Full wwPDB EM Validation Report (i)

Oct 14, 2021 – 11:04 pm BST

PDB ID	:	7PJT
EMDB ID	:	EMD-13459
Title	:	Structure of the 70S ribosome with tRNAs in hybrid state 1 (H1)
Authors	:	Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.
Deposited on	:	2021-08-24
Resolution	:	6.00 Å(reported)
Based on initial models	:	4AQY, 6YSS, 5LZD

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

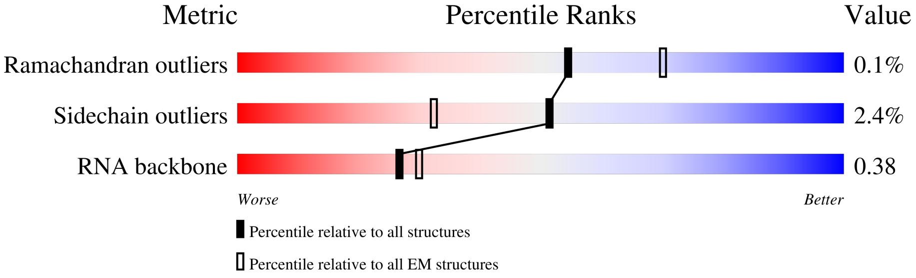
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: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

1 Overall quality at a glance (i)

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

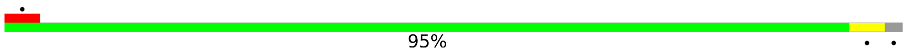
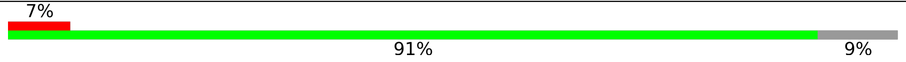
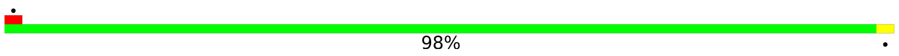
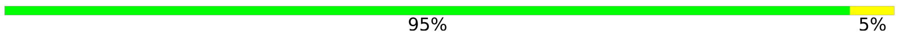
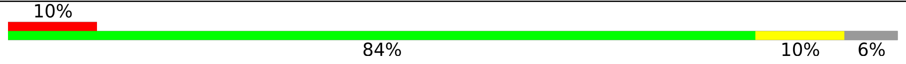
The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	0	57	
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	

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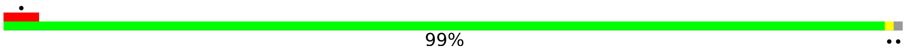
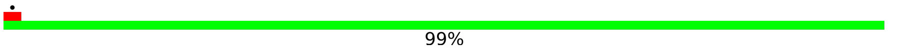
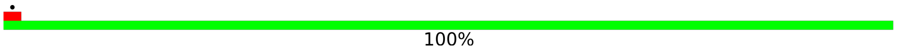
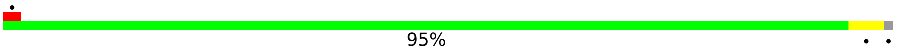
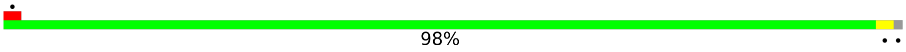
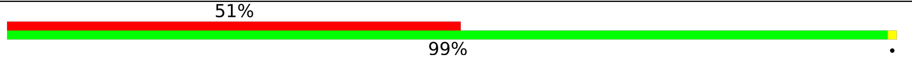
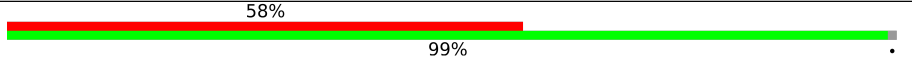
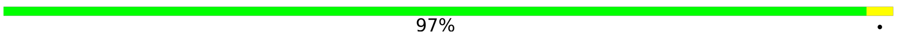
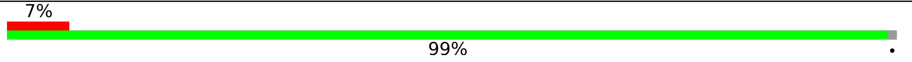
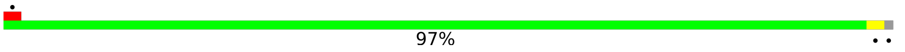
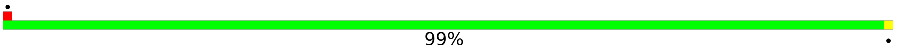
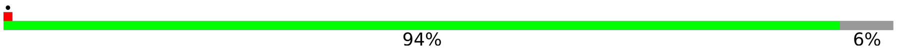
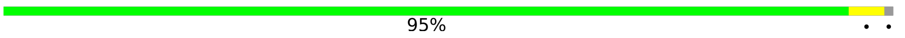
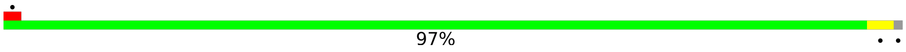
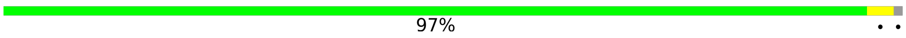
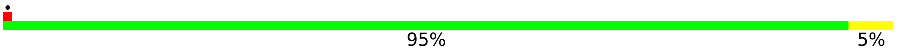
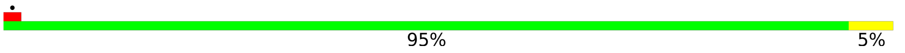
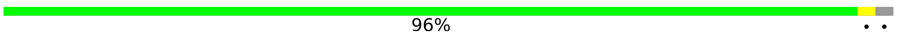
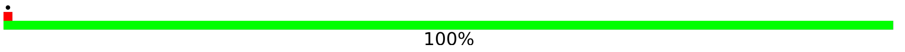
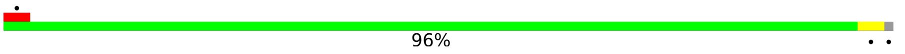
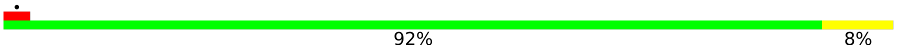
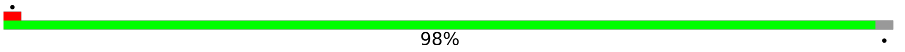
Mol	Chain	Length	Quality of chain
9	B	120	 60% 39%
10	C	273	 99%
11	D	209	 99%
12	E	201	 100%
13	F	179	 95%
14	G	177	 98%
15	H	149	 51% 99%
16	I	142	 58% 99%
17	J	142	 97%
18	K	123	 7% 99%
19	L	144	 97%
20	M	136	 99%
21	N	127	 94% 6%
22	O	117	 95%
23	P	115	 97%
24	Q	118	 97%
25	R	103	 95% 5%
26	S	110	 95% 5%
27	T	100	 91% 7%
28	U	104	 96%
29	V	94	 100%
30	W	85	 87% 12%
31	X	78	 96%
32	Y	63	 92% 8%
33	Z	59	 98%

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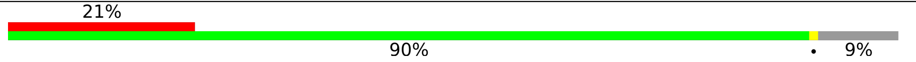
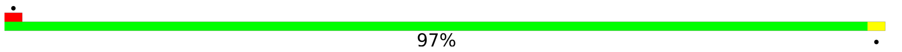
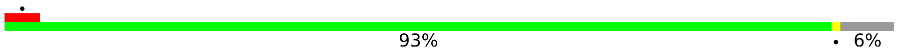
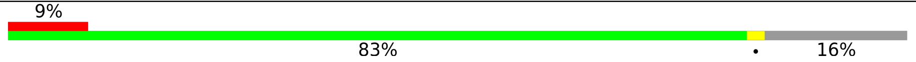
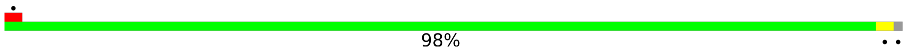
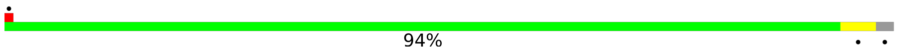
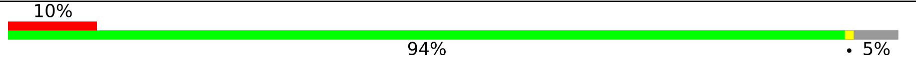
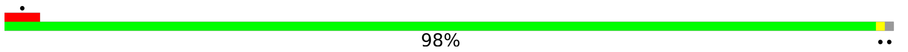
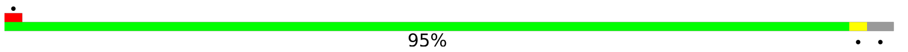
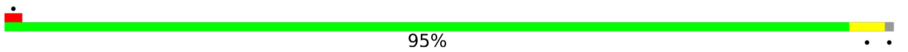
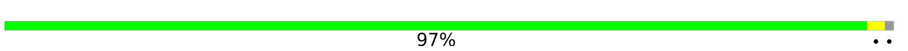
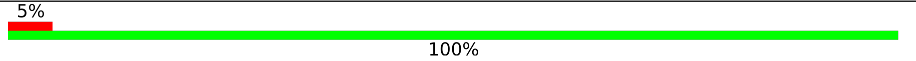
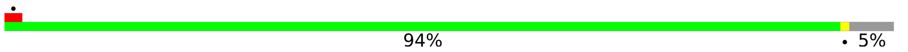
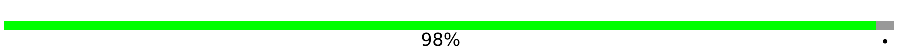
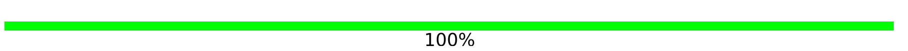
Mol	Chain	Length	Quality of chain
34	a	1542	
35	b	240	
36	c	233	
37	d	206	
38	e	167	
39	f	135	
40	g	179	
41	h	130	
42	i	130	
43	j	103	
44	k	129	
45	l	124	
46	m	118	
47	n	102	
48	o	89	
49	p	82	
50	q	84	
51	r	75	
52	s	92	
53	t	87	
54	u	71	
55	v	77	
56	w	76	
57	y	2	
58	z	33	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 147222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	A	2902	62317	27806	11469	20140	2902	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 57 is a protein called Dipeptide (FME-PHE).

