-C2-O2	5.24	122.04	118.90
33	a	537	C	C5-C6-N1	5.24	123.62	121.00
1	A	458	G	P-O3'-C3'	5.24	125.98	119.70
1	A	2277	C	C6-N1-C2	-5.24	118.20	120.30
1	A	2591	U	N1-C2-O2	5.24	126.46	122.80
1	A	1336	C	N1-C2-O2	5.23	122.04	118.90
1	A	1701	C	C5-C6-N1	5.23	123.62	121.00
1	A	1559	C	C2-N1-C1'	5.23	124.56	118.80
1	A	1671	G	N3-C4-C5	-5.23	125.98	128.60
33	a	1460	U	C5-C6-N1	5.23	125.31	122.70
53	x	53	G	N3-C4-N9	5.23	129.14	126.00
4	D	12	MET	CA-CB-CG	5.23	122.19	113.30
1	A	1970	C	N1-C2-O2	5.22	122.03	118.90
33	a	1462	U	P-O3'-C3'	5.22	125.97	119.70
1	A	1223	C	C5-C6-N1	5.22	123.61	121.00
1	A	2114	C	N1-C2-O2	5.22	122.03	118.90
33	a	1286	C	N3-C2-O2	-5.22	118.25	121.90
1	A	1448	U	P-O3'-C3'	5.22	125.96	119.70
1	A	2189	G	C6-C5-N7	-5.22	127.27	130.40
33	a	545	C	N1-C2-O2	5.22	122.03	118.90
1	A	309	U	N3-C2-O2	-5.21	118.55	122.20
33	a	901	U	N3-C2-O2	-5.21	118.55	122.20
1	A	1804	U	N1-C2-O2	5.21	126.45	122.80
1	A	1437	C	C6-N1-C2	-5.21	118.22	120.30
33	a	944	C	O4'-C1'-N1	-5.21	104.03	108.20
1	A	2114	C	C6-N1-C1'	-5.21	114.55	120.80
33	a	476	U	N3-C2-O2	-5.21	118.55	122.20
2	B	49	G	P-O3'-C3'	5.21	125.95	119.70
33	a	773	C	C5-C6-N1	5.20	123.60	121.00
1	A	686	C	C2-N1-C1'	5.20	124.52	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	A	O4'-C1'-N9	-5.20	104.04	108.20
2	B	15	C	N1-C2-O2	5.20	122.02	118.90
1	A	1344	C	N3-C2-O2	-5.20	118.26	121.90
1	A	1922	C	N1-C2-O2	5.20	122.02	118.90
2	B	62	U	N3-C2-O2	-5.20	118.56	122.20
33	a	113	G	P-O3'-C3'	5.20	125.94	119.70
1	A	501	A	OP2-P-O3'	5.20	116.63	105.20
1	A	895	G	N3-C4-N9	5.20	129.12	126.00
1	A	914	C	N1-C2-O2	5.20	122.02	118.90
1	A	83	G	N3-C4-N9	-5.19	122.88	126.00
1	A	1422	C	C6-N1-C2	-5.19	118.22	120.30
33	a	332	G	N3-C4-C5	-5.19	126.00	128.60
1	A	1343	C	C6-N1-C1'	-5.19	114.57	120.80
33	a	746	C	N1-C2-O2	5.19	122.01	118.90
1	A	830	A	C4-C5-N7	5.19	113.30	110.70
1	A	1794	C	C6-N1-C2	-5.19	118.22	120.30
1	A	769	A	C6-N1-C2	5.19	121.71	118.60
1	A	2348	C	N1-C2-O2	5.19	122.01	118.90
33	a	445	U	C5-C6-N1	5.19	125.29	122.70
1	A	2254	A	OP2-P-O3'	5.19	116.61	105.20
1	A	3	U	C5-C6-N1	5.18	125.29	122.70
1	A	93	C	C6-N1-C1'	5.18	127.02	120.80
1	A	2333	G	C8-N9-C1'	-5.18	120.27	127.00
1	A	2712	C	N3-C2-O2	-5.18	118.28	121.90
33	a	989	C	C2-N1-C1'	5.18	124.50	118.80
1	A	284	C	OP2-P-O3'	5.18	116.59	105.20
1	A	1671	G	P-O3'-C3'	5.18	125.91	119.70
1	A	442	C	C2-N1-C1'	5.17	124.49	118.80
1	A	2839	C	N1-C2-O2	5.17	122.00	118.90
33	a	563	U	P-O3'-C3'	5.17	125.91	119.70
33	a	966	U	C5-C6-N1	5.17	125.29	122.70
33	a	981	G	O4'-C1'-N9	5.17	112.34	108.20
1	A	1067	A	C4-C5-N7	5.17	113.28	110.70
1	A	2445	C	C6-N1-C2	-5.17	118.23	120.30
33	a	467	C	C5-C6-N1	5.17	123.58	121.00
2	B	29	C	C6-N1-C1'	-5.17	114.60	120.80
33	a	155	C	C5-C6-N1	5.17	123.58	121.00
33	a	563	U	OP1-P-O3'	5.17	116.56	105.20
1	A	1117	G	N3-C4-C5	-5.16	126.02	128.60
1	A	1156	G	N7-C8-N9	5.16	115.68	113.10
1	A	2454	A	P-O3'-C3'	5.16	125.89	119.70
44	l	94	LEU	CA-CB-CG	5.16	127.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2509	C	C6-N1-C2	-5.16	118.24	120.30
33	a	1018	U	P-O3'-C3'	5.16	125.89	119.70
1	A	2620	C	C5-C6-N1	5.16	123.58	121.00
1	A	195	C	C5-C6-N1	5.15	123.58	121.00
1	A	1759	U	O4'-C1'-N1	5.15	112.32	108.20
33	a	1110	C	N1-C2-O2	5.15	121.99	118.90
33	a	1392	C	C6-N1-C2	-5.15	118.24	120.30
33	a	1469	C	C6-N1-C2	-5.15	118.24	120.30
1	A	177	G	O5'-P-OP2	-5.15	101.06	105.70
33	a	130	C	C6-N1-C2	-5.15	118.24	120.30
1	A	2277	C	C2-N1-C1'	5.15	124.46	118.80
1	A	2675	C	C6-N1-C2	-5.15	118.24	120.30
6	F	79	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	2840	C	C2-N3-C4	5.15	122.47	119.90
1	A	211	C	C2-N3-C4	5.14	122.47	119.90
1	A	2604	C	C5-C6-N1	5.14	123.57	121.00
1	A	1028	C	C6-N1-C2	-5.14	118.24	120.30
1	A	1557	G	N3-C4-C5	-5.14	126.03	128.60
1	A	2523	G	C2-N3-C4	5.14	114.47	111.90
33	a	859	C	N1-C2-O2	5.14	121.98	118.90
33	a	1420	C	N3-C2-O2	-5.14	118.30	121.90
1	A	2827	A	N1-C6-N6	5.13	121.68	118.60
1	A	2920	C	C5-C6-N1	5.13	123.57	121.00
1	A	2323	C	N1-C2-O2	5.13	121.98	118.90
33	a	1398	C	C6-N1-C2	-5.13	118.25	120.30
1	A	1613	C	C2-N1-C1'	5.13	124.44	118.80
33	a	1010	U	N1-C2-O2	5.13	126.39	122.80
1	A	393	U	N1-C2-O2	5.13	126.39	122.80
1	A	1246	G	O4'-C1'-N9	5.13	112.30	108.20
1	A	1831	A	C5-N7-C8	-5.13	101.34	103.90
33	a	167	G	N3-C4-N9	5.13	129.08	126.00
33	a	174	C	N1-C2-O2	5.13	121.98	118.90
33	a	982	C	C6-N1-C2	-5.13	118.25	120.30
33	a	1502	A	C5-N7-C8	-5.13	101.34	103.90
33	a	21	C	C2-N1-C1'	5.12	124.43	118.80
33	a	1390	U	N3-C2-O2	-5.12	118.61	122.20
33	a	439	A	C2-N3-C4	5.12	113.16	110.60
1	A	2126	G	N7-C8-N9	5.11	115.66	113.10
33	a	746	C	N3-C2-O2	-5.11	118.32	121.90
1	A	113	U	N3-C2-O2	-5.11	118.62	122.20
1	A	299	U	N1-C2-N3	5.11	117.97	114.90
33	a	466	G	N1-C6-O6	-5.11	116.83	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	1022	A	C2-N3-C4	5.11	113.16	110.60
41	i	87	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	1805	G	C4-N9-C1'	5.11	133.14	126.50
2	B	49	G	OP1-P-O3'	5.11	116.44	105.20
33	a	967	U	C2-N1-C1'	5.11	123.83	117.70
1	A	1671	G	C6-C5-N7	-5.11	127.34	130.40
1	A	2822	C	N1-C2-O2	5.11	121.96	118.90
33	a	223	C	O4'-C1'-N1	5.11	112.28	108.20
33	a	361	A	OP2-P-O3'	5.11	116.43	105.20
33	a	521	U	C5-C6-N1	5.11	125.25	122.70
1	A	185	A	P-O5'-C5'	5.10	129.06	120.90
1	A	1644	C	N1-C2-O2	5.10	121.96	118.90
1	A	2617	G	C4-C5-N7	5.10	112.84	110.80
1	A	203	U	N1-C2-O2	5.10	126.37	122.80
1	A	104	C	N1-C2-O2	5.10	121.96	118.90
1	A	1626	U	N1-C2-O2	5.10	126.37	122.80
1	A	1307	U	C2-N1-C1'	5.10	123.82	117.70
1	A	309	U	N1-C2-O2	5.09	126.37	122.80
33	a	363	C	C6-N1-C2	-5.09	118.26	120.30
1	A	136	C	C5-C6-N1	5.09	123.55	121.00
1	A	1597	C	C5-C6-N1	5.09	123.55	121.00
33	a	572	A	O4'-C1'-N9	5.09	112.28	108.20
33	a	934	C	C5-C6-N1	5.09	123.55	121.00
1	A	549	A	P-O3'-C3'	5.09	125.81	119.70
1	A	2072	C	C2-N3-C4	5.09	122.44	119.90
33	a	1420	C	C6-N1-C2	-5.09	118.26	120.30
1	A	136	C	C6-N1-C2	-5.09	118.27	120.30
1	A	1199	C	N1-C2-O2	5.09	121.95	118.90
1	A	2203	C	C2-N1-C1'	5.09	124.40	118.80
1	A	2452	U	N3-C2-O2	-5.09	118.64	122.20
1	A	2711	G	N3-C4-N9	5.09	129.05	126.00
1	A	1779	G	C8-N9-C1'	-5.08	120.39	127.00
1	A	1223	C	C6-N1-C2	-5.08	118.27	120.30
1	A	2774	C	N1-C2-O2	5.08	121.95	118.90
33	a	1501	G	N3-C4-N9	-5.08	122.95	126.00
1	A	8	U	N3-C4-O4	5.08	122.96	119.40
1	A	2468	A	P-O3'-C3'	5.08	125.80	119.70
33	a	338	C	N1-C2-O2	5.08	121.95	118.90
1	A	1452	C	C6-N1-C2	-5.08	118.27	120.30
1	A	237	U	C2-N1-C1'	5.08	123.79	117.70
1	A	393	U	N3-C2-O2	-5.08	118.65	122.20
1	A	1534	A	C8-N9-C4	-5.07	103.77	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	2	ARG	NE-CZ-NH1	-5.07	117.76	120.30
33	a	963	G	C4-N9-C1'	5.07	133.09	126.50
33	a	1021	U	C5-C6-N1	5.07	125.23	122.70
33	a	1457	C	C5-C6-N1	5.07	123.53	121.00
1	A	1037	C	C5-C6-N1	5.07	123.53	121.00
33	a	820	C	C2-N1-C1'	5.07	124.37	118.80
33	a	855	G	P-O3'-C3'	5.06	125.78	119.70
1	A	2077	G	C4-N9-C1'	5.06	133.08	126.50
1	A	2648	U	N1-C2-O2	5.06	126.34	122.80
1	A	1998	A	OP1-P-O3'	5.06	116.33	105.20
1	A	981	C	C6-N1-C2	-5.06	118.28	120.30
33	a	369	G	C6-C5-N7	-5.06	127.37	130.40
33	a	854	C	N1-C2-O2	5.06	121.93	118.90
1	A	2076	C	C6-N1-C2	-5.05	118.28	120.30
33	a	1499	G	P-O3'-C3'	5.05	125.76	119.70
1	A	1715	C	C5-C6-N1	5.05	123.52	121.00
1	A	2365	A	N1-C6-N6	5.04	121.63	118.60
1	A	529	C	C5-C6-N1	5.04	123.52	121.00
33	a	336	C	N3-C2-O2	-5.04	118.37	121.90
1	A	624	C	N1-C2-O2	5.04	121.92	118.90
6	F	112	ARG	CA-CB-CG	5.04	124.49	113.40
33	a	982	C	N3-C2-O2	-5.04	118.37	121.90
1	A	508	C	C6-N1-C1'	-5.04	114.75	120.80
1	A	1565	U	P-O3'-C3'	5.04	125.74	119.70
33	a	982	C	N1-C2-O2	5.04	121.92	118.90
1	A	309	U	P-O3'-C3'	5.03	125.74	119.70
33	a	589	C	C6-N1-C2	-5.03	118.29	120.30
1	A	2420	G	O5'-P-OP2	-5.03	101.17	105.70
33	a	1293	C	C6-N1-C2	-5.03	118.29	120.30
1	A	18	C	C5-C6-N1	5.03	123.51	121.00
1	A	1727	A	O5'-P-OP1	-5.03	101.17	105.70
1	A	2733	C	C5-C6-N1	5.03	123.51	121.00
1	A	698	C	O4'-C1'-N1	5.02	112.22	108.20
17	S	40	PRO	N-CA-C	5.02	125.16	112.10
33	a	481	C	C5-C6-N1	5.02	123.51	121.00
1	A	506	U	N3-C2-O2	-5.02	118.69	122.20
1	A	946	G	C4-N9-C1'	5.02	133.02	126.50
33	a	319	C	N3-C2-O2	-5.02	118.39	121.90
1	A	1175	A	OP2-P-O3'	5.02	116.24	105.20
1	A	1250	G	P-O3'-C3'	5.02	125.72	119.70
1	A	1803	C	C5-C6-N1	5.02	123.51	121.00
1	A	1117	G	C4-N9-C1'	5.01	133.02	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1529	G	P-O3'-C3'	5.01	125.72	119.70
1	A	2313	C	N1-C2-O2	5.01	121.91	118.90
33	a	1078	G	N3-C4-N9	5.01	129.01	126.00
1	A	2296	A	O5'-P-OP2	5.01	116.71	110.70
1	A	648	G	C5'-C4'-C3'	-5.00	107.99	116.00
1	A	1160	G	O4'-C1'-N9	5.00	112.20	108.20
1	A	1333	C	C6-N1-C2	-5.00	118.30	120.30
33	a	1078	G	C6-C5-N7	-5.00	127.40	130.40
1	A	1239	U	C2-N1-C1'	5.00	123.70	117.70
33	a	182	U	C2-N1-C1'	5.00	123.70	117.70

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	0	50	ASN	Peptide
25	0	51	GLY	Peptide
30	6	59	PHE	Peptide
3	C	153	GLN	Peptide
4	D	53	PHE	Peptide
6	F	117	VAL	Peptide
6	F	138	PHE	Peptide
6	F	53	ALA	Peptide
8	J	132	PRO	Peptide
10	L	18	ARG	Peptide
10	L	35	HIS	Peptide
13	O	1	MET	Peptide
15	Q	102	ASP	Peptide
16	R	50	ASN	Peptide
16	R	51	PRO	Peptide
17	S	39	THR	Peptide
20	V	15	LYS	Peptide
20	V	19	VAL	Peptide
20	V	278	ARG	Peptide
20	V	279	PHE	Peptide
20	V	281	ILE	Peptide
20	V	342	THR	Peptide
20	V	405	LYS	Peptide
20	V	412	ARG	Peptide
20	V	521	ALA	Peptide
20	V	75	THR	Peptide
20	V	98	LEU	Peptide

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Mol	Chain	Res	Type	Group
34	b	148	LEU	Peptide
34	b	16	PHE	Peptide
34	b	18	HIS	Peptide
34	b	65	GLY	Peptide
34	b	66	LYS	Peptide
36	d	117	GLY	Peptide
36	d	192	ALA	Peptide
36	d	31	TYR	Peptide
36	d	32	ALA	Peptide
36	d	33	PRO	Peptide
37	e	20	ARG	Peptide
38	f	33	ASN	Peptide
39	g	114	LYS	Peptide
39	g	129	ASN	Peptide
40	h	98	LEU	Peptide
44	l	34	GLU	Peptide
44	l	57	LYS	Peptide
45	m	104	ASN	Peptide
45	m	3	ARG	Peptide
45	m	65	VAL	Peptide
47	o	24	SER	Peptide
49	q	30	TYR	Peptide
50	r	24	THR	Peptide
50	r	25	HIS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	270/277 (98%)	253 (94%)	17 (6%)	0	100	100
4	D	204/209 (98%)	195 (96%)	9 (4%)	0	100	100
5	E	203/207 (98%)	187 (92%)	16 (8%)	0	100	100
6	F	174/179 (97%)	159 (91%)	15 (9%)	0	100	100
7	G	173/179 (97%)	153 (88%)	20 (12%)	0	100	100
8	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	11	46
9	K	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
10	L	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
11	M	133/144 (92%)	125 (94%)	8 (6%)	0	100	100
12	N	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
13	O	118/120 (98%)	107 (91%)	11 (9%)	0	100	100
14	P	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
15	Q	115/119 (97%)	107 (93%)	6 (5%)	2 (2%)	9	42
16	R	99/102 (97%)	83 (84%)	15 (15%)	1 (1%)	15	54
17	S	107/113 (95%)	92 (86%)	13 (12%)	2 (2%)	8	40
18	T	88/95 (93%)	84 (96%)	4 (4%)	0	100	100
19	U	99/103 (96%)	86 (87%)	13 (13%)	0	100	100
20	V	539/548 (98%)	464 (86%)	73 (14%)	2 (0%)	34	72
21	W	80/94 (85%)	71 (89%)	9 (11%)	0	100	100
22	X	56/62 (90%)	46 (82%)	10 (18%)	0	100	100
23	Y	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
24	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
25	0	52/59 (88%)	49 (94%)	2 (4%)	1 (2%)	8	40
26	1	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
27	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
28	3	62/66 (94%)	60 (97%)	2 (3%)	0	100	100
29	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
30	6	61/66 (92%)	53 (87%)	8 (13%)	0	100	100
32	8	210/232 (90%)	192 (91%)	18 (9%)	0	100	100
34	b	216/246 (88%)	188 (87%)	24 (11%)	4 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	c	204/218 (94%)	185 (91%)	19 (9%)	0	100	100
36	d	193/200 (96%)	173 (90%)	18 (9%)	2 (1%)	15	54
37	e	162/166 (98%)	150 (93%)	12 (7%)	0	100	100
38	f	90/95 (95%)	83 (92%)	7 (8%)	0	100	100
39	g	147/156 (94%)	136 (92%)	11 (8%)	0	100	100
40	h	129/132 (98%)	107 (83%)	20 (16%)	2 (2%)	9	43
41	i	123/130 (95%)	104 (85%)	18 (15%)	1 (1%)	19	58
42	j	93/102 (91%)	83 (89%)	9 (10%)	1 (1%)	14	52
43	k	112/131 (86%)	100 (89%)	12 (11%)	0	100	100
44	l	134/138 (97%)	117 (87%)	16 (12%)	1 (1%)	22	61
45	m	106/121 (88%)	94 (89%)	11 (10%)	1 (1%)	17	56
46	n	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	9	42
47	o	83/89 (93%)	79 (95%)	3 (4%)	1 (1%)	13	50
48	p	86/90 (96%)	76 (88%)	7 (8%)	3 (4%)	3	27
49	q	82/87 (94%)	77 (94%)	5 (6%)	0	100	100
50	r	62/79 (78%)	57 (92%)	5 (8%)	0	100	100
51	s	76/92 (83%)	66 (87%)	10 (13%)	0	100	100
52	t	81/88 (92%)	76 (94%)	3 (4%)	2 (2%)	5	34
All	All	5956/6298 (95%)	5382 (90%)	545 (9%)	29 (0%)	32	68

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	133	HIS
15	Q	93	LYS
17	S	40	PRO
20	V	280	SER
34	b	18	HIS
34	b	19	GLN
36	d	32	ALA
40	h	99	ASN
48	p	47	ALA
52	t	69	LYS
8	J	132	PRO
15	Q	92	ARG
34	b	67	ILE

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Mol	Chain	Res	Type
36	d	33	PRO
40	h	4	THR
46	n	32	SER
34	b	66	LYS
45	m	105	ASN
17	S	39	THR
25	0	51	GLY
44	l	135	PRO
48	p	48	GLU
52	t	68	HIS
16	R	50	ASN
41	i	125	PRO
48	p	46	PRO
20	V	281	ILE
42	j	79	PRO
47	o	25	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	220/225 (98%)	218 (99%)	2 (1%)	78 90
4	D	167/170 (98%)	166 (99%)	1 (1%)	86 94
5	E	169/170 (99%)	164 (97%)	5 (3%)	41 71
6	F	151/154 (98%)	144 (95%)	7 (5%)	27 61
7	G	148/151 (98%)	148 (100%)	0	100 100
8	J	120/123 (98%)	118 (98%)	2 (2%)	60 82
9	K	101/101 (100%)	101 (100%)	0	100 100
10	L	110/110 (100%)	108 (98%)	2 (2%)	59 81
11	M	109/116 (94%)	108 (99%)	1 (1%)	78 90
12	N	99/100 (99%)	99 (100%)	0	100 100
13	O	93/93 (100%)	91 (98%)	2 (2%)	52 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	P	100/100 (100%)	97 (97%)	3 (3%)	41	71
15	Q	96/98 (98%)	96 (100%)	0	100	100
16	R	83/84 (99%)	81 (98%)	2 (2%)	49	76
17	S	90/93 (97%)	90 (100%)	0	100	100
18	T	81/85 (95%)	79 (98%)	2 (2%)	47	75
19	U	85/87 (98%)	85 (100%)	0	100	100
20	V	424/431 (98%)	417 (98%)	7 (2%)	60	82
21	W	64/74 (86%)	61 (95%)	3 (5%)	26	60
22	X	47/50 (94%)	44 (94%)	3 (6%)	17	50
23	Y	56/57 (98%)	56 (100%)	0	100	100
24	Z	52/53 (98%)	51 (98%)	1 (2%)	57	80
25	0	48/53 (91%)	45 (94%)	3 (6%)	18	51
26	1	46/47 (98%)	46 (100%)	0	100	100
27	2	39/39 (100%)	38 (97%)	1 (3%)	46	74
28	3	54/56 (96%)	52 (96%)	2 (4%)	34	65
29	4	35/35 (100%)	35 (100%)	0	100	100
30	6	53/55 (96%)	53 (100%)	0	100	100
32	8	169/185 (91%)	168 (99%)	1 (1%)	86	94
34	b	189/212 (89%)	182 (96%)	7 (4%)	34	65
35	c	168/178 (94%)	166 (99%)	2 (1%)	71	87
36	d	169/173 (98%)	165 (98%)	4 (2%)	49	76
37	e	128/130 (98%)	126 (98%)	2 (2%)	62	83
38	f	81/84 (96%)	80 (99%)	1 (1%)	71	87
39	g	125/132 (95%)	124 (99%)	1 (1%)	81	91
40	h	111/112 (99%)	109 (98%)	2 (2%)	59	81
41	i	98/102 (96%)	96 (98%)	2 (2%)	55	79
42	j	86/92 (94%)	86 (100%)	0	100	100
43	k	86/100 (86%)	85 (99%)	1 (1%)	71	87
44	l	114/116 (98%)	111 (97%)	3 (3%)	46	74
45	m	94/104 (90%)	94 (100%)	0	100	100
46	n	53/54 (98%)	52 (98%)	1 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	o	80/83 (96%)	79 (99%)	1 (1%)	69	86
48	p	74/76 (97%)	72 (97%)	2 (3%)	44	73
49	q	77/80 (96%)	74 (96%)	3 (4%)	32	64
50	r	56/64 (88%)	54 (96%)	2 (4%)	35	66
51	s	70/81 (86%)	69 (99%)	1 (1%)	67	85
52	t	66/70 (94%)	65 (98%)	1 (2%)	65	84
All	All	5034/5238 (96%)	4948 (98%)	86 (2%)	62	82

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	221	ARG
3	C	273	ARG
4	D	199	LEU
5	E	10	ASN
5	E	29	ASN
5	E	188	ASN
5	E	192	LEU
5	E	194	ILE
6	F	3	ARG
6	F	4	LEU
6	F	78	ARG
6	F	119	LYS
6	F	133	LYS
6	F	136	LEU
6	F	165	GLU
8	J	26	LEU
8	J	123	LEU
10	L	18	ARG
10	L	47	ARG
11	M	124	LYS
13	O	4	LYS
13	O	61	LYS
14	P	36	ASN
14	P	39	ARG
14	P	51	ARG
16	R	47	LYS
16	R	48	VAL
18	T	65	ARG
18	T	68	ARG