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

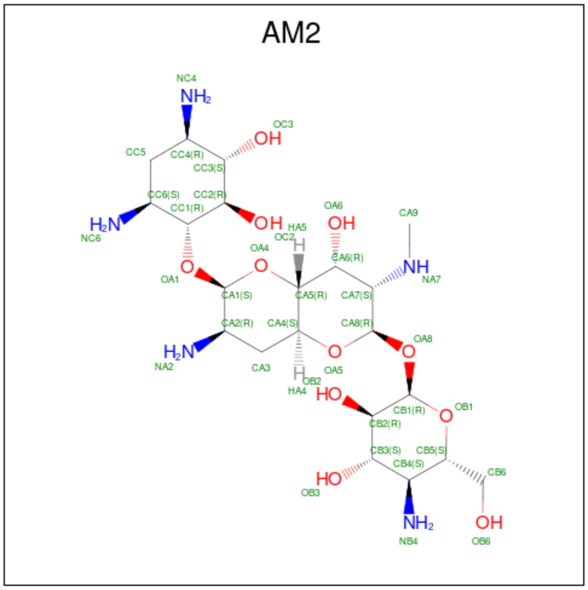
- Molecule 58 is a RNA chain called mRNA.

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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
59	4	1	Total Zn 1 1	0
59	6	1	Total Zn 1 1	0

- Molecule 60 is APRAMYCIN (three-letter code: AM2) (formula: $C_{21}H_{41}N_5O_{11}$).



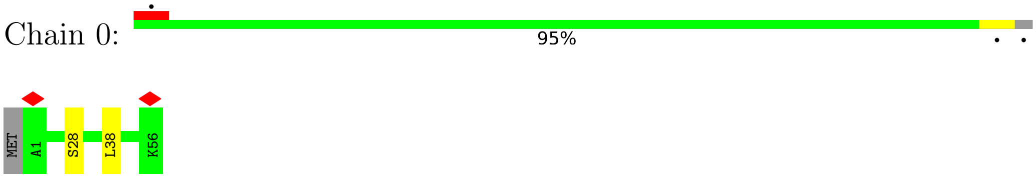
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
60	a	1	37	21	5	11	0

3 Residue-property plots ⓘ

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

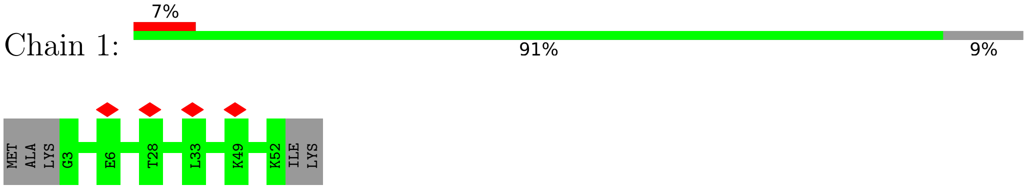
- Molecule 1: 50S ribosomal protein L32

Chain 0:



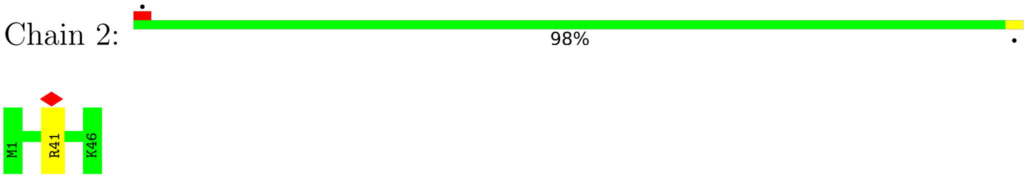
- Molecule 2: 50S ribosomal protein L33

Chain 1:



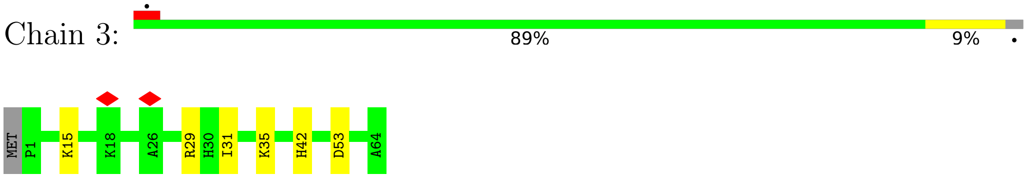
- Molecule 3: 50S ribosomal protein L34

Chain 2:



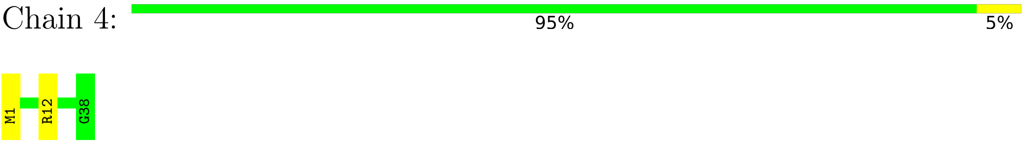
- Molecule 4: 50S ribosomal protein L35

Chain 3:



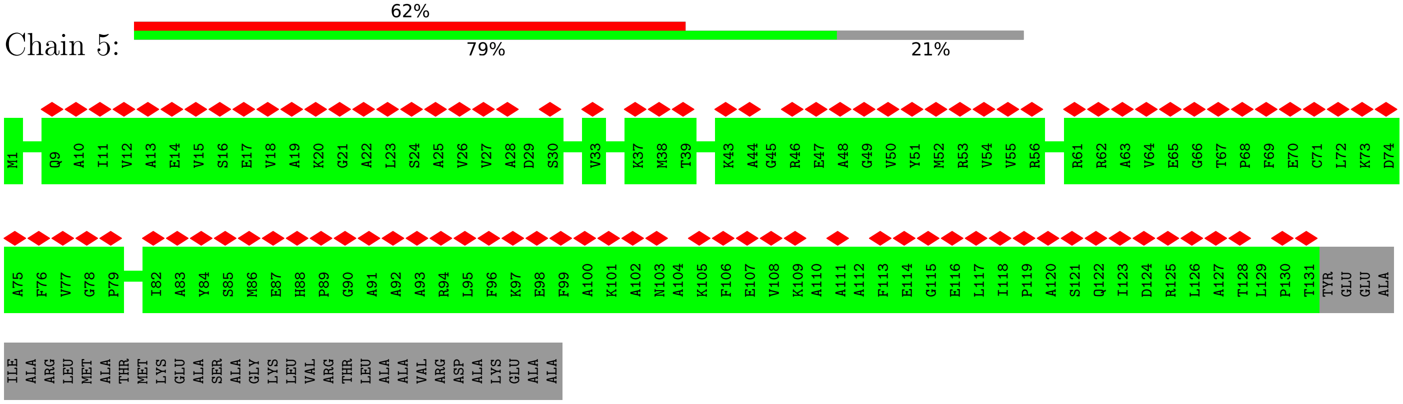
- Molecule 5: 50S ribosomal protein L36

Chain 4:



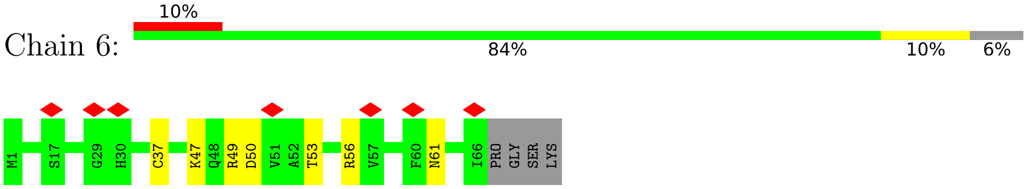
- Molecule 6: 50S ribosomal protein L10

Chain 5:



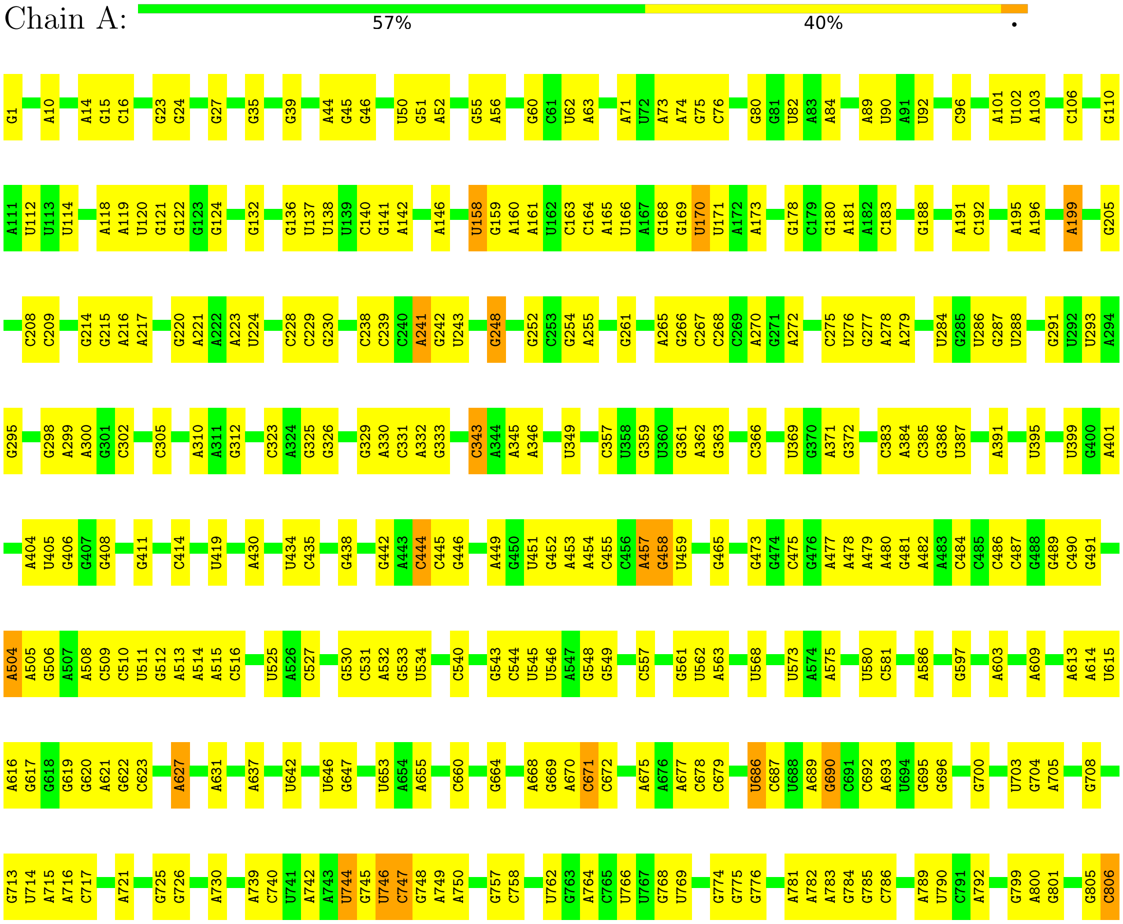
- Molecule 7: 50S ribosomal protein L31

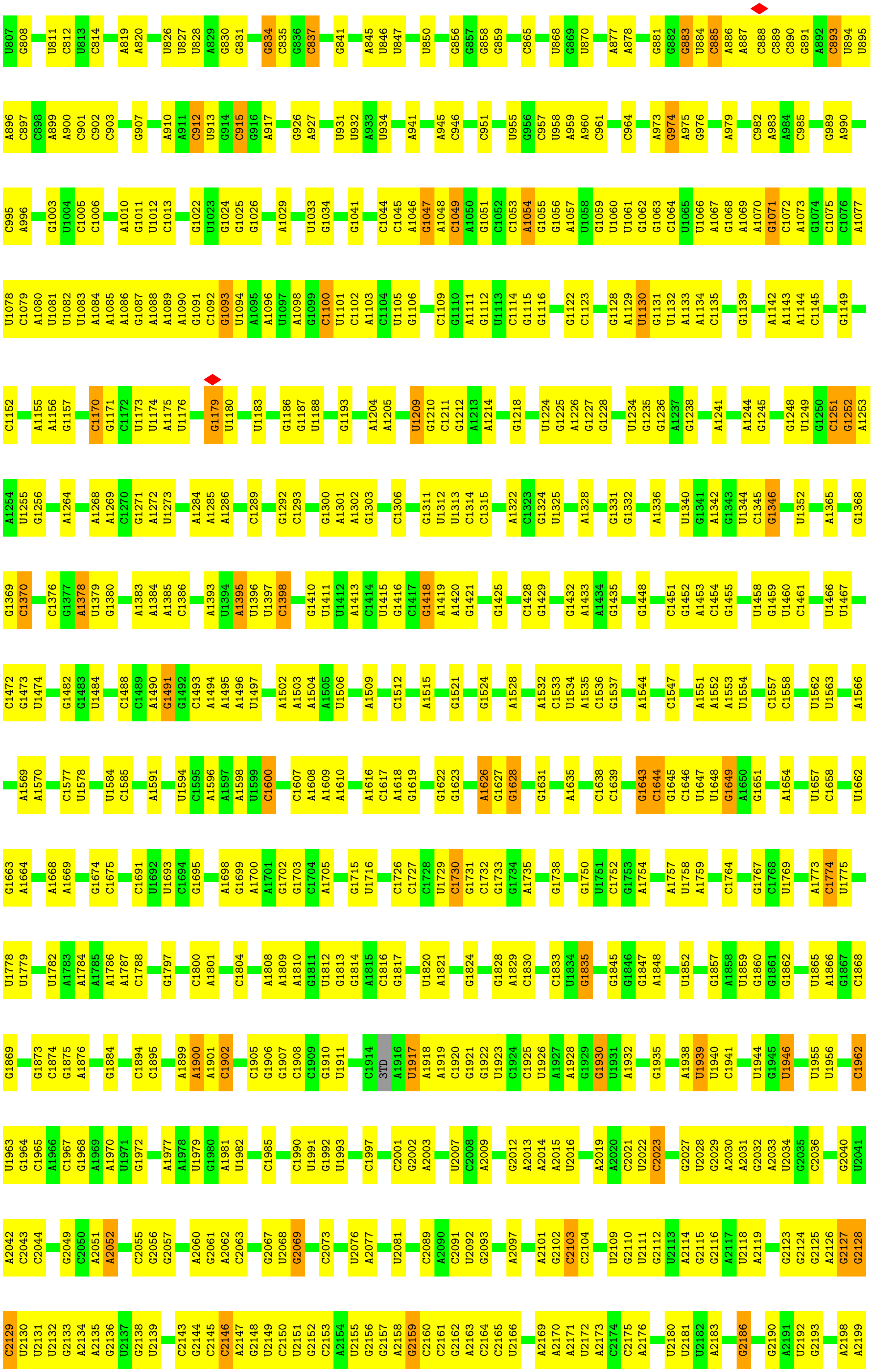
Chain 6:



- Molecule 8: 23S ribosomal RNA

Chain A:

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G836
C837
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U850
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G859
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U868
G869
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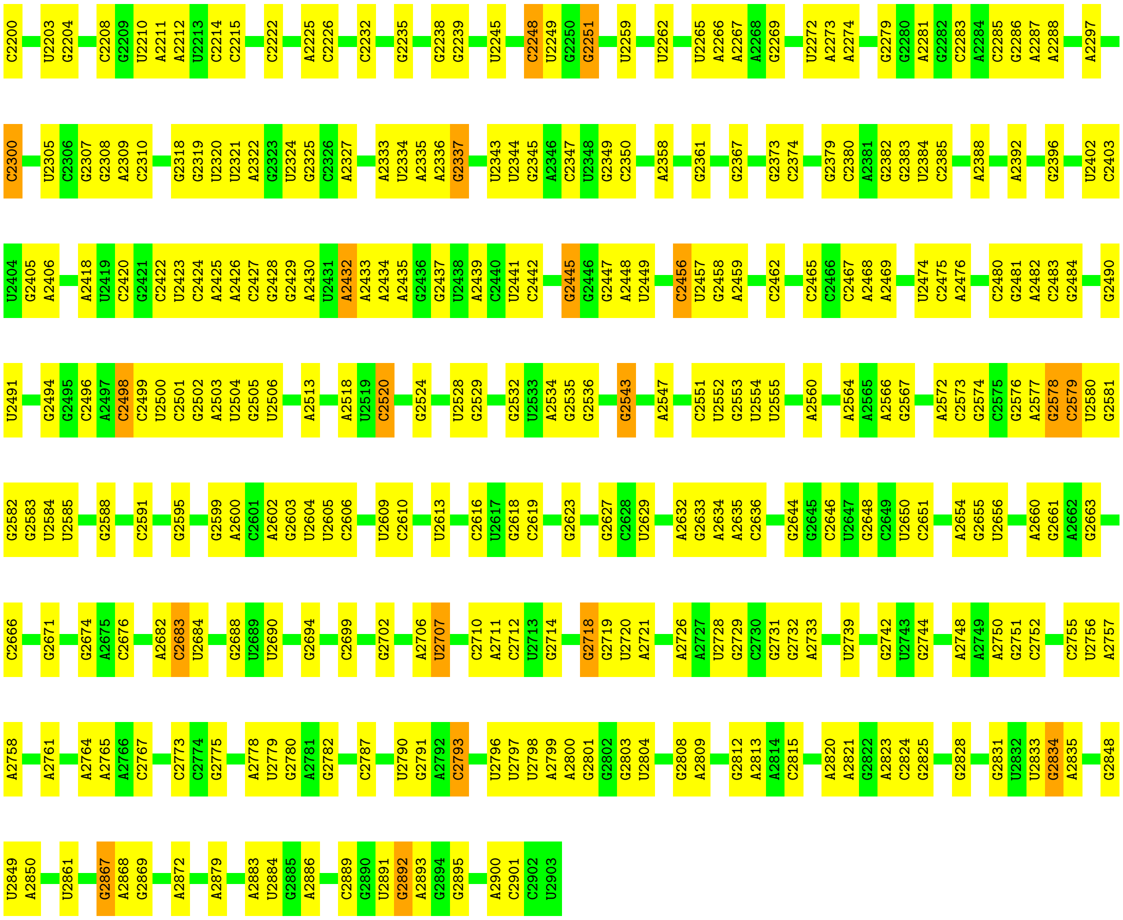
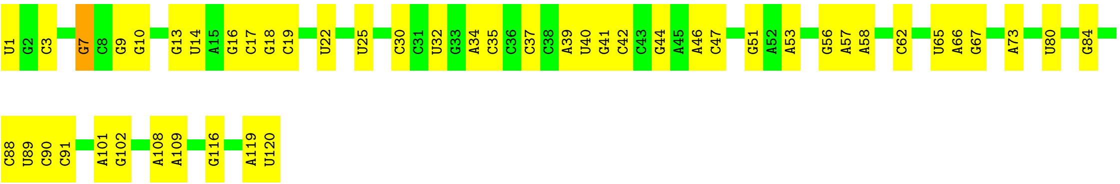


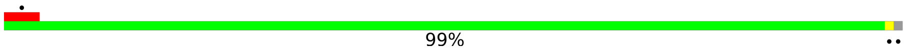
- Molecule 9: 5S ribosomal RNA

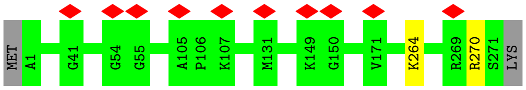
Chain B:



- Molecule 10: 50S ribosomal protein L2

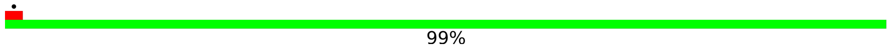
Chain C:

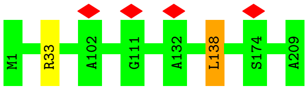




- Molecule 11: 50S ribosomal protein L3

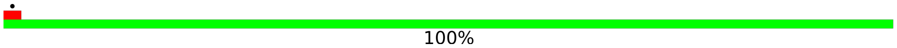
Chain D:

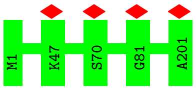




- Molecule 12: 50S ribosomal protein L4

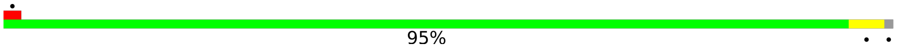
Chain E:

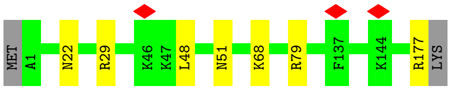




- Molecule 13: 50S ribosomal protein L5

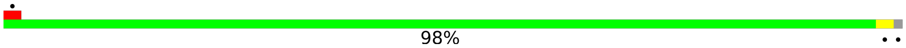
Chain F:

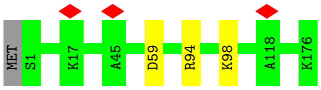




- Molecule 14: 50S ribosomal protein L6

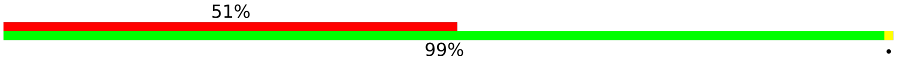
Chain G:

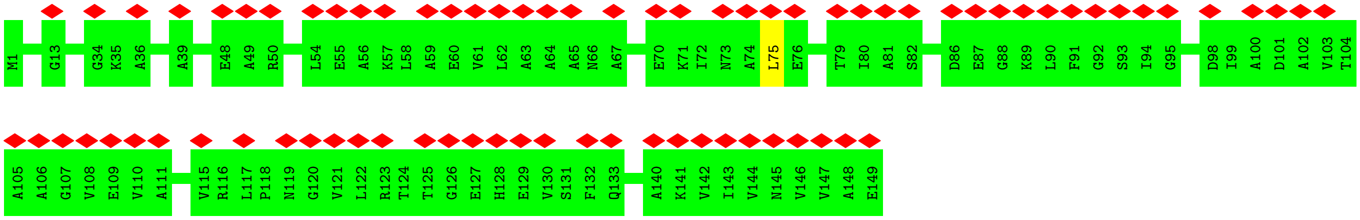




- Molecule 15: 50S ribosomal protein L9

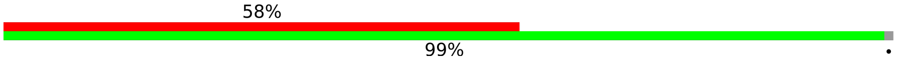
Chain H:

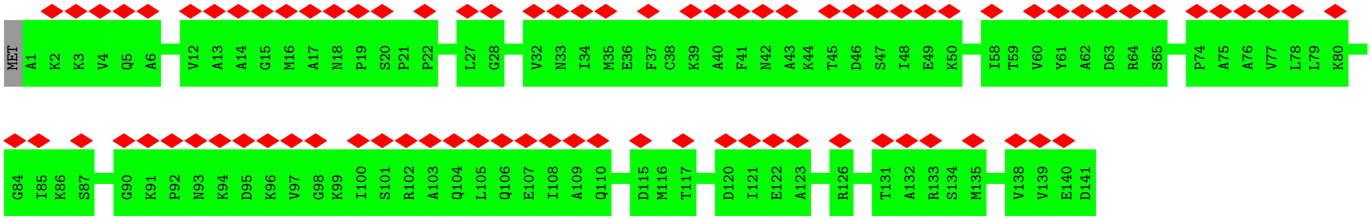




- Molecule 16: 50S ribosomal protein L11

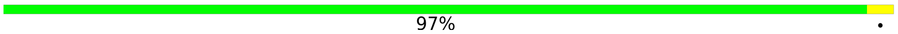
Chain I:

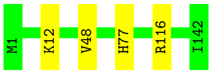




- Molecule 17: 50S ribosomal protein L13

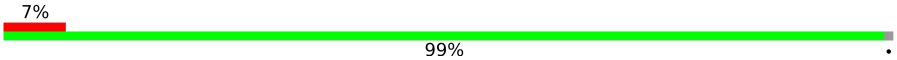
Chain J:

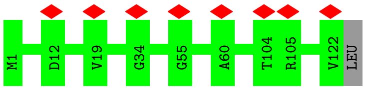




- Molecule 18: 50S ribosomal protein L14

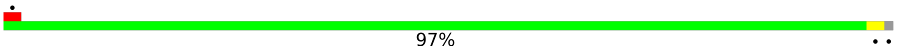
Chain K:

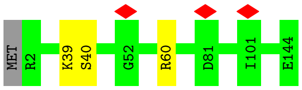




- Molecule 19: 50S ribosomal protein L15

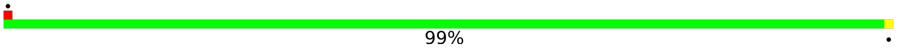
Chain L:

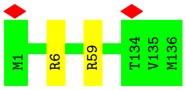




- Molecule 20: 50S ribosomal protein L16

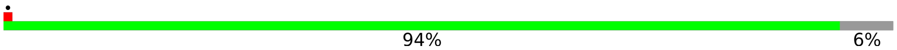
Chain M:

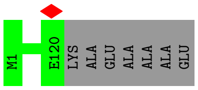




- Molecule 21: 50S ribosomal protein L17

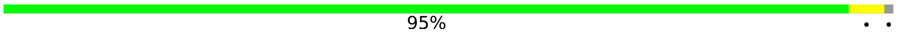
Chain N:

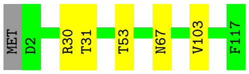




- Molecule 22: 50S ribosomal protein L18

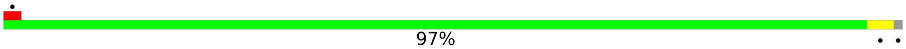
Chain O:

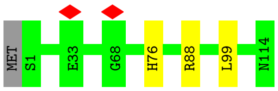




- Molecule 23: 50S ribosomal protein L19

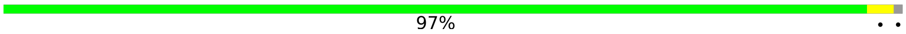
Chain P:

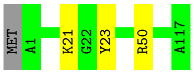




- Molecule 24: 50S ribosomal protein L20

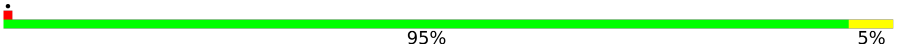
Chain Q:

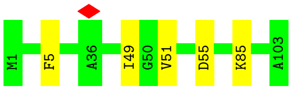




- Molecule 25: 50S ribosomal protein L21

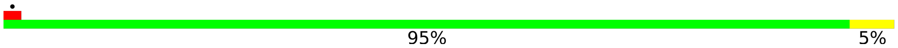
Chain R:

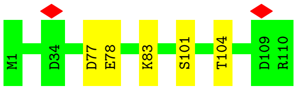




- Molecule 26: 50S ribosomal protein L22

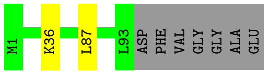
Chain S:





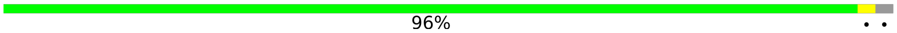
- Molecule 27: 50S ribosomal protein L23

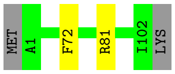
Chain T:



- Molecule 28: 50S ribosomal protein L24

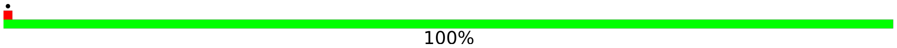
Chain U:

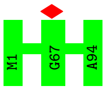




- Molecule 29: 50S ribosomal protein L25

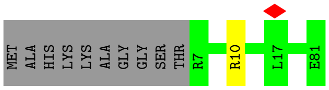
Chain V:



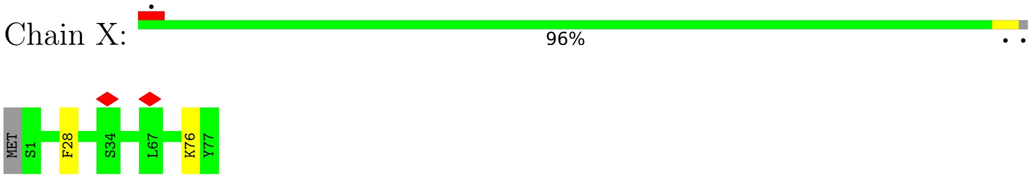


- Molecule 30: 50S ribosomal protein L27

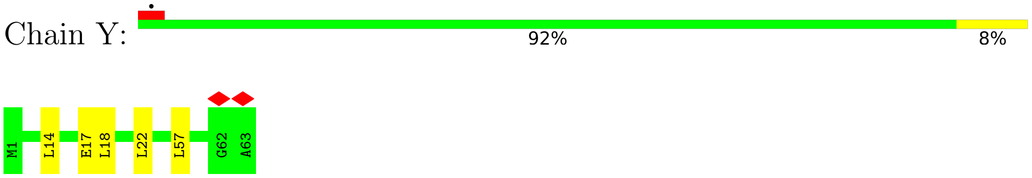
Chain W:



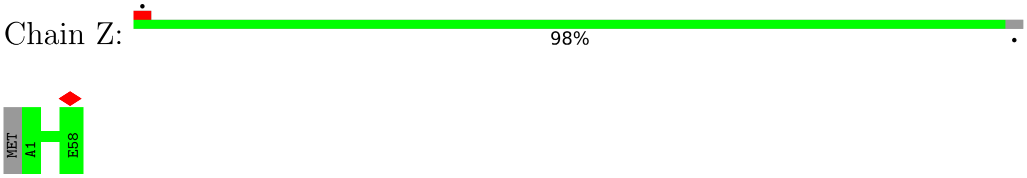
- Molecule 31: 50S ribosomal protein L28



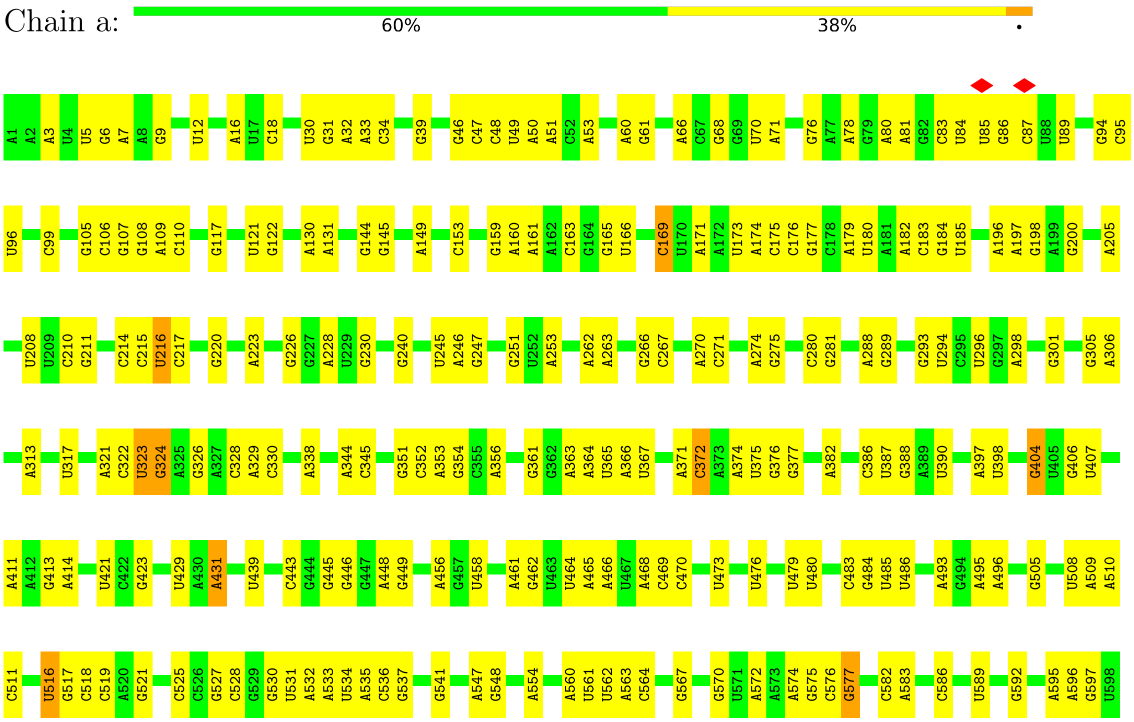
- Molecule 32: 50S ribosomal protein L29