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Mol	Chain	Res	Type
20	V	14	VAL
20	V	63	ARG
20	V	160	ARG
20	V	182	LYS
20	V	309	ASN
20	V	380	PHE
20	V	388	ASN
21	W	22	ARG
21	W	28	ARG
21	W	79	ARG
22	X	4	LYS
22	X	17	ASN
22	X	27	ARG
24	Z	9	LYS
25	0	22	LEU
25	0	38	LEU
25	0	50	ASN
27	2	28	ARG
28	3	32	LEU
28	3	62	LEU
32	8	121	MET
34	b	24	ASN
34	b	36	ASN
34	b	113	ARG
34	b	123	ASN
34	b	154	MET
34	b	179	LEU
34	b	203	ASN
35	c	71	LYS
35	c	163	ARG
36	d	54	LYS
36	d	147	ASN
36	d	172	LEU
36	d	182	ARG
37	e	36	LEU
37	e	95	LEU
38	f	77	ARG
39	g	9	LYS
40	h	57	GLN
40	h	96	ARG
41	i	12	ARG
41	i	106	ARG

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Mol	Chain	Res	Type
43	k	95	ARG
44	l	44	ARG
44	l	56	LYS
44	l	96	ARG
46	n	29	ARG
47	o	54	ARG
48	p	32	ARG
48	p	71	ARG
49	q	32	LYS
49	q	67	ARG
49	q	76	ARG
50	r	29	LYS
50	r	48	ARG
51	s	5	LEU
52	t	78	ARG

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

Mol	Chain	Res	Type
3	C	86	ASN
3	C	177	ASN
3	C	230	HIS
3	C	232	HIS
4	D	33	ASN
5	E	10	ASN
5	E	29	ASN
5	E	188	ASN
6	F	45	GLN
7	G	148	ASN
10	L	126	ASN
12	N	27	ASN
12	N	61	GLN
12	N	68	ASN
13	O	15	HIS
14	P	36	ASN
15	Q	29	HIS
15	Q	37	GLN
15	Q	66	ASN
16	R	83	HIS
17	S	102	HIS
19	U	64	HIS
20	V	73	GLN

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Mol	Chain	Res	Type
20	V	158	HIS
20	V	207	GLN
20	V	218	ASN
20	V	296	ASN
20	V	309	ASN
20	V	335	ASN
20	V	360	GLN
20	V	388	ASN
20	V	406	HIS
20	V	435	ASN
20	V	461	HIS
21	W	37	GLN
22	X	17	ASN
22	X	23	ASN
25	0	40	HIS
25	0	50	ASN
26	1	22	ASN
26	1	26	ASN
28	3	60	GLN
32	8	67	ASN
32	8	106	GLN
32	8	188	ASN
34	b	18	HIS
34	b	24	ASN
34	b	36	ASN
34	b	123	ASN
34	b	203	ASN
35	c	136	GLN
36	d	96	ASN
36	d	112	GLN
36	d	118	HIS
36	d	147	ASN
37	e	83	HIS
38	f	33	ASN
38	f	61	GLN
39	g	84	ASN
39	g	142	HIS
40	h	57	GLN
41	i	81	HIS
41	i	126	GLN
44	l	59	ASN
44	l	85	HIS

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Mol	Chain	Res	Type
44	l	90	HIS
44	l	109	HIS
45	m	76	ASN
46	n	10	GLN
47	o	28	GLN
47	o	37	ASN
47	o	42	HIS
47	o	46	HIS
47	o	51	HIS
47	o	83	ASN
49	q	49	HIS
52	t	70	ASN
52	t	84	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2876/2928 (98%)	857 (29%)	90 (3%)
2	B	111/112 (99%)	40 (36%)	3 (2%)
31	7	2/3 (66%)	0	0
33	a	1532/1554 (98%)	411 (26%)	0
53	x	73/75 (97%)	29 (39%)	0
All	All	4594/4672 (98%)	1337 (29%)	93 (2%)

All (1337) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	U
1	A	10	A
1	A	13	A
1	A	18	C
1	A	26	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	45	G
1	A	46	C
1	A	55	G
1	A	60	G
1	A	61	A

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Mol	Chain	Res	Type
1	A	62	C
1	A	63	G
1	A	64	A
1	A	65	A
1	A	66	C
1	A	71	A
1	A	74	U
1	A	75	G
1	A	76	C
1	A	77	U
1	A	78	U
1	A	79	C
1	A	83	G
1	A	84	A
1	A	85	G
1	A	86	C
1	A	87	U
1	A	89	U
1	A	90	A
1	A	92	G
1	A	93	C
1	A	96	G
1	A	99	U
1	A	100	U
1	A	101	G
1	A	117	A
1	A	118	A
1	A	119	U
1	A	124	A
1	A	125	A
1	A	126	A
1	A	127	C
1	A	134	C
1	A	141	U
1	A	156	A
1	A	162	A
1	A	163	U
1	A	164	U
1	A	167	U
1	A	174	U
1	A	175	G
1	A	176	A

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Mol	Chain	Res	Type
1	A	177	G
1	A	178	A
1	A	179	A
1	A	182	C
1	A	187	C
1	A	188	C
1	A	196	U
1	A	199	A
1	A	202	A
1	A	207	A
1	A	216	A
1	A	218	G
1	A	219	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	229	A
1	A	231	A
1	A	232	U
1	A	233	G
1	A	234	C
1	A	236	A
1	A	237	U
1	A	244	A
1	A	247	A
1	A	248	G
1	A	251	G
1	A	252	C
1	A	253	G
1	A	255	G
1	A	258	A
1	A	266	U
1	A	267	C
1	A	268	A
1	A	269	G
1	A	270	C
1	A	272	C
1	A	275	A
1	A	282	G
1	A	283	G
1	A	284	C
1	A	285	U

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Mol	Chain	Res	Type
1	A	286	U
1	A	290	U
1	A	291	C
1	A	298	U
1	A	299	U
1	A	301	U
1	A	302	A
1	A	308	C
1	A	309	U
1	A	310	C
1	A	337	A
1	A	345	A
1	A	346	G
1	A	348	U
1	A	349	C
1	A	352	G
1	A	354	A
1	A	360	C
1	A	361	G
1	A	366	A
1	A	367	G
1	A	373	A
1	A	374	A
1	A	375	C
1	A	382	G
1	A	389	A
1	A	395	C
1	A	396	G
1	A	398	U
1	A	409	U
1	A	411	G
1	A	412	A
1	A	418	A
1	A	419	G
1	A	420	U
1	A	421	A
1	A	430	C
1	A	433	G
1	A	434	U
1	A	436	A
1	A	442	C
1	A	444	U

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Mol	Chain	Res	Type
1	A	445	C
1	A	453	G
1	A	458	G
1	A	459	A
1	A	469	A
1	A	471	G
1	A	482	C
1	A	483	C
1	A	489	G
1	A	490	A
1	A	494	A
1	A	498	U
1	A	502	C
1	A	503	C
1	A	504	A
1	A	506	U
1	A	508	C
1	A	511	U
1	A	524	A
1	A	526	A
1	A	527	A
1	A	528	G
1	A	529	C
1	A	548	A
1	A	550	G
1	A	551	A
1	A	552	G
1	A	554	U
1	A	555	C
1	A	556	C
1	A	558	G
1	A	568	G
1	A	573	C
1	A	575	A
1	A	577	U
1	A	578	A
1	A	583	G
1	A	584	A
1	A	590	U
1	A	591	U
1	A	592	A
1	A	593	A

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Mol	Chain	Res	Type
1	A	594	C
1	A	595	G
1	A	599	G
1	A	607	G
1	A	613	U
1	A	617	G
1	A	618	A
1	A	619	A
1	A	622	A
1	A	630	A
1	A	632	U
1	A	646	A
1	A	647	A
1	A	648	G
1	A	649	G
1	A	655	C
1	A	658	A
1	A	659	A
1	A	662	U
1	A	667	A
1	A	668	G
1	A	673	A
1	A	680	G
1	A	683	A
1	A	686	C
1	A	689	A
1	A	690	A
1	A	691	U
1	A	698	C
1	A	699	A
1	A	700	U
1	A	701	G
1	A	703	G
1	A	715	A
1	A	716	G
1	A	717	A
1	A	718	C
1	A	733	U
1	A	741	U
1	A	749	G
1	A	764	C
1	A	765	A

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Mol	Chain	Res	Type
1	A	766	C
1	A	777	C
1	A	787	C
1	A	788	G
1	A	790	A
1	A	794	U
1	A	804	G
1	A	810	G
1	A	811	A
1	A	812	G
1	A	822	G
1	A	823	G
1	A	824	G
1	A	829	A
1	A	830	A
1	A	831	U
1	A	832	G
1	A	837	U
1	A	839	G
1	A	847	A
1	A	852	G
1	A	853	C
1	A	858	U
1	A	859	C
1	A	866	A
1	A	874	U
1	A	875	U
1	A	878	G
1	A	890	G
1	A	891	G
1	A	892	U
1	A	893	A
1	A	906	G
1	A	908	A
1	A	913	A
1	A	914	C
1	A	916	G
1	A	919	U
1	A	923	C
1	A	928	G
1	A	929	G
1	A	931	C

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Mol	Chain	Res	Type
1	A	933	C
1	A	934	U
1	A	935	A
1	A	936	C
1	A	937	C
1	A	939	G
1	A	940	G
1	A	941	U
1	A	942	U
1	A	943	A
1	A	944	C
1	A	948	A
1	A	953	G
1	A	954	U
1	A	957	A
1	A	958	A
1	A	959	C
1	A	962	C
1	A	964	A
1	A	970	A
1	A	973	G
1	A	975	C
1	A	977	U
1	A	980	C
1	A	987	A
1	A	992	G
1	A	999	A
1	A	1003	A
1	A	1006	A
1	A	1007	G
1	A	1019	A
1	A	1020	A
1	A	1026	A
1	A	1029	A
1	A	1031	C
1	A	1036	A
1	A	1037	C
1	A	1042	A
1	A	1051	C
1	A	1054	A
1	A	1055	A
1	A	1058	U

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Mol	Chain	Res	Type
1	A	1059	A
1	A	1067	A
1	A	1068	G
1	A	1069	U
1	A	1070	G
1	A	1071	G
1	A	1072	A
1	A	1073	A
1	A	1079	U
1	A	1086	U
1	A	1091	U
1	A	1101	G
1	A	1102	G
1	A	1103	A
1	A	1106	U
1	A	1110	C
1	A	1111	U
1	A	1116	A
1	A	1117	G
1	A	1118	C
1	A	1119	A
1	A	1120	G
1	A	1121	C
1	A	1122	C
1	A	1123	A
1	A	1124	C
1	A	1125	C
1	A	1127	U
1	A	1128	U
1	A	1134	A
1	A	1142	A
1	A	1143	U
1	A	1145	G
1	A	1146	C
1	A	1157	A
1	A	1158	G
1	A	1159	U
1	A	1160	G
1	A	1161	A
1	A	1173	A
1	A	1174	A
1	A	1176	U

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Mol	Chain	Res	Type
1	A	1178	U
1	A	1179	A
1	A	1180	C
1	A	1181	C
1	A	1182	G
1	A	1185	G
1	A	1188	A
1	A	1197	A
1	A	1201	A
1	A	1203	G
1	A	1210	A
1	A	1221	A
1	A	1235	A
1	A	1236	G
1	A	1244	A
1	A	1245	G
1	A	1248	C
1	A	1249	U
1	A	1250	G
1	A	1251	U
1	A	1252	G
1	A	1259	G
1	A	1260	A
1	A	1261	C
1	A	1270	C
1	A	1276	G
1	A	1278	G
1	A	1280	G
1	A	1281	C
1	A	1282	U
1	A	1290	G
1	A	1293	A
1	A	1294	A
1	A	1295	U
1	A	1296	G
1	A	1306	G
1	A	1307	U
1	A	1311	G
1	A	1312	A
1	A	1313	A
1	A	1314	A
1	A	1315	G

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Mol	Chain	Res	Type
1	A	1323	A
1	A	1325	A
1	A	1330	C
1	A	1333	C
1	A	1339	A
1	A	1340	A
1	A	1341	U
1	A	1343	C
1	A	1344	C
1	A	1346	A
1	A	1351	U
1	A	1352	U
1	A	1354	C
1	A	1362	G
1	A	1363	G
1	A	1364	C
1	A	1365	U
1	A	1366	C
1	A	1368	U
1	A	1369	C
1	A	1370	C
1	A	1371	G
1	A	1372	C
1	A	1375	A
1	A	1376	G
1	A	1384	C
1	A	1385	G
1	A	1388	A
1	A	1389	C
1	A	1391	U
1	A	1404	A
1	A	1417	A
1	A	1418	U
1	A	1422	C
1	A	1423	A
1	A	1424	A
1	A	1425	C
1	A	1426	A
1	A	1435	U
1	A	1436	U
1	A	1442	A
1	A	1443	C

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Mol	Chain	Res	Type
1	A	1448	U
1	A	1449	C
1	A	1451	U
1	A	1457	U
1	A	1459	U
1	A	1460	G
1	A	1465	A
1	A	1467	G
1	A	1472	G
1	A	1473	A
1	A	1475	G
1	A	1481	G
1	A	1487	G
1	A	1489	U
1	A	1490	A
1	A	1499	A
1	A	1500	U
1	A	1502	G
1	A	1506	A
1	A	1507	U
1	A	1508	C
1	A	1516	A
1	A	1522	U
1	A	1525	G
1	A	1526	G
1	A	1527	C
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	G
1	A	1532	A
1	A	1536	A
1	A	1539	C
1	A	1540	A
1	A	1542	A
1	A	1543	U
1	A	1544	C
1	A	1545	C
1	A	1549	U
1	A	1550	C
1	A	1551	C
1	A	1553	A

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Mol	Chain	Res	Type
1	A	1556	A
1	A	1557	G
1	A	1558	G
1	A	1559	C
1	A	1560	U
1	A	1561	G
1	A	1562	A
1	A	1563	G
1	A	1566	G
1	A	1568	G
1	A	1569	A
1	A	1570	U
1	A	1571	G
1	A	1573	C
1	A	1602	U
1	A	1606	A
1	A	1607	C
1	A	1608	A
1	A	1613	C
1	A	1617	A
1	A	1626	U
1	A	1628	G
1	A	1631	A
1	A	1632	G
1	A	1645	C
1	A	1653	A
1	A	1655	A
1	A	1657	C
1	A	1658	G
1	A	1661	A
1	A	1672	A
1	A	1679	A
1	A	1680	A
1	A	1691	A
1	A	1692	U
1	A	1693	C
1	A	1694	G
1	A	1696	G
1	A	1697	A
1	A	1699	A
1	A	1700	A
1	A	1708	U

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Mol	Chain	Res	Type
1	A	1709	A
1	A	1712	G
1	A	1717	C
1	A	1719	G
1	A	1720	C
1	A	1727	A
1	A	1738	U
1	A	1740	G
1	A	1745	A
1	A	1746	A
1	A	1748	G
1	A	1750	G
1	A	1752	G
1	A	1753	C
1	A	1757	G
1	A	1758	U
1	A	1759	U
1	A	1760	A
1	A	1762	G
1	A	1766	C
1	A	1768	A
1	A	1771	C
1	A	1776	A
1	A	1777	G
1	A	1778	A
1	A	1779	G
1	A	1781	C
1	A	1782	G
1	A	1783	C
1	A	1785	G
1	A	1789	A
1	A	1790	U
1	A	1792	G
1	A	1793	G
1	A	1797	A
1	A	1802	A
1	A	1810	G
1	A	1811	C
1	A	1812	A
1	A	1813	A
1	A	1814	A
1	A	1815	A

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Mol	Chain	Res	Type
1	A	1829	C
1	A	1830	G
1	A	1831	A
1	A	1833	G
1	A	1839	A
1	A	1843	G
1	A	1845	A
1	A	1846	G
1	A	1849	U
1	A	1858	A
1	A	1867	C
1	A	1872	C
1	A	1877	A
1	A	1882	A
1	A	1883	A
1	A	1884	G
1	A	1885	A
1	A	1887	G
1	A	1895	A
1	A	1899	U
1	A	1902	G
1	A	1904	G
1	A	1932	G
1	A	1935	G
1	A	1941	A
1	A	1942	A
1	A	1943	C
1	A	1944	U
1	A	1946	U
1	A	1952	U
1	A	1956	A
1	A	1958	G
1	A	1959	G
1	A	1966	A
1	A	1967	A
1	A	1968	U
1	A	1969	U
1	A	1970	C
1	A	1972	U
1	A	1973	U
1	A	1984	U
1	A	1992	C

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Mol	Chain	Res	Type
1	A	1993	G
1	A	1995	A
1	A	1996	C
1	A	1999	A
1	A	2000	A
1	A	2001	G
1	A	2004	G
1	A	2010	A
1	A	2020	U
1	A	2022	U
1	A	2025	C
1	A	2026	A
1	A	2033	G
1	A	2050	G
1	A	2051	U
1	A	2052	A
1	A	2053	C
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2064	G
1	A	2065	C
1	A	2068	G
1	A	2070	U
1	A	2072	C
1	A	2079	C
1	A	2080	A
1	A	2081	G
1	A	2084	C
1	A	2085	G
1	A	2089	A
1	A	2090	G
1	A	2098	G
1	A	2101	G
1	A	2121	U
1	A	2123	A
1	A	2125	U
1	A	2128	U
1	A	2131	U
1	A	2134	A
1	A	2135	G

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Mol	Chain	Res	Type
1	A	2136	C
1	A	2139	G
1	A	2140	U
1	A	2145	G
1	A	2146	A
1	A	2147	U
1	A	2149	G
1	A	2156	G
1	A	2160	U
1	A	2161	G
1	A	2162	G
1	A	2166	C
1	A	2174	C
1	A	2175	C
1	A	2176	A
1	A	2177	G
1	A	2185	G
1	A	2187	A
1	A	2198	G
1	A	2200	A
1	A	2201	U
1	A	2202	A
1	A	2203	C
1	A	2205	A
1	A	2206	C
1	A	2208	C
1	A	2210	G
1	A	2212	C
1	A	2213	U
1	A	2217	U
1	A	2219	G
1	A	2228	A
1	A	2232	G
1	A	2233	C
1	A	2240	U
1	A	2241	A
1	A	2242	U
1	A	2244	G
1	A	2245	G
1	A	2246	G
1	A	2249	G
1	A	2252	A

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Mol	Chain	Res	Type
1	A	2254	A
1	A	2255	C
1	A	2260	U
1	A	2267	G
1	A	2268	G
1	A	2295	A
1	A	2296	A
1	A	2307	A
1	A	2308	G
1	A	2311	G
1	A	2312	C
1	A	2316	A
1	A	2317	A
1	A	2323	C
1	A	2324	C
1	A	2325	U
1	A	2327	A
1	A	2331	U
1	A	2332	G
1	A	2333	G
1	A	2334	U
1	A	2335	U
1	A	2336	G
1	A	2338	A
1	A	2340	A
1	A	2341	U
1	A	2342	C
1	A	2343	A
1	A	2344	U
1	A	2345	U
1	A	2348	C
1	A	2349	A
1	A	2350	G
1	A	2354	G
1	A	2356	A
1	A	2357	A
1	A	2363	C
1	A	2364	A
1	A	2368	G
1	A	2374	G
1	A	2376	C
1	A	2379	C

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Mol	Chain	Res	Type
1	A	2381	A
1	A	2387	A
1	A	2390	A
1	A	2401	G
1	A	2406	A
1	A	2408	G
1	A	2412	G
1	A	2413	G
1	A	2414	C
1	A	2418	G
1	A	2420	G
1	A	2431	U
1	A	2432	C
1	A	2435	C
1	A	2448	U
1	A	2451	C
1	A	2452	U
1	A	2453	C
1	A	2454	A
1	A	2455	A
1	A	2458	G
1	A	2459	A
1	A	2460	U
1	A	2464	A
1	A	2468	A
1	A	2469	C
1	A	2470	C
1	A	2476	G
1	A	2477	A
1	A	2488	A
1	A	2497	A
1	A	2503	C
1	A	2505	A
1	A	2506	C
1	A	2507	A
1	A	2511	A
1	A	2523	G
1	A	2524	G
1	A	2525	C
1	A	2527	C
1	A	2531	G
1	A	2532	A

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Mol	Chain	Res	Type
1	A	2533	U
1	A	2534	G
1	A	2547	A
1	A	2554	G
1	A	2558	G
1	A	2563	C
1	A	2564	G
1	A	2570	A
1	A	2583	U
1	A	2593	A
1	A	2595	A
1	A	2596	G
1	A	2598	G
1	A	2601	A
1	A	2602	C
1	A	2607	G
1	A	2612	G
1	A	2613	U
1	A	2614	U
1	A	2615	C
1	A	2630	C
1	A	2631	A
1	A	2638	U
1	A	2642	U
1	A	2644	U
1	A	2654	G
1	A	2659	G
1	A	2660	G
1	A	2667	G
1	A	2674	G
1	A	2675	C
1	A	2689	A
1	A	2692	G
1	A	2696	C
1	A	2702	G
1	A	2711	G
1	A	2714	G
1	A	2718	U
1	A	2720	C
1	A	2743	G
1	A	2747	G
1	A	2753	U

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Mol	Chain	Res	Type
1	A	2755	U
1	A	2760	G
1	A	2762	A
1	A	2764	G
1	A	2765	G
1	A	2766	G
1	A	2773	G
1	A	2777	A
1	A	2784	C
1	A	2785	U
1	A	2786	A
1	A	2789	C
1	A	2794	A
1	A	2795	G
1	A	2806	G
1	A	2807	A
1	A	2808	U
1	A	2818	C
1	A	2821	U
1	A	2822	C
1	A	2823	C
1	A	2824	G
1	A	2826	A
1	A	2828	G
1	A	2831	A
1	A	2832	G
1	A	2833	U
1	A	2843	G
1	A	2855	G
1	A	2859	G
1	A	2860	A
1	A	2862	A
1	A	2866	C
1	A	2868	G
1	A	2874	G
1	A	2886	C
1	A	2891	G
1	A	2892	G
1	A	2897	G
1	A	2900	A
1	A	2901	G
1	A	2905	C

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Mol	Chain	Res	Type
1	A	2908	A
1	A	2916	A
1	A	2917	G
2	B	10	G
2	B	12	U
2	B	15	C
2	B	22	G
2	B	23	U
2	B	28	C
2	B	31	G
2	B	32	U
2	B	33	U
2	B	34	C
2	B	38	U
2	B	39	A
2	B	40	C
2	B	41	C
2	B	42	G
2	B	47	C
2	B	48	G
2	B	49	G
2	B	50	A
2	B	52	G
2	B	53	U
2	B	54	U
2	B	55	A
2	B	59	U
2	B	60	C
2	B	62	U
2	B	63	C
2	B	64	A
2	B	65	G
2	B	66	C
2	B	85	U
2	B	86	U
2	B	87	U
2	B	88	C
2	B	97	A
2	B	101	U
2	B	106	C
2	B	107	G
2	B	110	G

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Mol	Chain	Res	Type
2	B	114	A
33	a	9	G
33	a	10	A
33	a	11	G
33	a	24	G
33	a	32	C
33	a	33	G
33	a	34	A
33	a	41	G
33	a	46	G
33	a	49	C
33	a	50	C
33	a	51	U
33	a	52	A
33	a	53	A
33	a	60	C
33	a	65	C
33	a	66	G
33	a	72	A
33	a	75	G
33	a	77	U
33	a	80	G
33	a	84	U
33	a	85	U
33	a	86	G
33	a	87	C
33	a	88	U
33	a	89	C
33	a	90	C
33	a	92	U
33	a	93	G
33	a	99	A
33	a	114	A
33	a	117	A
33	a	118	A
33	a	119	C
33	a	120	A
33	a	128	A
33	a	129	A
33	a	130	C
33	a	136	U
33	a	137	G

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Mol	Chain	Res	Type
33	a	140	A
33	a	141	G
33	a	142	A
33	a	144	U
33	a	153	U
33	a	154	C
33	a	158	G
33	a	162	C
33	a	167	G
33	a	172	U
33	a	176	G
33	a	181	G
33	a	182	U
33	a	189	A
33	a	190	A
33	a	193	G
33	a	194	C
33	a	197	G
33	a	207	U
33	a	208	A
33	a	209	A
33	a	211	A
33	a	218	U
33	a	219	U
33	a	220	C
33	a	221	G
33	a	222	G
33	a	249	G
33	a	253	U
33	a	255	G
33	a	259	G
33	a	262	G
33	a	274	G
33	a	275	C
33	a	277	C
33	a	280	C
33	a	287	A
33	a	288	C
33	a	297	G
33	a	306	A
33	a	314	A
33	a	316	C

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Mol	Chain	Res	Type
33	a	321	A
33	a	329	A
33	a	336	C
33	a	337	A
33	a	338	C
33	a	340	G
33	a	352	A
33	a	353	C
33	a	355	G
33	a	357	A
33	a	359	G
33	a	360	C
33	a	362	G
33	a	371	A
33	a	373	U
33	a	375	U
33	a	380	C
33	a	383	U
33	a	385	G
33	a	390	A
33	a	392	G
33	a	396	G
33	a	400	G
33	a	405	A
33	a	406	C
33	a	414	G
33	a	419	A
33	a	420	U
33	a	421	G
33	a	426	U
33	a	429	U
33	a	430	C
33	a	432	G
33	a	436	G
33	a	437	U
33	a	438	A
33	a	439	A
33	a	442	C
33	a	447	U
33	a	456	A
33	a	457	A
33	a	459	A