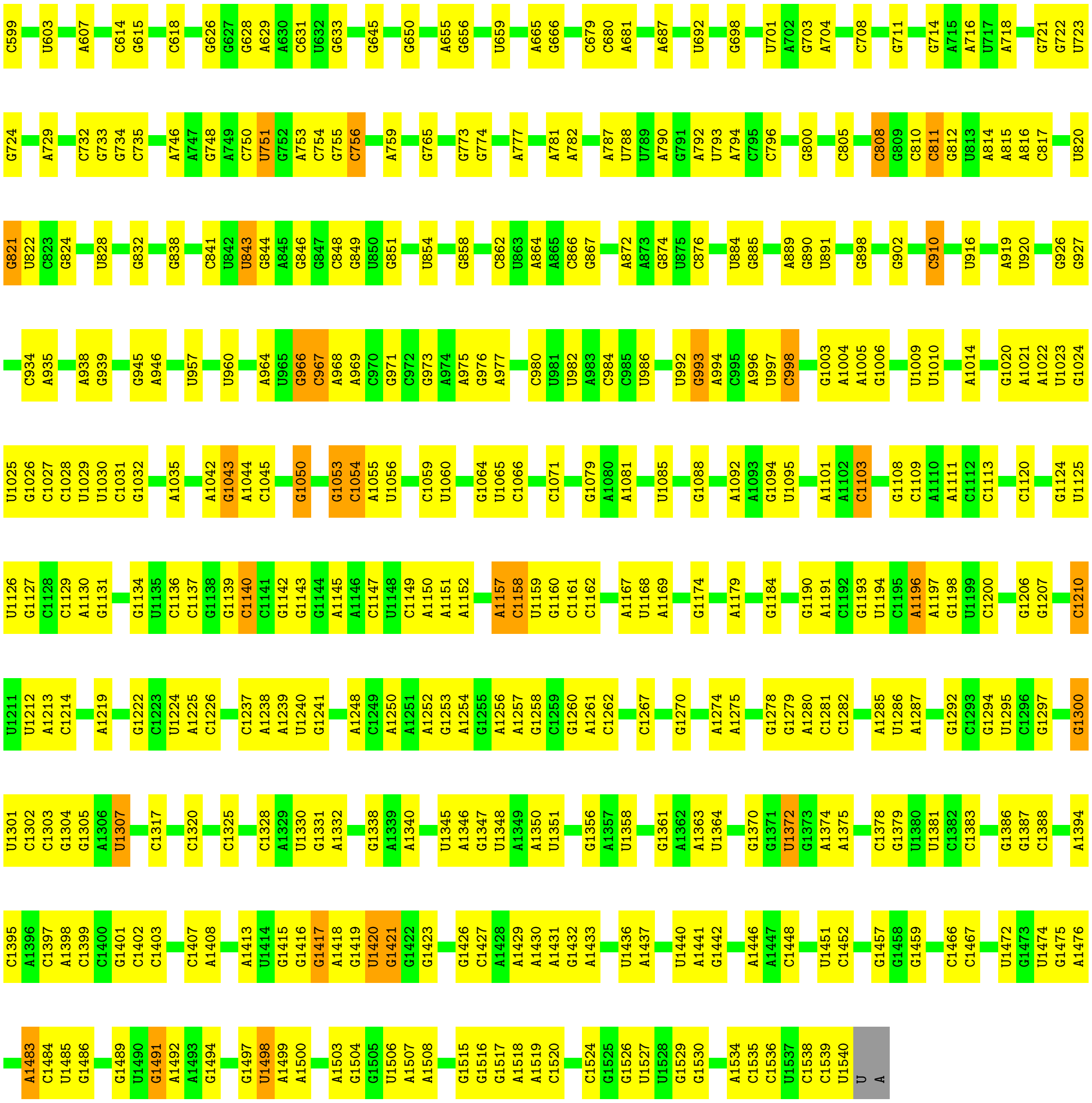


- Molecule 33: 50S ribosomal protein L30



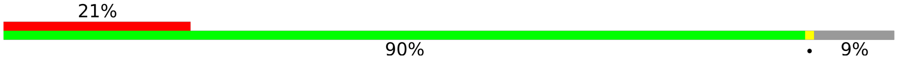
- Molecule 34: 16S ribosomal RNA

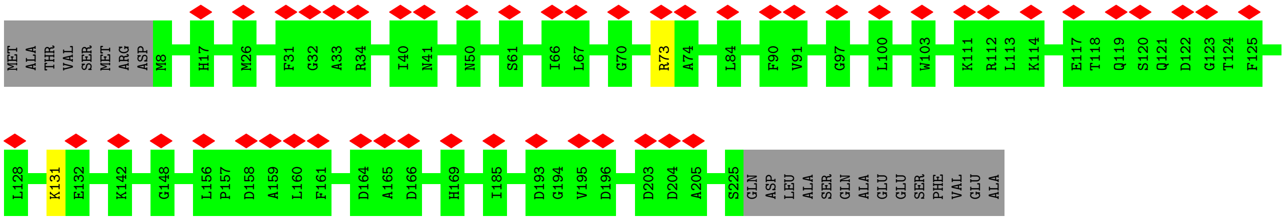




- Molecule 35: 30S ribosomal protein S2

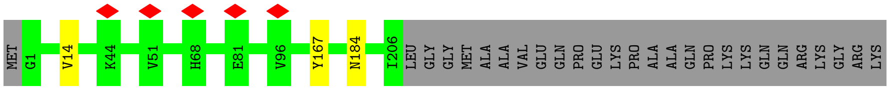
Chain b:





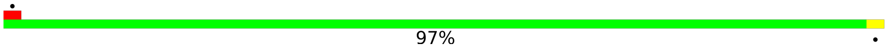
- Molecule 36: 30S ribosomal protein S3

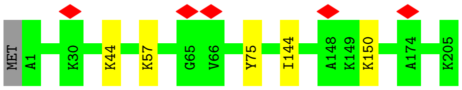
Chain c:



- Molecule 37: 30S ribosomal protein S4

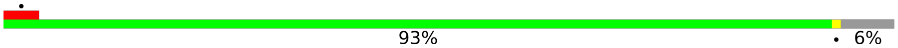
Chain d:

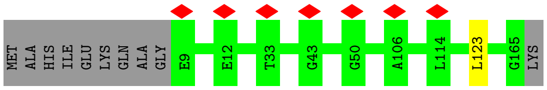




- Molecule 38: 30S ribosomal protein S5

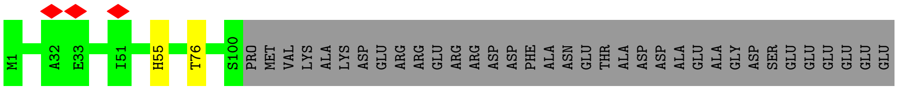
Chain e:





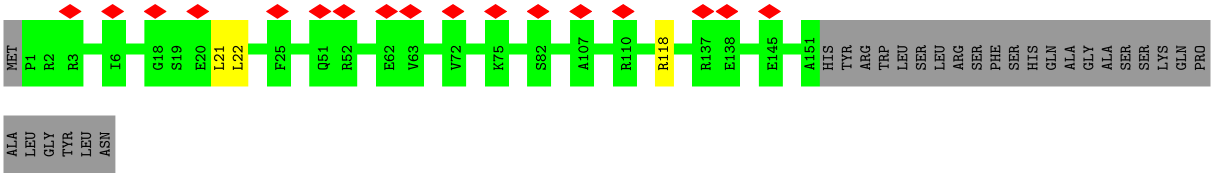
- Molecule 39: 30S ribosomal protein S6

Chain f:



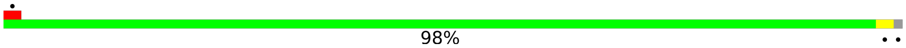
- Molecule 40: 30S ribosomal protein S7

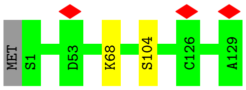
Chain g:



- Molecule 41: 30S ribosomal protein S8

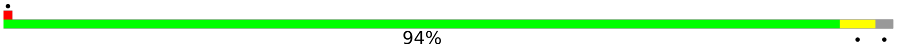
Chain h:

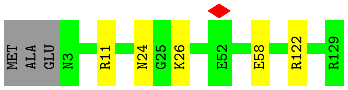




- Molecule 42: 30S ribosomal protein S9

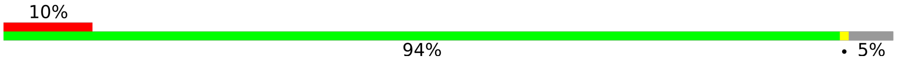
Chain i:

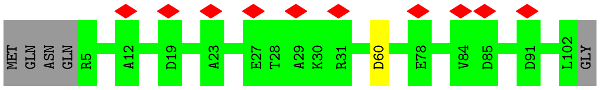




- Molecule 43: 30S ribosomal protein S10

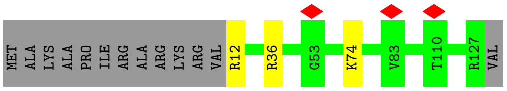
Chain j:





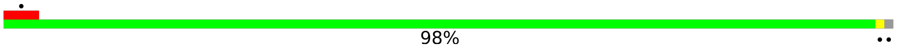
- Molecule 44: 30S ribosomal protein S11

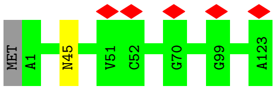
Chain k:



- Molecule 45: 30S ribosomal protein S12

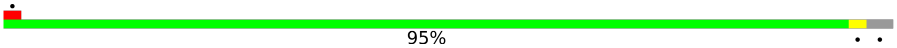
Chain l:

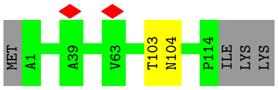




- Molecule 46: 30S ribosomal protein S13

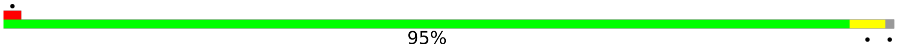
Chain m:

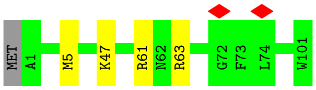




- Molecule 47: 30S ribosomal protein S14

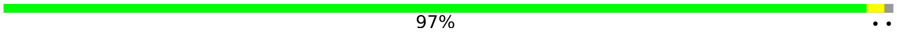
Chain n:

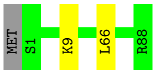




- Molecule 48: 30S ribosomal protein S15

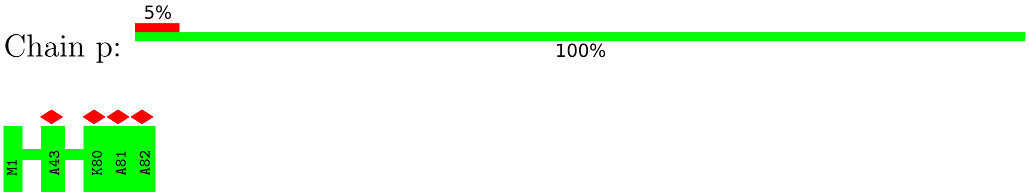
Chain o:





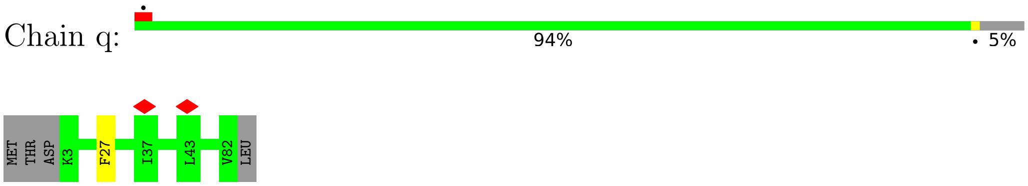
- Molecule 49: 30S ribosomal protein S16

Chain p:



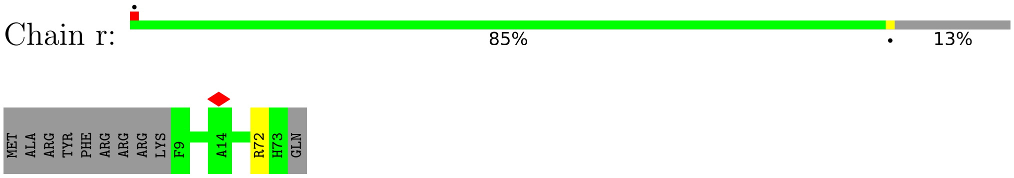
- Molecule 50: 30S ribosomal protein S17

Chain q:



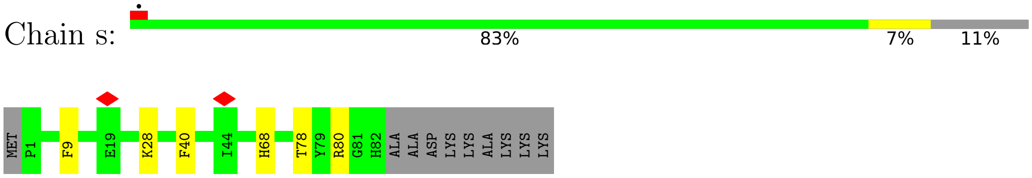
- Molecule 51: 30S ribosomal protein S18

Chain r:



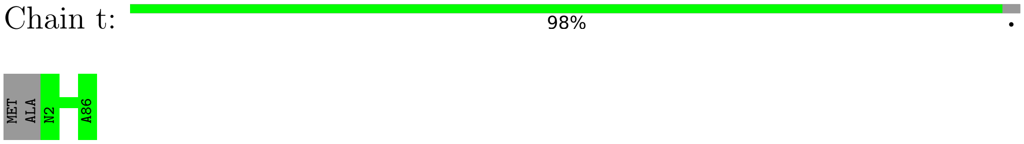
- Molecule 52: 30S ribosomal protein S19

Chain s:



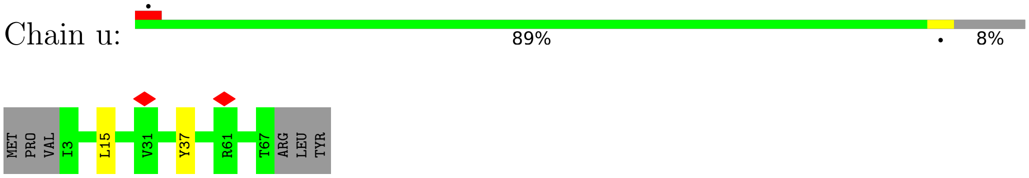
- Molecule 53: 30S ribosomal protein S20

Chain t:



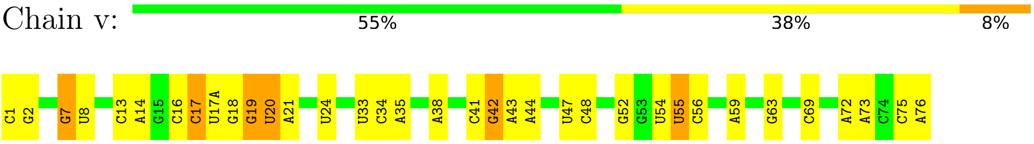
- Molecule 54: 30S ribosomal protein S21

Chain u:



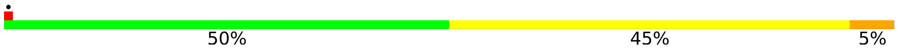
- Molecule 55: P-site tRNA(fMet)

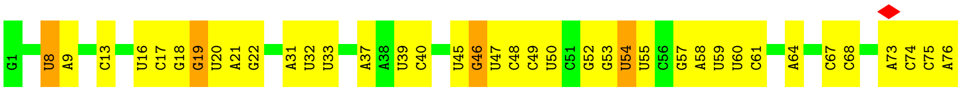
Chain v:



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

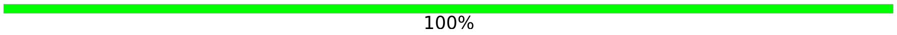
Chain w:





- Molecule 57: Dipeptide (FME-PHE)

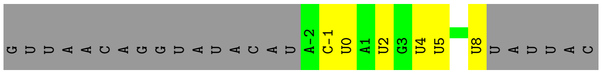
Chain y:



There are no outlier residues recorded for this chain.

- Molecule 58: mRNA

Chain z:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	11.607	Depositor
Minimum map value	-7.178	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	0	0.53	0/450	0.60	0/599
2	1	0.39	0/416	0.52	0/554
3	2	0.46	0/380	0.66	0/498
4	3	0.50	0/513	0.69	0/676
5	4	0.43	0/303	0.60	0/397
6	5	0.26	0/646	0.51	0/898
7	6	0.49	0/531	0.73	0/709
8	A	1.04	22/69266 (0.0%)	1.20	242/108055 (0.2%)
9	B	0.87	2/2873 (0.1%)	1.10	1/4478 (0.0%)
10	C	0.48	0/2121	0.62	0/2852
11	D	0.47	0/1586	0.62	0/2134
12	E	0.46	0/1571	0.60	0/2113
13	F	0.43	0/1434	0.59	0/1926
14	G	0.40	0/1343	0.57	0/1816
15	H	0.38	0/1122	0.61	0/1515
16	I	0.26	0/692	0.50	0/960
17	J	0.50	0/1152	0.55	0/1551
18	K	0.43	0/947	0.61	0/1268
19	L	0.48	0/1054	0.69	1/1403 (0.1%)
20	M	0.46	0/1093	0.57	0/1460
21	N	0.42	0/973	0.62	0/1301
22	O	0.43	0/902	0.61	0/1209
23	P	0.47	0/929	0.63	2/1242 (0.2%)
24	Q	0.50	0/960	0.60	1/1278 (0.1%)
25	R	0.47	0/829	0.64	0/1107
26	S	0.44	0/864	0.61	0/1156
27	T	0.42	0/744	0.62	0/994
28	U	0.46	0/787	0.61	0/1051
29	V	0.46	0/766	0.57	0/1025
30	W	0.45	0/582	0.63	0/769
31	X	0.44	0/635	0.66	1/848 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Y	0.41	0/510	0.64	0/677
33	Z	0.40	0/453	0.55	0/605
34	a	0.91	3/36725 (0.0%)	1.17	121/57285 (0.2%)
35	b	0.37	0/1735	0.57	0/2338
36	c	0.43	0/1651	0.56	1/2225 (0.0%)
37	d	0.39	0/1665	0.59	0/2227
38	e	0.42	0/1154	0.58	0/1554
39	f	0.38	0/835	0.56	0/1128
40	g	0.37	0/1195	0.54	0/1602
41	h	0.41	0/989	0.59	0/1326
42	i	0.42	0/1034	0.60	0/1375
43	j	0.37	0/796	0.62	0/1077
44	k	0.43	0/885	0.61	0/1195
45	l	0.44	0/969	0.60	0/1300
46	m	0.37	0/892	0.60	0/1193
47	n	0.45	0/811	0.69	0/1081
48	o	0.40	0/722	0.63	1/964 (0.1%)
49	p	0.40	0/659	0.58	0/884
50	q	0.41	0/657	0.59	0/881
51	r	0.42	0/544	0.60	0/731
52	s	0.46	0/675	0.69	0/908
53	t	0.38	0/671	0.51	0/888
54	u	0.40	0/512	0.56	0/683
55	v	0.83	1/1745 (0.1%)	1.17	7/2716 (0.3%)
56	w	0.69	0/1650	1.17	5/2569 (0.2%)
57	y	0.63	0/11	0.43	0/13
58	z	0.53	0/255	0.95	0/394
All	All	0.86	28/158864 (0.0%)	1.07	383/237661 (0.2%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	1	C	OP3-P	-10.75	1.48	1.61
9	B	1	U	OP3-P	-10.74	1.48	1.61
8	A	1	G	OP3-P	-10.73	1.48	1.61
8	A	1786	A	N9-C4	-7.76	1.33	1.37
8	A	195	A	N9-C4	-6.71	1.33	1.37
8	A	1378	A	N9-C4	-6.71	1.33	1.37
34	a	1196	A	O3'-P	6.17	1.68	1.61
8	A	2726	A	N9-C4	-6.07	1.34	1.37
34	a	1483	A	N9-C4	-5.81	1.34	1.37
8	A	1156	A	N9-C4	-5.73	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	679	C	N1-C6	-5.61	1.33	1.37
8	A	241	A	N9-C4	-5.58	1.34	1.37
8	A	1286	A	N9-C4	-5.49	1.34	1.37
8	A	1626	A	N9-C4	-5.40	1.34	1.37
34	a	288	A	N9-C4	-5.35	1.34	1.37
9	B	39	A	N9-C4	-5.33	1.34	1.37
8	A	270	A	N9-C4	-5.31	1.34	1.37
8	A	2616	C	N1-C6	-5.30	1.33	1.37
8	A	457	A	N9-C4	-5.25	1.34	1.37
8	A	627	A	N9-C4	-5.15	1.34	1.37
8	A	1029	A	N9-C4	-5.13	1.34	1.37
8	A	1378	A	C5-C6	-5.09	1.36	1.41
8	A	2014	A	N9-C4	-5.09	1.34	1.37
8	A	2456	C	N1-C6	-5.09	1.34	1.37
8	A	2432	A	N9-C4	-5.07	1.34	1.37
8	A	1662	U	C2-N3	-5.03	1.34	1.37
8	A	199	A	N9-C4	-5.03	1.34	1.37
8	A	454	A	N9-C4	-5.01	1.34	1.37

All (383) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1054	C	O5'-P-OP1	14.14	127.67	110.70
34	a	1196	A	C2'-C3'-O3'	9.93	131.35	109.50
34	a	1053	G	O3'-P-O5'	-9.74	85.50	104.00
34	a	1421	G	N9-C4-C5	9.61	109.24	105.40
34	a	1421	G	C8-N9-C1'	9.46	139.30	127.00
8	A	2731	G	C4-C5-N7	9.19	114.47	110.80
31	X	28	PHE	C-N-CA	-8.89	99.47	121.70
34	a	1421	G	N3-C4-N9	-8.74	120.76	126.00
34	a	1420	U	C2-N1-C1'	8.59	128.01	117.70
34	a	1466	C	N3-C2-O2	-8.57	115.90	121.90
34	a	811	C	C2-N1-C1'	8.53	128.18	118.80
55	v	17	C	N1-C1'-C2'	-8.52	102.63	112.00
8	A	951	C	C6-N1-C2	8.36	123.64	120.30
8	A	1902	C	N1-C2-O2	8.36	123.92	118.90
8	A	2129	C	C2-N1-C1'	8.25	127.88	118.80
8	A	1730	C	N1-C2-O2	8.24	123.84	118.90
8	A	1985	C	C6-N1-C2	8.20	123.58	120.30
8	A	1730	C	C2-N1-C1'	8.15	127.77	118.80
8	A	2731	G	C6-C5-N7	-8.06	125.57	130.40
55	v	42	G	O4'-C1'-N9	8.05	114.64	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2129	C	N1-C2-O2	7.87	123.62	118.90
8	A	799	G	N1-C2-N3	7.85	128.61	123.90
8	A	1533	C	N3-C2-O2	-7.78	116.46	121.90
8	A	1643	G	N1-C6-O6	-7.64	115.32	119.90
34	a	431	A	N1-C6-N6	-7.63	114.02	118.60
8	A	2683	C	N1-C2-O2	7.56	123.44	118.90
34	a	1421	G	C4-N9-C1'	-7.54	116.69	126.50
8	A	1418	G	N7-C8-N9	7.50	116.85	113.10
34	a	176	C	N3-C2-O2	-7.50	116.65	121.90
34	a	1053	G	OP1-P-O3'	-7.39	88.94	105.20
8	A	2506	U	C2-N1-C1'	7.39	126.57	117.70
8	A	1703	G	C8-N9-C4	7.38	109.35	106.40
34	a	1421	G	C6-C5-N7	7.35	134.81	130.40
8	A	686	U	O4'-C1'-N1	-7.33	102.33	108.20
8	A	2245	U	C5-C6-N1	-7.33	119.04	122.70
8	A	2731	G	N9-C4-C5	-7.26	102.50	105.40
34	a	176	C	N3-C4-N4	-7.23	112.94	118.00
8	A	1985	C	C5-C6-N1	-7.15	117.42	121.00
8	A	2159	G	N3-C4-N9	-7.11	121.73	126.00
8	A	2501	C	C2-N1-C1'	-7.08	111.01	118.80
34	a	106	C	N3-C2-O2	-7.06	116.96	121.90
34	a	1421	G	O4'-C1'-N9	7.05	113.84	108.20
8	A	964	C	C6-N1-C2	7.03	123.11	120.30
8	A	2052	A	N9-C4-C5	-7.02	102.99	105.80
8	A	183	C	N3-C2-O2	-7.01	116.99	121.90
8	A	2506	U	N1-C2-O2	7.01	127.70	122.80
8	A	799	G	C6-N1-C2	-6.99	120.91	125.10
8	A	214	G	N1-C2-N2	-6.92	109.97	116.20
34	a	1210	C	N3-C2-O2	-6.84	117.11	121.90
34	a	176	C	C2-N1-C1'	-6.81	111.31	118.80
8	A	2103	C	C2-N1-C1'	6.80	126.28	118.80
8	A	2731	G	C8-N9-C1'	-6.80	118.16	127.00
8	A	2731	G	N3-C4-N9	6.79	130.07	126.00
8	A	2731	G	C4-N9-C1'	6.78	135.31	126.50
34	a	866	C	N3-C2-O2	-6.78	117.15	121.90
8	A	1774	C	C2-N1-C1'	6.77	126.25	118.80
8	A	2159	G	N3-C4-C5	6.75	131.98	128.60
34	a	1158	C	N1-C2-O2	6.75	122.95	118.90
34	a	1420	U	C6-N1-C1'	-6.73	111.77	121.20
8	A	170	U	C2-N1-C1'	6.70	125.73	117.70
34	a	1043	G	N3-C4-N9	-6.69	121.98	126.00
8	A	1902	C	N3-C2-O2	-6.69	117.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1043	G	N9-C4-C5	6.69	108.08	105.40
8	A	1577	C	N3-C2-O2	-6.68	117.22	121.90
19	L	60	ARG	C-N-CA	-6.67	105.02	121.70
34	a	215	C	N1-C2-O2	6.66	122.90	118.90
8	A	2129	C	N3-C2-O2	-6.66	117.24	121.90
34	a	811	C	C6-N1-C1’	-6.65	112.82	120.80
34	a	751	U	C2-N1-C1’	6.62	125.64	117.70
8	A	2834	G	C8-N9-C4	6.60	109.04	106.40
8	A	2040	G	C8-N9-C4	6.59	109.03	106.40
8	A	1336	A	C8-N9-C4	6.58	108.43	105.80
8	A	2674	G	C8-N9-C4	6.56	109.02	106.40
56	w	19	G	N9-C4-C5	-6.52	102.79	105.40
8	A	238	C	C6-N1-C2	6.51	122.91	120.30
8	A	1779	U	C5-C6-N1	-6.48	119.46	122.70
34	a	811	C	N1-C2-O2	6.47	122.78	118.90
8	A	2103	C	N1-C2-O2	6.46	122.78	118.90
34	a	1053	G	OP2-P-O3’	-6.46	90.99	105.20
8	A	1398	C	N1-C2-O2	6.45	122.77	118.90
8	A	192	C	N3-C2-O2	-6.39	117.42	121.90
23	P	76	HIS	C-N-CA	-6.36	105.79	121.70
34	a	754	C	N1-C2-O2	6.36	122.72	118.90
8	A	964	C	C5-C6-N1	-6.34	117.83	121.00
8	A	1418	G	C5-N7-C8	-6.33	101.14	104.30
8	A	2248	C	N1-C2-O2	6.32	122.69	118.90
8	A	414	C	C6-N1-C2	6.32	122.83	120.30
34	a	577	G	C8-N9-C4	6.32	108.93	106.40
8	A	799	G	N1-C6-O6	-6.30	116.12	119.90
34	a	993	G	C6-C5-N7	-6.29	126.63	130.40
34	a	1421	G	N1-C6-O6	-6.28	116.13	119.90
8	A	192	C	N1-C2-O2	6.28	122.67	118.90
8	A	806	C	C6-N1-C2	6.27	122.81	120.30
8	A	2248	C	N3-C2-O2	-6.27	117.51	121.90
8	A	883	G	N3-C4-N9	-6.25	122.25	126.00
34	a	993	G	C4-N9-C1’	6.24	134.61	126.50
34	a	1356	G	N9-C4-C5	-6.23	102.91	105.40
8	A	1774	C	C6-N1-C1’	-6.22	113.33	120.80
8	A	2165	C	N1-C2-O2	6.22	122.63	118.90
34	a	176	C	C5-C6-N1	-6.21	117.89	121.00
8	A	2272	U	C5-C6-N1	-6.20	119.60	122.70
34	a	603	U	N3-C2-O2	-6.19	117.87	122.20
8	A	183	C	N1-C2-O2	6.19	122.61	118.90
8	A	627	A	C8-N9-C4	6.16	108.26	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2683	C	N3-C2-O2	-6.15	117.59	121.90
34	a	1307	U	C2-N1-C1’	6.15	125.08	117.70
36	c	14	VAL	C-N-CA	-6.14	106.35	121.70
8	A	806	C	C2-N3-C4	-6.14	116.83	119.90
8	A	1730	C	N3-C2-O2	-6.11	117.62	121.90
34	a	756	C	N3-C2-O2	-6.10	117.63	121.90
48	o	66	LEU	CA-CB-CG	-6.10	101.27	115.30
8	A	2159	G	C4-N9-C1’	-6.09	118.58	126.50
8	A	678	C	N3-C2-O2	-6.09	117.64	121.90
34	a	998	C	C6-N1-C1’	6.09	128.11	120.80
34	a	1043	G	C8-N9-C1’	6.09	134.91	127.00
8	A	2103	C	C6-N1-C2	-6.08	117.87	120.30
8	A	357	C	N3-C2-O2	-6.07	117.65	121.90
8	A	214	G	N1-C6-O6	-6.05	116.27	119.90
8	A	2731	G	C5-C6-O6	-6.04	124.97	128.60
34	a	754	C	N3-C2-O2	-6.04	117.68	121.90
8	A	2591	C	C6-N1-C2	-6.03	117.89	120.30
8	A	2588	G	C2-N3-C4	-6.03	108.89	111.90
34	a	1421	G	N3-C2-N2	-6.03	115.68	119.90
8	A	1730	C	C6-N1-C1’	-6.01	113.59	120.80
8	A	2129	C	C6-N1-C2	-6.01	117.90	120.30
8	A	893	C	C2-N3-C4	-6.01	116.89	119.90
34	a	1356	G	C6-C5-N7	-6.00	126.80	130.40
8	A	2023	C	N3-C4-C5	5.99	124.30	121.90
34	a	1421	G	C8-N9-C4	-5.99	104.00	106.40
8	A	2619	C	C6-N1-C2	5.99	122.69	120.30
8	A	696	G	C8-N9-C4	5.97	108.79	106.40
8	A	343	C	C2-N1-C1’	5.95	125.34	118.80
34	a	1466	C	N1-C2-O2	5.94	122.47	118.90
8	A	1324	G	O4’-C1’-N9	5.94	112.95	108.20
8	A	1054	A	N9-C4-C5	-5.93	103.43	105.80
8	A	1905	C	C5-C6-N1	-5.93	118.04	121.00
8	A	1234	U	N3-C2-O2	-5.92	118.05	122.20
8	A	742	A	C8-N9-C4	5.92	108.17	105.80
34	a	216	U	N1-C2-O2	5.90	126.93	122.80