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Mol	Chain	Res	Type
33	a	460	A
33	a	461	C
33	a	465	U
33	a	466	G
33	a	467	C
33	a	473	G
33	a	474	A
33	a	476	U
33	a	477	A
33	a	478	G
33	a	480	G
33	a	483	G
33	a	484	U
33	a	485	A
33	a	487	C
33	a	488	U
33	a	490	G
33	a	491	A
33	a	494	G
33	a	506	A
33	a	508	A
33	a	518	A
33	a	519	A
33	a	520	C
33	a	526	G
33	a	527	C
33	a	530	G
33	a	533	G
33	a	536	G
33	a	539	G
33	a	540	U
33	a	541	A
33	a	542	A
33	a	553	G
33	a	554	C
33	a	556	A
33	a	563	U
33	a	564	C
33	a	568	A
33	a	571	U
33	a	573	U
33	a	581	A

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Mol	Chain	Res	Type
33	a	582	A
33	a	585	G
33	a	586	G
33	a	588	U
33	a	591	C
33	a	597	G
33	a	616	A
33	a	627	C
33	a	628	U
33	a	629	C
33	a	641	G
33	a	642	U
33	a	643	C
33	a	648	G
33	a	650	A
33	a	661	U
33	a	662	U
33	a	670	G
33	a	674	A
33	a	694	G
33	a	696	A
33	a	704	A
33	a	727	A
33	a	732	U
33	a	733	G
33	a	740	G
33	a	742	G
33	a	745	U
33	a	756	U
33	a	757	A
33	a	758	A
33	a	762	A
33	a	764	G
33	a	768	A
33	a	787	G
33	a	802	U
33	a	803	A
33	a	806	C
33	a	815	C
33	a	821	G
33	a	824	A
33	a	826	C

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Mol	Chain	Res	Type
33	a	828	A
33	a	829	U
33	a	841	G
33	a	845	G
33	a	849	G
33	a	853	C
33	a	855	G
33	a	856	C
33	a	861	U
33	a	880	U
33	a	884	G
33	a	885	C
33	a	895	G
33	a	899	A
33	a	909	C
33	a	924	A
33	a	932	G
33	a	936	G
33	a	944	C
33	a	945	A
33	a	952	G
33	a	964	G
33	a	966	U
33	a	967	U
33	a	968	A
33	a	970	U
33	a	975	A
33	a	976	G
33	a	978	A
33	a	979	A
33	a	981	G
33	a	984	A
33	a	985	A
33	a	986	G
33	a	987	A
33	a	992	U
33	a	993	A
33	a	999	U
33	a	1000	C
33	a	1002	U
33	a	1003	G
33	a	1006	A

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Mol	Chain	Res	Type
33	a	1008	C
33	a	1009	C
33	a	1010	U
33	a	1011	C
33	a	1012	U
33	a	1014	A
33	a	1015	C
33	a	1017	A
33	a	1019	C
33	a	1020	C
33	a	1023	G
33	a	1024	A
33	a	1027	U
33	a	1028	A
33	a	1030	G
33	a	1031	A
33	a	1033	G
33	a	1035	C
33	a	1036	C
33	a	1039	U
33	a	1040	U
33	a	1041	C
33	a	1042	G
33	a	1043	G
33	a	1046	G
33	a	1047	C
33	a	1050	A
33	a	1051	G
33	a	1052	U
33	a	1053	G
33	a	1056	A
33	a	1058	G
33	a	1060	G
33	a	1064	C
33	a	1071	G
33	a	1074	G
33	a	1075	U
33	a	1095	U
33	a	1102	A
33	a	1104	G
33	a	1105	U
33	a	1110	C

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Mol	Chain	Res	Type
33	a	1111	A
33	a	1112	A
33	a	1114	G
33	a	1118	G
33	a	1124	C
33	a	1128	A
33	a	1134	G
33	a	1136	U
33	a	1140	A
33	a	1141	G
33	a	1142	C
33	a	1143	A
33	a	1145	U
33	a	1148	G
33	a	1149	U
33	a	1150	U
33	a	1151	G
33	a	1153	G
33	a	1155	A
33	a	1163	G
33	a	1166	A
33	a	1167	C
33	a	1168	U
33	a	1169	G
33	a	1170	C
33	a	1176	A
33	a	1177	C
33	a	1178	A
33	a	1180	A
33	a	1190	G
33	a	1192	U
33	a	1193	G
33	a	1205	A
33	a	1206	A
33	a	1209	C
33	a	1211	U
33	a	1214	U
33	a	1221	U
33	a	1222	A
33	a	1224	G
33	a	1233	U
33	a	1235	C

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Mol	Chain	Res	Type
33	a	1236	A
33	a	1237	C
33	a	1238	A
33	a	1239	C
33	a	1245	A
33	a	1247	A
33	a	1258	C
33	a	1259	A
33	a	1265	C
33	a	1266	A
33	a	1267	G
33	a	1269	G
33	a	1279	G
33	a	1288	A
33	a	1289	A
33	a	1291	C
33	a	1294	A
33	a	1295	C
33	a	1296	A
33	a	1299	U
33	a	1307	C
33	a	1308	A
33	a	1309	G
33	a	1311	U
33	a	1312	C
33	a	1313	G
33	a	1314	G
33	a	1323	C
33	a	1326	C
33	a	1329	C
33	a	1331	C
33	a	1332	G
33	a	1336	G
33	a	1340	G
33	a	1345	U
33	a	1347	G
33	a	1349	A
33	a	1354	U
33	a	1355	A
33	a	1362	G
33	a	1366	A
33	a	1371	C

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Mol	Chain	Res	Type
33	a	1372	A
33	a	1373	U
33	a	1377	G
33	a	1379	G
33	a	1387	C
33	a	1403	A
33	a	1406	C
33	a	1407	A
33	a	1413	C
33	a	1428	G
33	a	1435	A
33	a	1451	A
33	a	1452	G
33	a	1455	A
33	a	1461	U
33	a	1462	U
33	a	1463	A
33	a	1464	G
33	a	1478	A
33	a	1494	U
33	a	1496	G
33	a	1497	G
33	a	1500	U
33	a	1502	A
33	a	1503	A
33	a	1507	G
33	a	1513	A
33	a	1515	G
33	a	1516	U
33	a	1517	A
33	a	1527	G
33	a	1529	A
33	a	1539	G
33	a	1540	G
53	x	6	G
53	x	8	U
53	x	9	G
53	x	13	G
53	x	16	U
53	x	17	U
53	x	17(A)	G
53	x	18	G

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Mol	Chain	Res	Type
53	x	19	U
53	x	20	A
53	x	21	G
53	x	22	A
53	x	23	C
53	x	25	C
53	x	26	G
53	x	36	G
53	x	41	U
53	x	43	G
53	x	44	U
53	x	51	G
53	x	52	G
53	x	53	G
53	x	56	C
53	x	60	U
53	x	61	C
53	x	63	C
53	x	70	G
53	x	75	C
53	x	76	A

All (93) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	62	C
1	A	88	G
1	A	92	G
1	A	118	A
1	A	163	U
1	A	181	G
1	A	199	A
1	A	236	A
1	A	252	C
1	A	347	G
1	A	410	G
1	A	411	G
1	A	441	C
1	A	455	G
1	A	458	G
1	A	459	A
1	A	482	C

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Mol	Chain	Res	Type
1	A	525	A
1	A	549	A
1	A	554	U
1	A	576	G
1	A	594	C
1	A	666	G
1	A	689	A
1	A	702	A
1	A	732	A
1	A	756	U
1	A	810	G
1	A	831	U
1	A	848	G
1	A	855	G
1	A	933	C
1	A	1028	C
1	A	1032	C
1	A	1036	A
1	A	1041	C
1	A	1172	A
1	A	1176	U
1	A	1187	U
1	A	1210	A
1	A	1226	U
1	A	1243	A
1	A	1250	G
1	A	1260	A
1	A	1266	A
1	A	1269	A
1	A	1294	A
1	A	1305	A
1	A	1325	A
1	A	1339	A
1	A	1351	U
1	A	1365	U
1	A	1448	U
1	A	1464	A
1	A	1507	U
1	A	1525	G
1	A	1529	G
1	A	1530	G
1	A	1535	U

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Mol	Chain	Res	Type
1	A	1543	U
1	A	1565	U
1	A	1570	U
1	A	1631	A
1	A	1671	G
1	A	1726	G
1	A	1751	U
1	A	1784	A
1	A	1813	A
1	A	1828	G
1	A	1844	A
1	A	1882	A
1	A	1883	A
1	A	1886	G
1	A	1991	C
1	A	2009	G
1	A	2127	U
1	A	2139	G
1	A	2155	A
1	A	2254	A
1	A	2295	A
1	A	2316	A
1	A	2356	A
1	A	2454	A
1	A	2456	C
1	A	2468	A
1	A	2531	G
1	A	2630	C
1	A	2710	C
1	A	2805	A
1	A	2904	A
2	B	37	A
2	B	48	G
2	B	49	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	TEL	A	3001	-	59,62,62	1.29	4 (6%)	77,92,92	1.97	13 (16%)
55	ATP	V	900	20	26,33,33	0.91	1 (3%)	31,52,52	1.66	6 (19%)
55	ATP	V	901	-	26,33,33	0.98	1 (3%)	31,52,52	1.83	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	TEL	A	3001	-	1/1/19/19	14/73/108/108	0/4/5/5
55	ATP	V	900	20	-	3/18/38/38	0/3/3/3
55	ATP	V	901	-	-	4/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A	3001	TEL	O5-C10	5.85	1.45	1.35
54	A	3001	TEL	O9-C15	4.91	1.45	1.34
54	A	3001	TEL	C36-N31	-2.79	1.34	1.38
54	A	3001	TEL	O5-C2	-2.74	1.43	1.47
55	V	901	ATP	C5-C4	2.38	1.47	1.40
55	V	900	ATP	C5-C4	2.13	1.46	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A	3001	TEL	O9-C15-C21	9.27	120.30	110.88
54	A	3001	TEL	C11-N6-C10	6.88	130.94	122.25
55	V	901	ATP	PB-O3B-PG	-6.13	111.78	132.83
54	A	3001	TEL	C17-C11-N6	-5.42	104.94	113.31
55	V	901	ATP	PA-O3A-PB	-5.15	115.17	132.83
55	V	900	ATP	PA-O3A-PB	-4.69	116.72	132.83
54	A	3001	TEL	C1-C2-C3	-4.60	111.15	116.69
54	A	3001	TEL	C4-O9-C15	-3.65	111.69	118.18
55	V	900	ATP	N3-C2-N1	-3.41	123.35	128.68
54	A	3001	TEL	O20-C15-C21	-3.21	120.55	124.77
55	V	901	ATP	N3-C2-N1	-3.19	123.69	128.68
54	A	3001	TEL	C8-C4-C2	-3.10	110.96	115.23
54	A	3001	TEL	C28-C24-C19	-2.97	111.07	116.11
55	V	900	ATP	PB-O3B-PG	-2.97	122.65	132.83
55	V	900	ATP	C4-C5-N7	-2.75	106.54	109.40
54	A	3001	TEL	O9-C15-O20	-2.56	119.15	123.94
54	A	3001	TEL	C56-N52-C47	2.50	121.17	116.85
54	A	3001	TEL	C42-O39-C34	-2.39	112.10	116.25
54	A	3001	TEL	C24-C19-C13	-2.29	109.38	113.32
55	V	901	ATP	C4-C5-N7	-2.26	107.05	109.40
54	A	3001	TEL	C54-C49-N53	-2.19	109.48	115.67
55	V	900	ATP	O2A-PA-O1A	2.07	122.50	112.24
55	V	900	ATP	O3G-PG-O2G	2.06	115.51	107.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
54	A	3001	TEL	C21

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	A	3001	TEL	C15-C21-C26-O29
54	A	3001	TEL	C15-C21-C26-C30
55	V	900	ATP	C5'-O5'-PA-O1A
55	V	901	ATP	C5'-O5'-PA-O1A
54	A	3001	TEL	C21-C15-O9-C4
54	A	3001	TEL	O20-C15-O9-C4
54	A	3001	TEL	O9-C4-C8-C14
54	A	3001	TEL	N6-C3-C7-C12
54	A	3001	TEL	C17-C22-C27-N31
54	A	3001	TEL	C17-C11-N6-C10
54	A	3001	TEL	O20-C15-C21-C25

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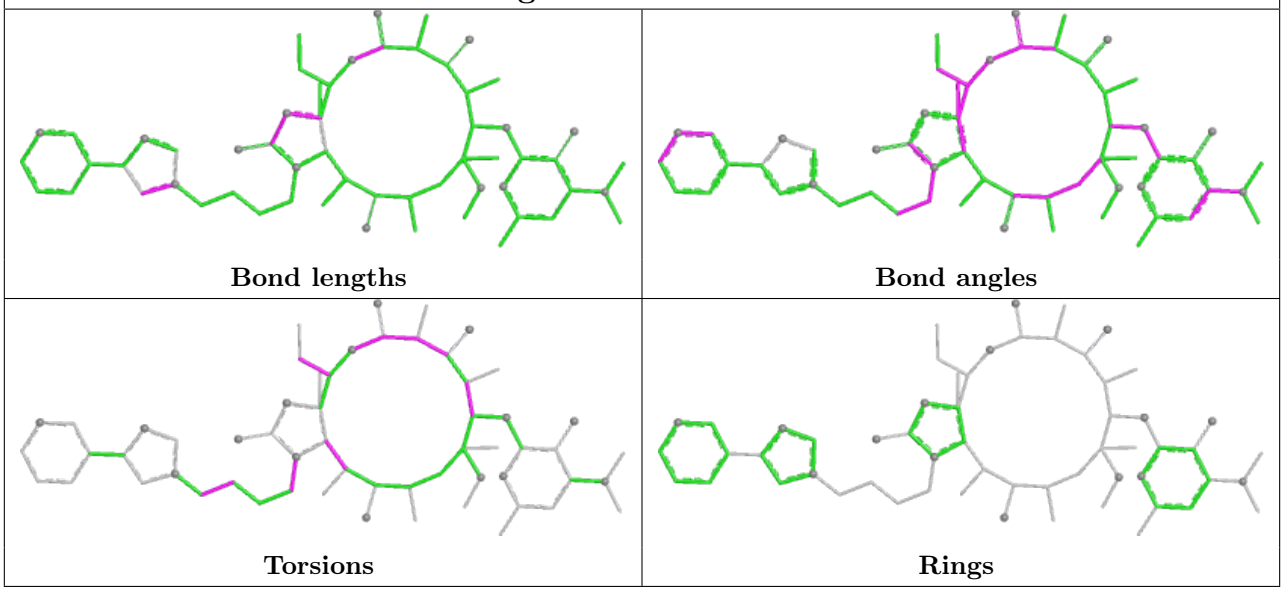
Mol	Chain	Res	Type	Atoms
54	A	3001	TEL	O9-C15-C21-C25
55	V	900	ATP	C5'-O5'-PA-O3A
55	V	901	ATP	C5'-O5'-PA-O3A
55	V	900	ATP	C5'-O5'-PA-O2A
55	V	901	ATP	C5'-O5'-PA-O2A
54	A	3001	TEL	C35-C30-C34-C28
54	A	3001	TEL	C2-C4-C8-C14
55	V	901	ATP	PB-O3A-PA-O1A
54	A	3001	TEL	O20-C15-C21-C26
54	A	3001	TEL	C26-C30-C34-C28

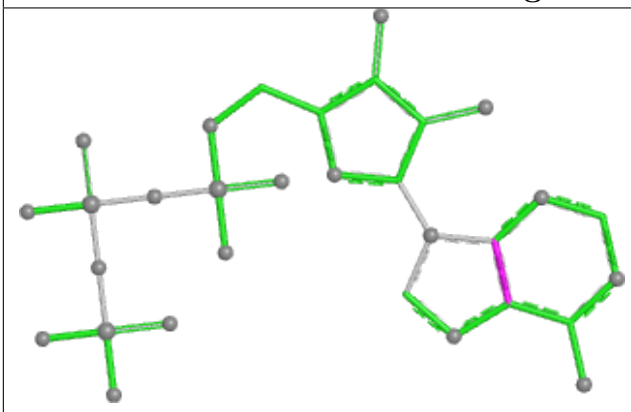
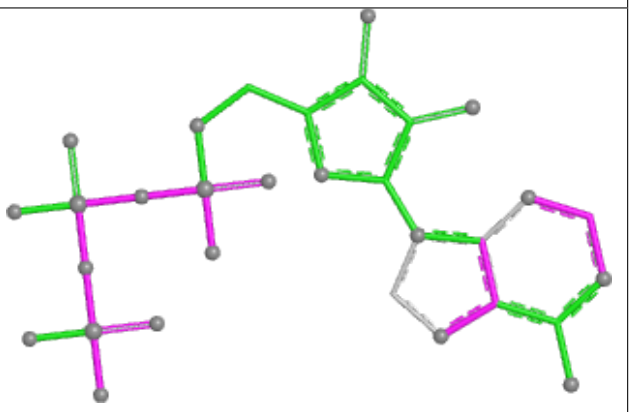
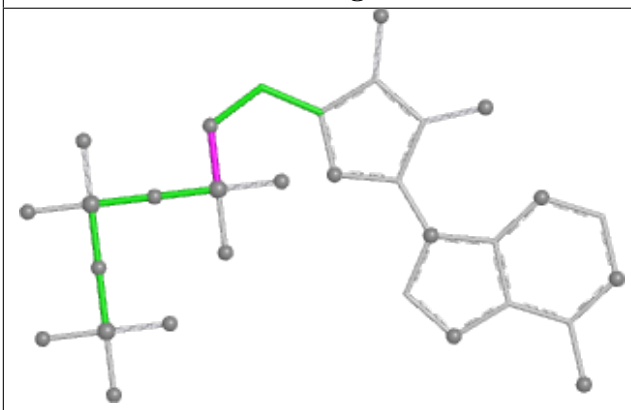
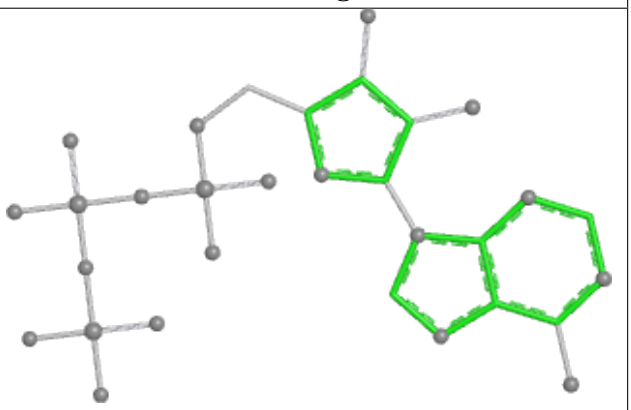
There are no ring outliers.

No monomer is involved in short contacts.

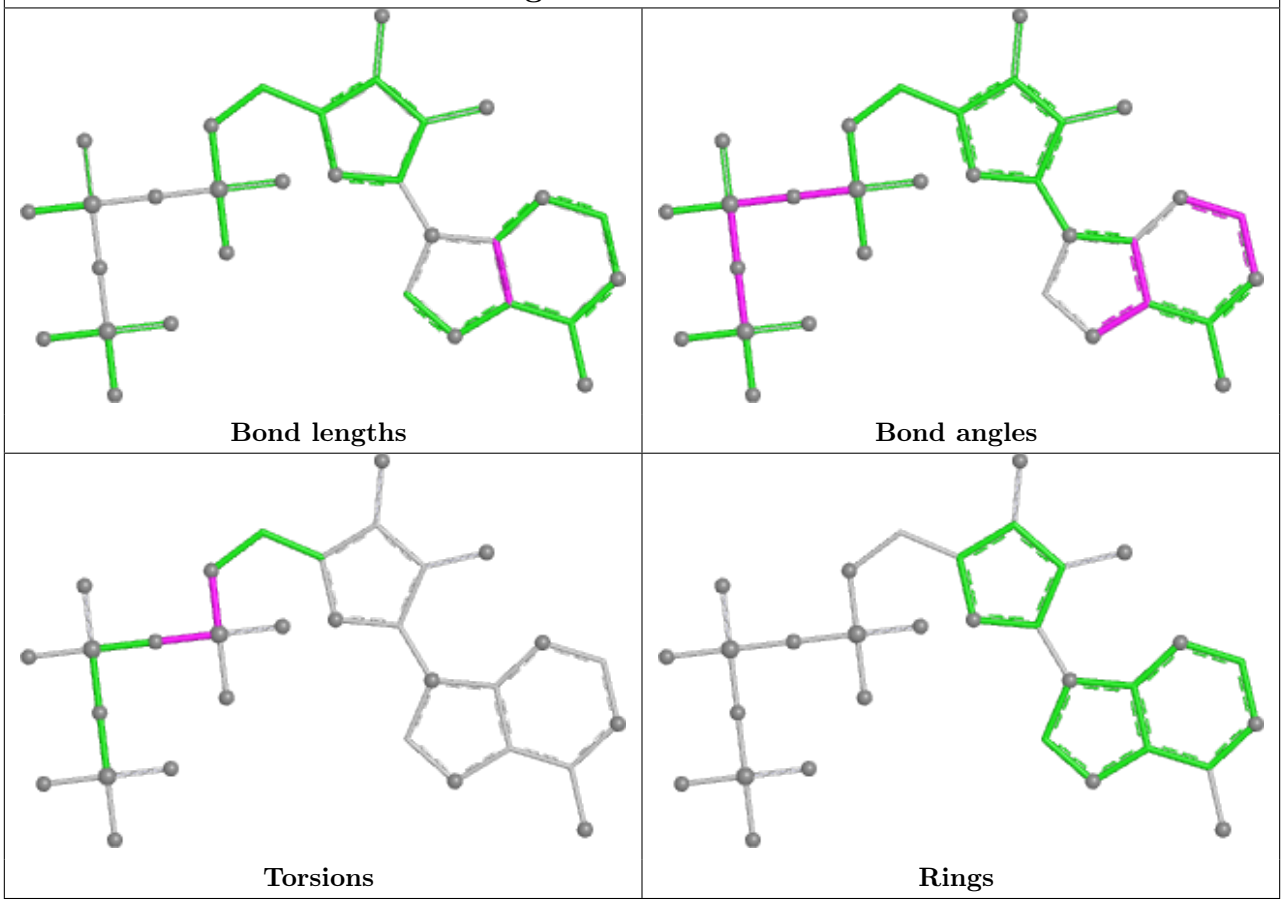
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 TEL A 3001



Ligand ATP V 900	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP V 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
53	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	44:U	O3'	47:U	P	14.81
1	A	182:C	O3'	183:A	P	6.43
1	A	1449:C	O3'	1450:C	P	4.34
1	A	1451:U	O3'	1452:C	P	3.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1452:C	O3'	1453:A	P	3.25
1	A	183:A	O3'	184:G	P	3.12

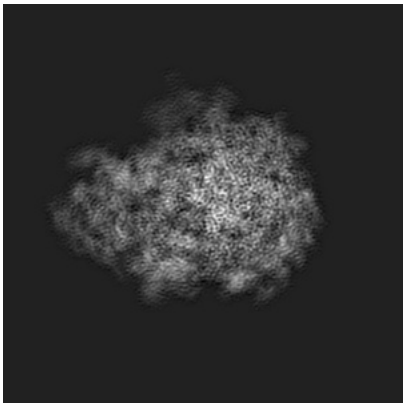
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0177. These allow visual inspection of the internal detail of the map and identification of artifacts.

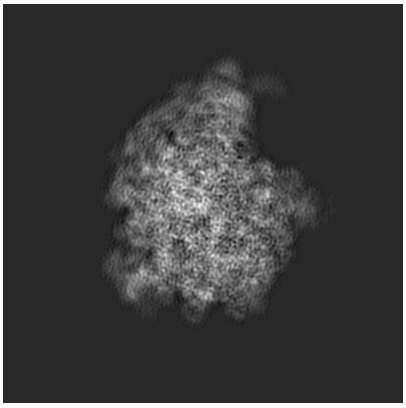
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

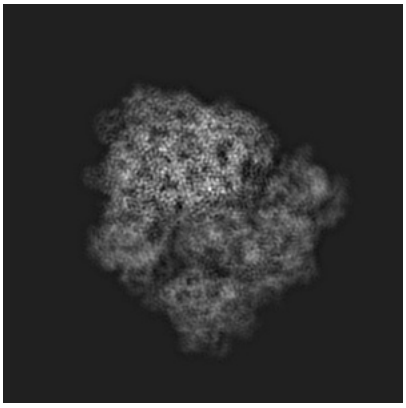
6.1.1 Primary map



X



Y

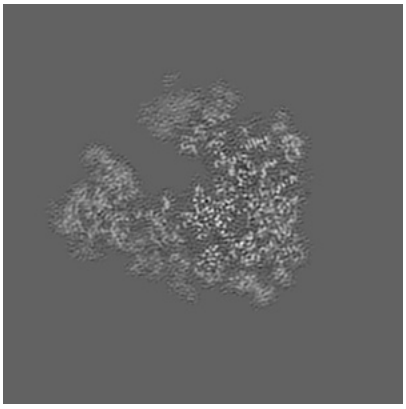


Z

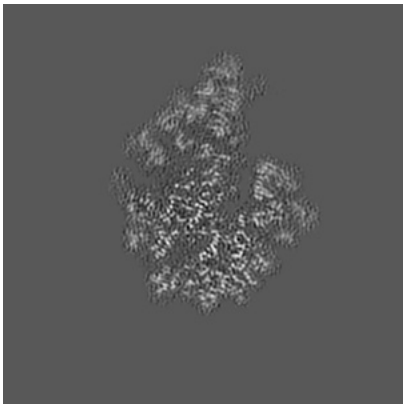
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

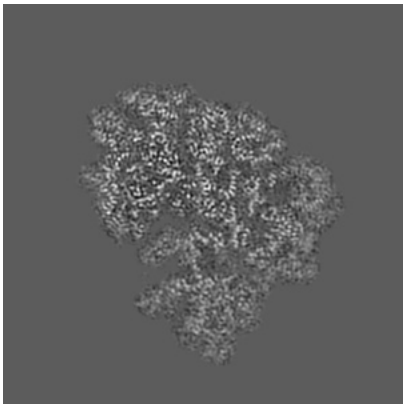
6.2.1 Primary map



X Index: 180



Y Index: 180

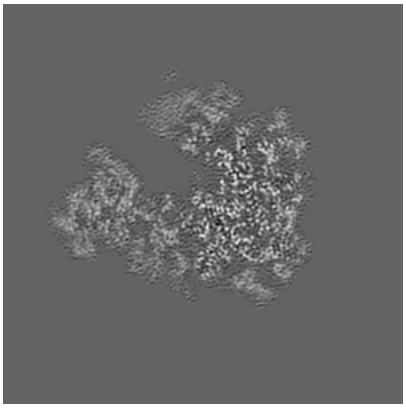


Z Index: 180

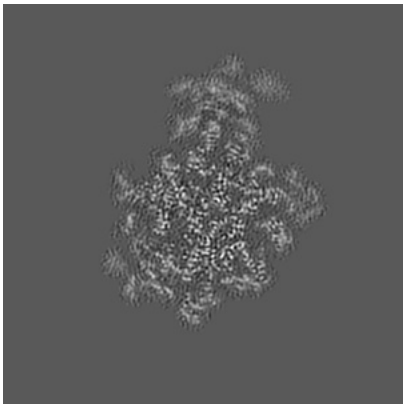
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

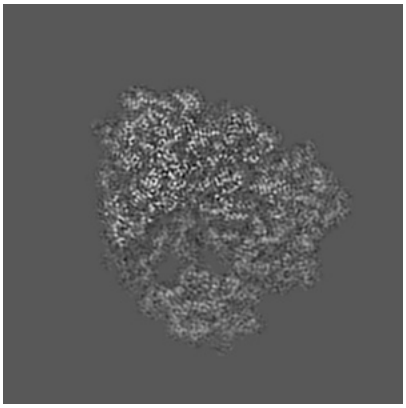
6.3.1 Primary map



X Index: 177



Y Index: 199

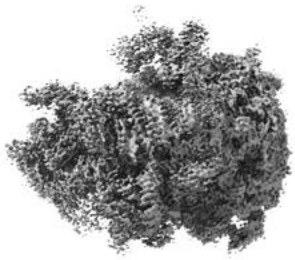


Z Index: 189

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

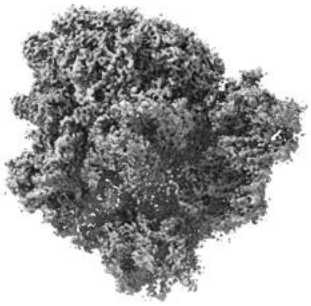
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

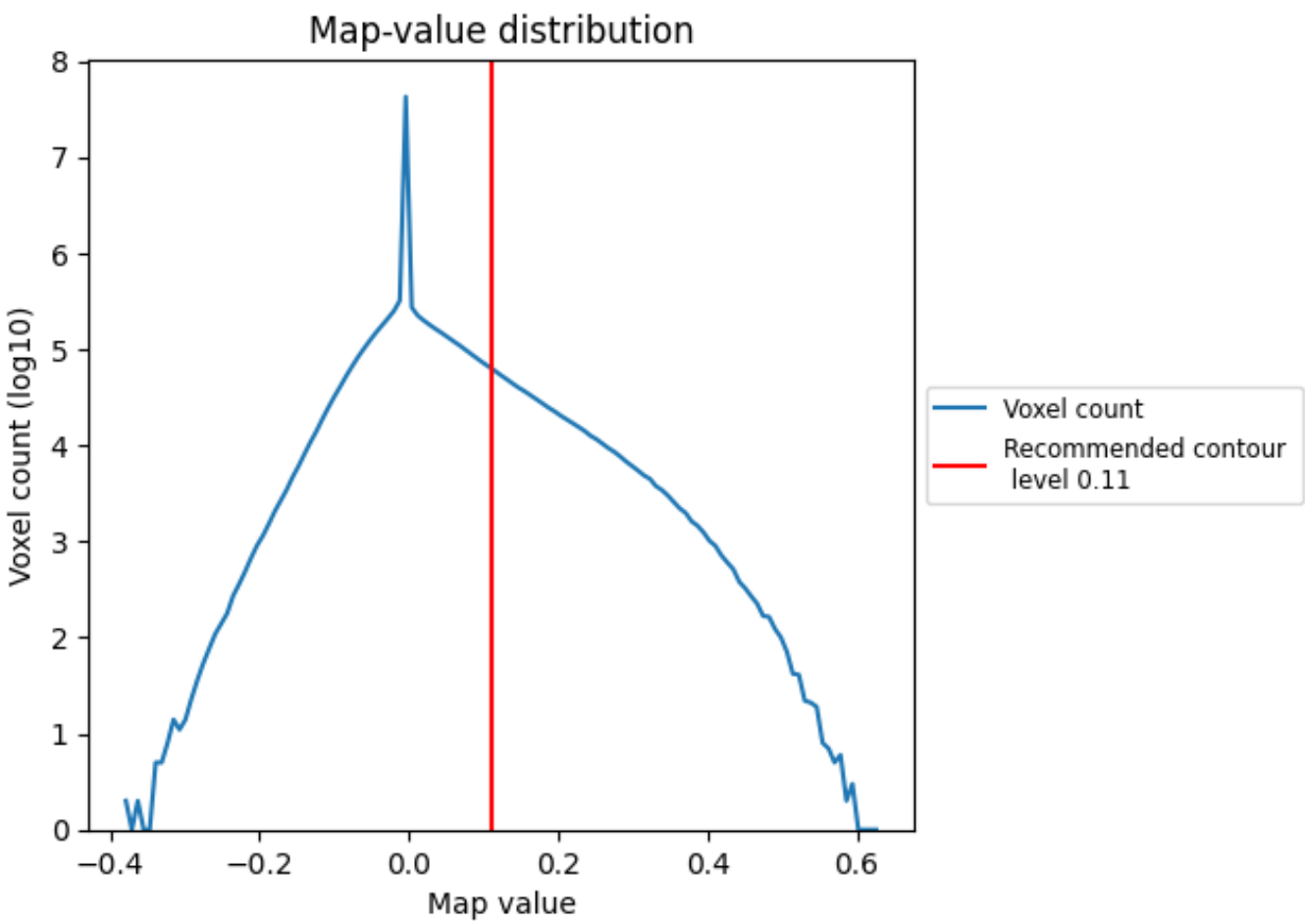
6.5 Mask visualisation (i)

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

7 Map analysis (i)

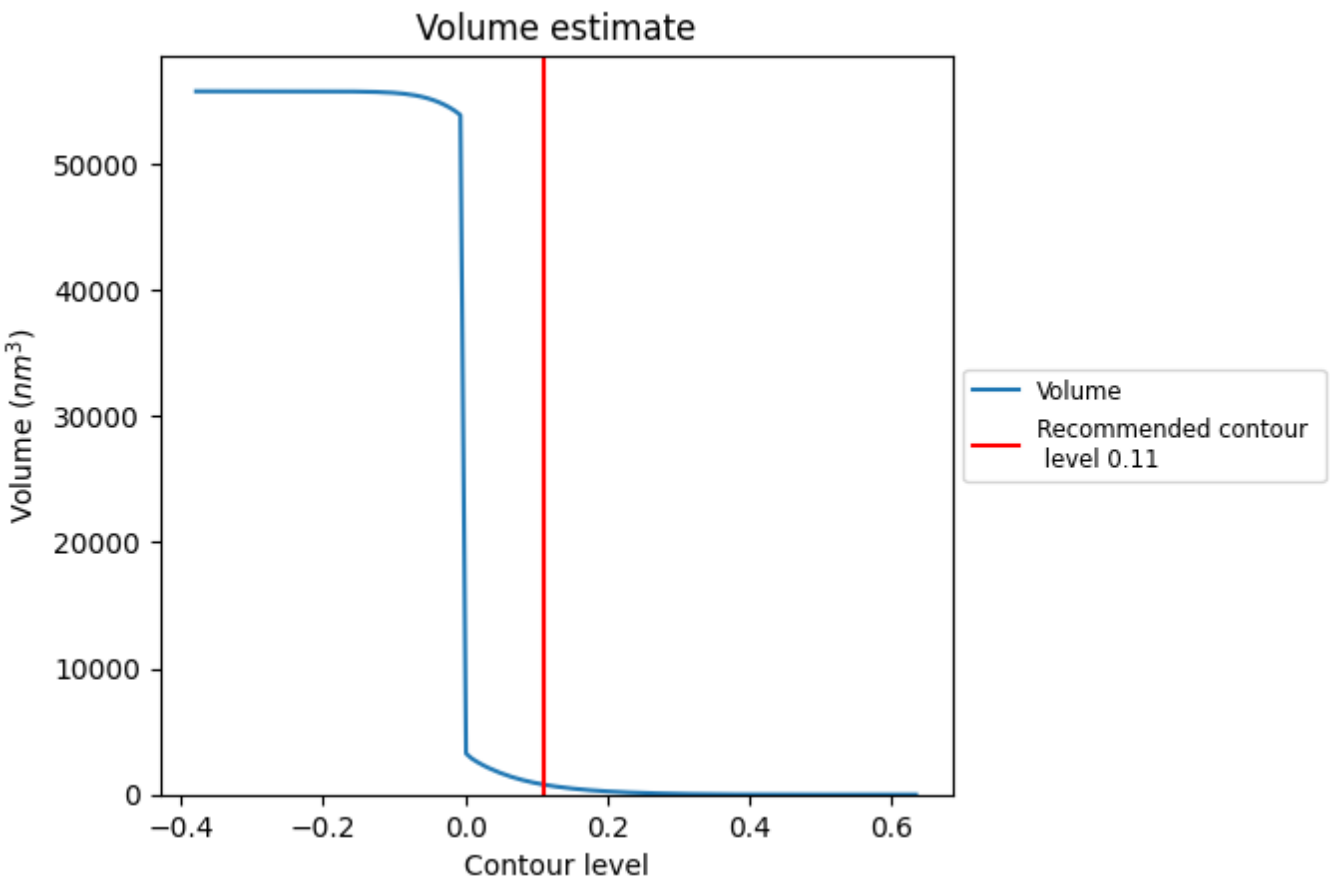
This section contains the results of statistical analysis of the map.

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.

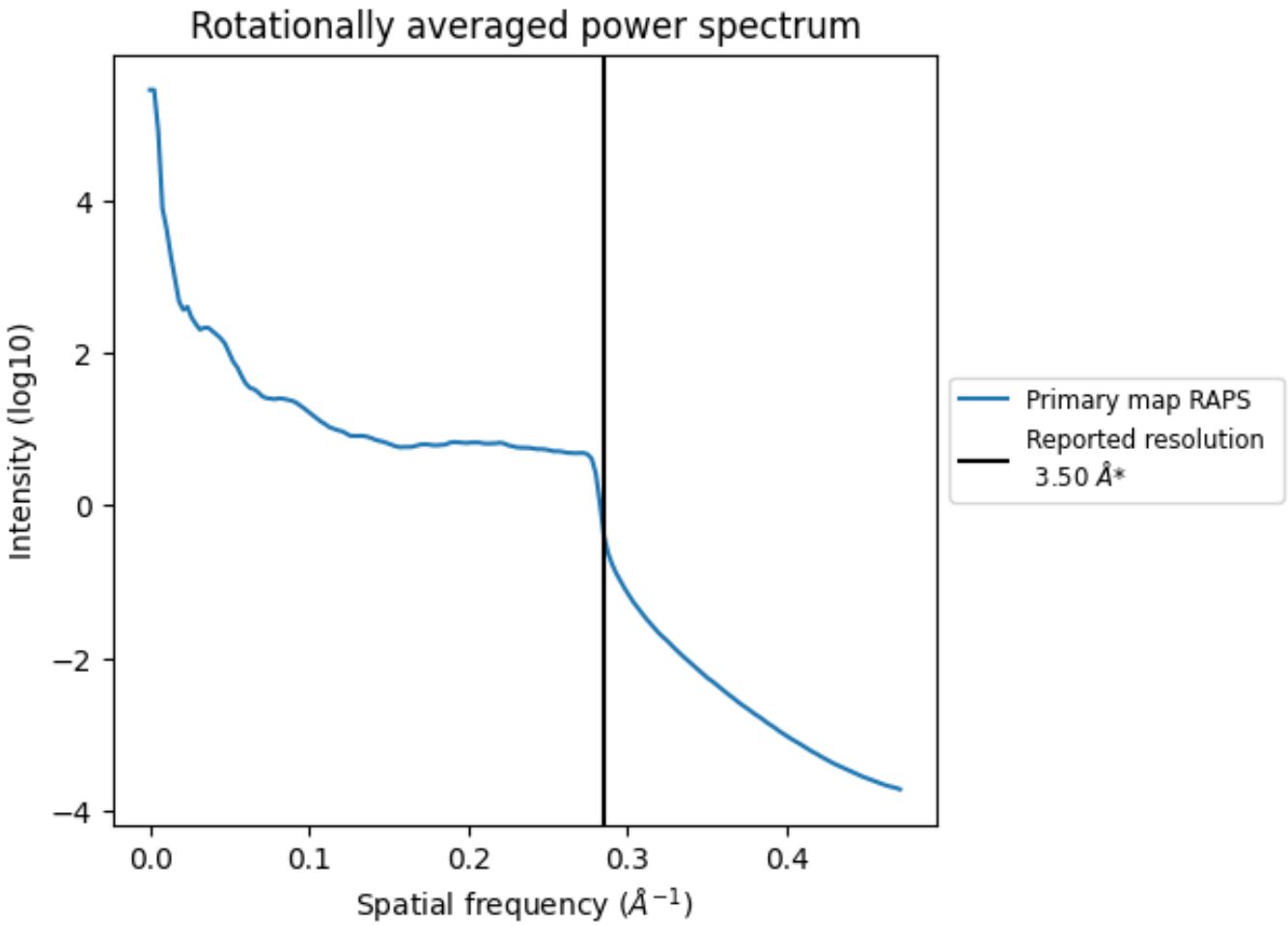
7.2 Volume estimate (i)



The volume at the recommended contour level is 793 nm^3; this corresponds to an approximate mass of 716 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

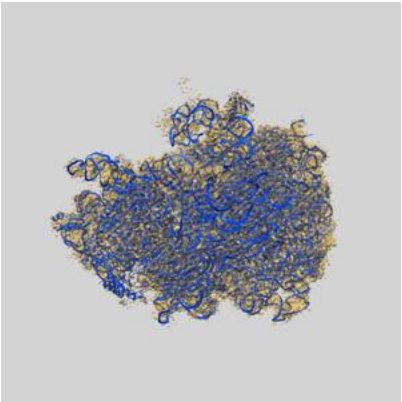
8 Fourier-Shell correlation (i)

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

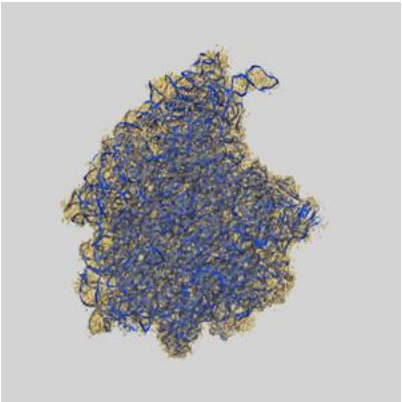
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0177 and PDB model 6HA8. Per-residue inclusion information can be found in section 3 on page 16.

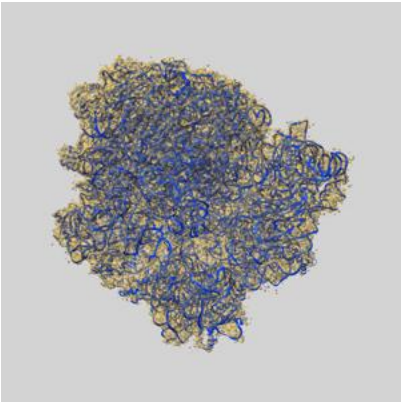
9.1 Map-model overlay (i)



X



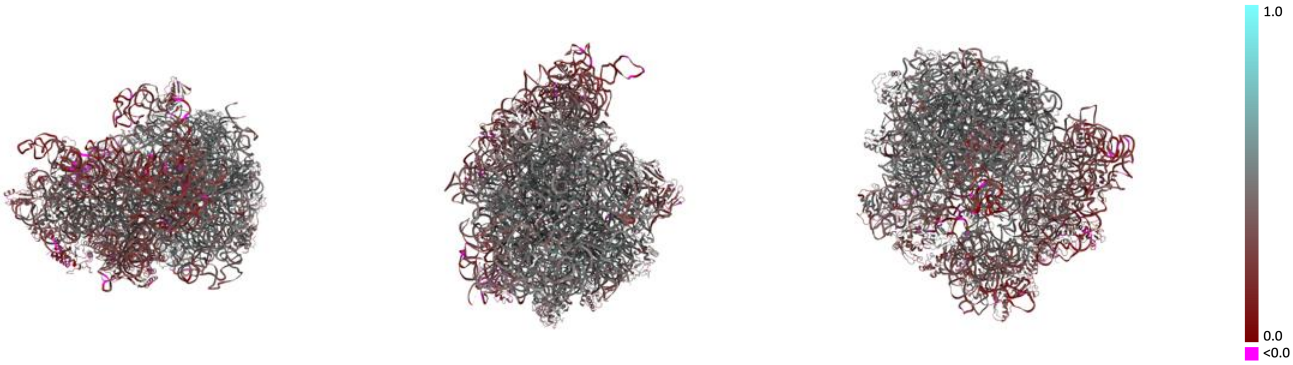
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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.

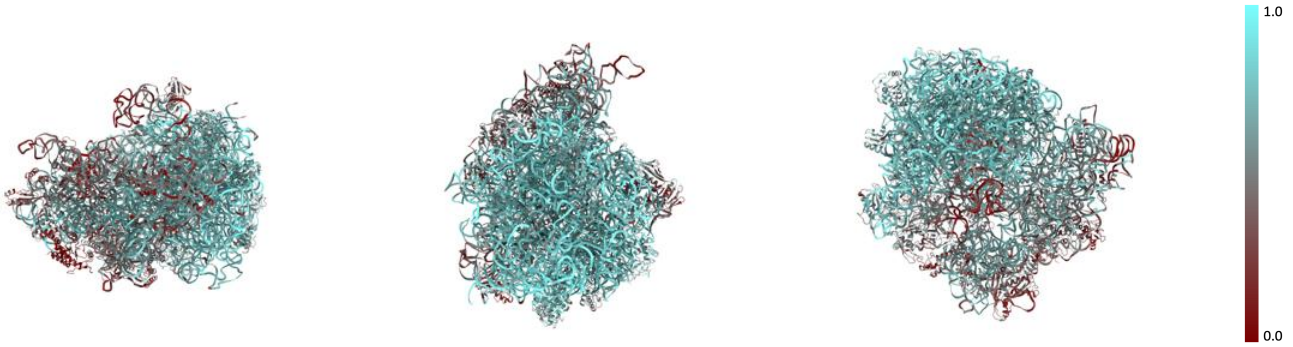
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

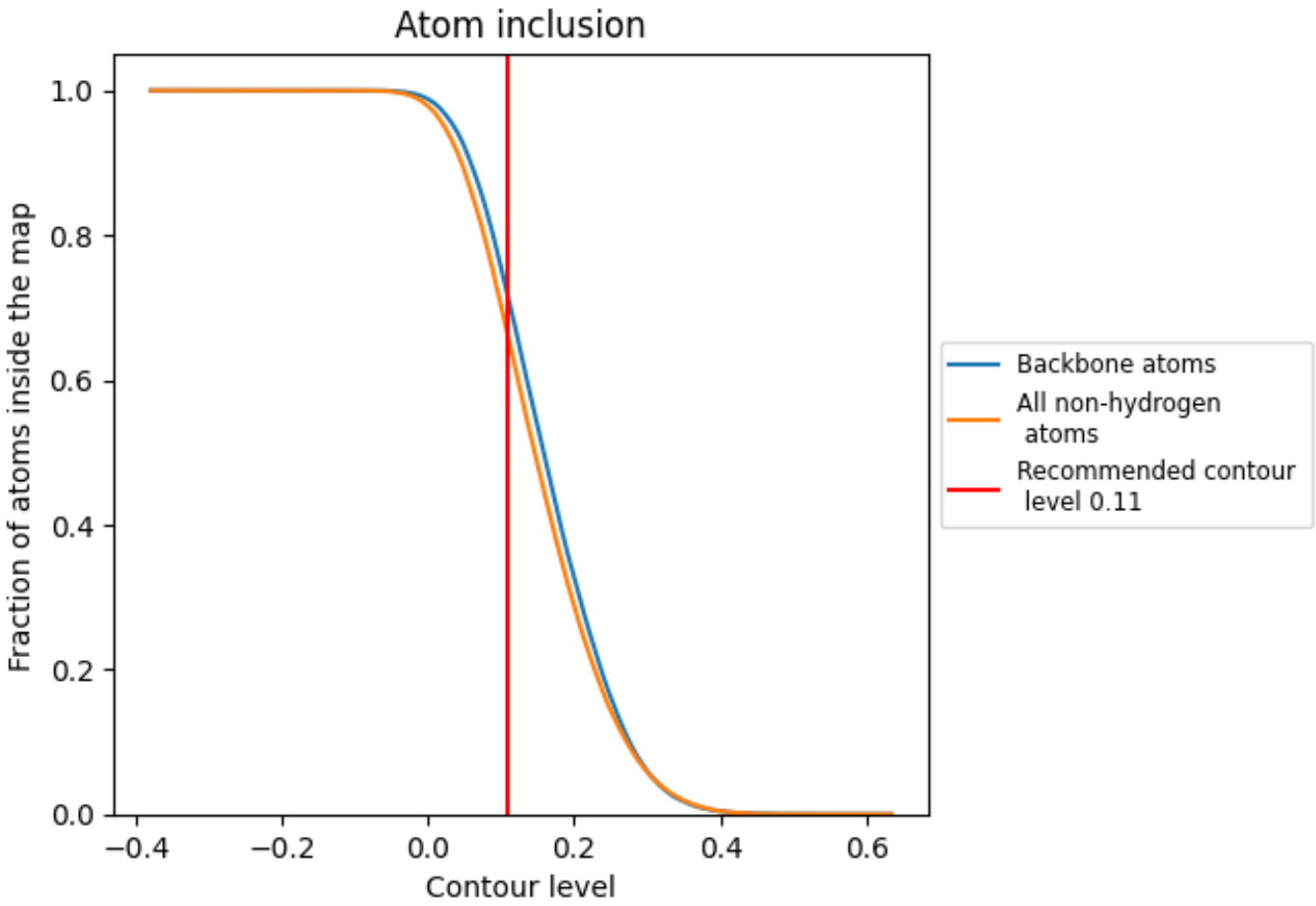
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6582	0.3890
0	0.7191	0.4870
1	0.6744	0.4410
2	0.7362	0.5030
3	0.7255	0.5080
4	0.6138	0.4620
6	0.2945	0.2640
7	0.6667	0.4050
8	0.0760	0.1430
A	0.7959	0.4370
B	0.7847	0.4020
C	0.6757	0.4800
D	0.6958	0.4810
E	0.6819	0.4500
F	0.4591	0.3260
G	0.4146	0.3170
J	0.7095	0.4720
K	0.6455	0.4620
L	0.6629	0.4490
M	0.6353	0.4500
N	0.6838	0.4640
O	0.5468	0.3630
P	0.6325	0.4500
Q	0.7074	0.4500
R	0.6894	0.4530
S	0.7033	0.4810
T	0.6136	0.4430
U	0.6146	0.4040
V	0.4241	0.3890
W	0.6486	0.4500
X	0.5231	0.4500
Y	0.5875	0.3610
Z	0.6360	0.4400
a	0.6450	0.3360
b	0.1212	0.1970

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Chain	Atom inclusion	Q-score
c	0.3994	0.3340
d	0.2454	0.2270
e	0.4966	0.3750
f	0.2840	0.2490
g	0.4504	0.3240
h	0.3958	0.2870
i	0.4339	0.3220
j	0.3405	0.3210
k	0.3794	0.2970
l	0.3722	0.3080
m	0.3810	0.2880
n	0.3812	0.3480
o	0.3852	0.2490
p	0.3260	0.2690
q	0.2853	0.2390
r	0.3406	0.2730
s	0.3457	0.2600
t	0.3714	0.2630
x	0.4336	0.3210