56	w	19	G	C4-C5-N7	5.90	113.16	110.80
8	A	1900	A	O4’-C1’-N9	5.90	112.92	108.20
34	a	1158	C	N3-C2-O2	-5.89	117.77	121.90
8	A	268	C	C6-N1-C2	5.89	122.66	120.30
8	A	2815	C	C6-N1-C2	5.88	122.65	120.30
8	A	1662	U	N3-C4-O4	-5.88	115.28	119.40
8	A	2420	C	N1-C2-O2	5.88	122.43	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	177	G	C8-N9-C1'	-5.88	119.36	127.00
8	A	2543	G	C8-N9-C4	-5.88	104.05	106.40
34	a	998	C	C2-N1-C1'	-5.87	112.34	118.80
8	A	2215	C	C6-N1-C2	5.87	122.65	120.30
34	a	993	G	C8-N9-C1'	-5.86	119.39	127.00
8	A	700	G	C8-N9-C4	5.85	108.74	106.40
8	A	2300	C	C2-N1-C1'	5.83	125.22	118.80
8	A	2506	U	C6-N1-C1'	-5.82	113.05	121.20
34	a	751	U	C5-C6-N1	5.82	125.61	122.70
8	A	2127	G	O4'-C1'-N9	5.81	112.85	108.20
8	A	2551	C	N3-C4-N4	-5.81	113.94	118.00
8	A	1533	C	N1-C2-O2	5.79	122.37	118.90
24	Q	23	TYR	CB-CA-C	5.79	121.97	110.40
8	A	1049	C	C5-C6-N1	5.78	123.89	121.00
34	a	404	G	C8-N9-C1'	5.77	134.50	127.00
8	A	1845	G	C8-N9-C4	5.77	108.71	106.40
8	A	2483	C	C6-N1-C2	5.76	122.61	120.30
8	A	834	G	N1-C6-O6	-5.74	116.45	119.90
8	A	915	C	C2-N1-C1'	5.73	125.10	118.80
8	A	1930	G	N3-C4-C5	5.71	131.46	128.60
34	a	1140	C	N1-C2-O2	5.71	122.33	118.90
8	A	2501	C	C6-N1-C1'	5.70	127.64	120.80
8	A	1378	A	C2-N3-C4	-5.70	107.75	110.60
34	a	1103	C	C6-N1-C2	5.69	122.58	120.30
8	A	2731	G	C5-N7-C8	-5.68	101.46	104.30
8	A	806	C	N3-C4-C5	5.67	124.17	121.90
8	A	1398	C	N3-C2-O2	-5.67	117.93	121.90
8	A	806	C	C5-C6-N1	-5.67	118.17	121.00
34	a	1431	A	O4'-C1'-N9	5.67	112.73	108.20
8	A	885	C	OP2-P-O3'	5.67	117.67	105.20
34	a	177	G	C4-N9-C1'	5.67	133.87	126.50
34	a	1174	G	N9-C4-C5	-5.67	103.13	105.40
8	A	2707	U	C5-C6-N1	-5.66	119.87	122.70
8	A	893	C	C2-N1-C1'	-5.66	112.58	118.80
34	a	1059	C	N3-C4-N4	-5.66	114.04	118.00
8	A	2123	G	N3-C4-C5	5.65	131.43	128.60
8	A	1049	C	C6-N1-C2	-5.64	118.05	120.30
8	A	2337	G	N9-C4-C5	-5.63	103.15	105.40
34	a	993	G	N3-C4-N9	5.63	129.38	126.00
8	A	2052	A	C6-C5-N7	-5.62	128.37	132.30
34	a	1307	U	C6-N1-C1'	-5.62	113.34	121.20
34	a	1157	A	O4'-C1'-N9	-5.58	103.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	2828	G	C8-N9-C4	5.57	108.63	106.40
8	A	1100	C	N1-C2-O2	5.57	122.24	118.90
8	A	1179	G	C4-N9-C1'	5.57	133.74	126.50
8	A	2159	G	C8-N9-C1'	5.57	134.24	127.00
8	A	2146	C	N1-C2-O2	5.56	122.24	118.90
34	a	1210	C	C6-N1-C2	-5.56	118.08	120.30
55	v	17	C	O4'-C1'-N1	5.56	112.65	108.20
8	A	837	C	N1-C2-O2	5.56	122.23	118.90
34	a	716	A	C8-N9-C4	5.55	108.02	105.80
34	a	1149	C	C5-C6-N1	5.55	123.77	121.00
8	A	2742	G	C8-N9-C4	5.54	108.62	106.40
8	A	2129	C	C6-N1-C1'	-5.53	114.17	120.80
34	a	305	G	N3-C4-N9	-5.52	122.69	126.00
8	A	214	G	N3-C2-N2	5.52	123.76	119.90
34	a	821	G	C8-N9-C4	5.51	108.61	106.40
8	A	814	C	C6-N1-C2	5.51	122.50	120.30
34	a	1103	C	C5-C6-N1	-5.51	118.25	121.00
55	v	19	G	O4'-C1'-N9	-5.50	103.80	108.20
8	A	2103	C	N3-C2-O2	-5.50	118.05	121.90
8	A	357	C	N1-C2-O2	5.50	122.20	118.90
34	a	105	G	C8-N9-C4	5.50	108.60	106.40
8	A	2052	A	C4-C5-N7	5.49	113.44	110.70
8	A	1252	G	C8-N9-C4	5.48	108.59	106.40
8	A	1071	G	C4-N9-C1'	5.48	133.62	126.50
8	A	678	C	N1-C2-O2	5.48	122.19	118.90
34	a	910	C	C6-N1-C2	5.48	122.49	120.30
8	A	1662	U	C5-C6-N1	-5.47	119.96	122.70
8	A	744	U	C2-N1-C1'	5.47	124.27	117.70
34	a	176	C	C5-C4-N4	5.47	124.03	120.20
56	w	9	A	O4'-C1'-N9	5.45	112.56	108.20
34	a	386	C	N3-C2-O2	-5.45	118.08	121.90
8	A	708	G	N3-C4-N9	-5.45	122.73	126.00
8	A	2892	G	C8-N9-C4	5.45	108.58	106.40
8	A	1491	G	N9-C4-C5	5.44	107.58	105.40
34	a	476	U	C2-N1-C1'	5.44	124.23	117.70
8	A	1649	G	N1-C6-O6	-5.43	116.64	119.90
8	A	775	G	N3-C4-C5	5.42	131.31	128.60
8	A	705	A	N1-C6-N6	5.41	121.85	118.60
8	A	238	C	C5-C6-N1	-5.40	118.30	121.00
34	a	1356	G	C4-C5-N7	5.40	112.96	110.80
34	a	1292	G	N9-C4-C5	-5.40	103.24	105.40
8	A	671	C	N3-C4-N4	-5.39	114.22	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	2867	G	O4'-C1'-N9	5.39	112.51	108.20
34	a	1401	G	N1-C6-O6	-5.39	116.67	119.90
34	a	1421	G	C4-C5-N7	-5.39	108.64	110.80
34	a	1292	G	C4-C5-N7	5.39	112.95	110.80
8	A	695	G	C8-N9-C4	5.38	108.55	106.40
8	A	1824	G	C8-N9-C4	5.38	108.55	106.40
8	A	2103	C	C5-C6-N1	5.38	123.69	121.00
8	A	2676	C	C6-N1-C2	5.38	122.45	120.30
8	A	721	A	C8-N9-C4	5.38	107.95	105.80
8	A	2465	C	C6-N1-C2	5.37	122.45	120.30
8	A	1644	C	O4'-C1'-N1	5.37	112.49	108.20
8	A	1990	C	N3-C2-O2	-5.37	118.14	121.90
8	A	2040	G	N9-C4-C5	-5.36	103.25	105.40
34	a	655	A	C8-N9-C4	5.36	107.94	105.80
34	a	1491	G	C8-N9-C4	-5.36	104.26	106.40
8	A	2128	G	C4-N9-C1'	5.35	133.45	126.50
8	A	1662	U	C2-N3-C4	-5.35	123.79	127.00
8	A	721	A	N9-C4-C5	-5.34	103.66	105.80
9	B	7	G	C4-N9-C1'	-5.34	119.56	126.50
8	A	1946	U	C5-C6-N1	-5.34	120.03	122.70
8	A	901	C	N1-C2-O2	5.33	122.10	118.90
8	A	2793	C	N1-C2-O2	5.33	122.10	118.90
8	A	2551	C	C5-C6-N1	-5.32	118.34	121.00
34	a	528	C	C2-N1-C1'	-5.32	112.94	118.80
8	A	1905	C	C6-N1-C2	5.32	122.43	120.30
8	A	1292	G	C8-N9-C4	5.31	108.53	106.40
8	A	1902	C	N3-C4-C5	5.31	124.02	121.90
34	a	169	C	N1-C2-O2	5.31	122.09	118.90
8	A	1902	C	C6-N1-C1'	-5.30	114.44	120.80
8	A	2551	C	C6-N1-C2	5.30	122.42	120.30
8	A	1170	C	N1-C2-O2	5.30	122.08	118.90
8	A	799	G	N1-C2-N2	-5.30	111.43	116.20
8	A	671	C	C5-C6-N1	-5.30	118.35	121.00
8	A	458	G	N3-C4-C5	5.29	131.25	128.60
34	a	1142	G	C8-N9-C4	5.29	108.52	106.40
8	A	1156	A	C8-N9-C4	5.29	107.92	105.80
8	A	2367	G	C8-N9-C4	5.29	108.52	106.40
8	A	2520	C	N3-C4-C5	5.29	124.02	121.90
56	w	48	C	C6-N1-C2	5.29	122.42	120.30
34	a	750	C	N3-C2-O2	-5.28	118.20	121.90
8	A	1905	C	C2-N3-C4	-5.28	117.26	119.90
8	A	504	A	C2'-C3'-O3'	5.27	122.13	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	628	G	N9-C4-C5	-5.26	103.29	105.40
8	A	1370	C	C2-N3-C4	-5.26	117.27	119.90
8	A	89	A	C2-N3-C4	-5.26	107.97	110.60
8	A	2215	C	N3-C4-C5	5.25	124.00	121.90
34	a	1174	G	C4-C5-N7	5.25	112.90	110.80
8	A	2773	C	C6-N1-C2	5.25	122.40	120.30
34	a	808	C	O4'-C1'-N1	5.25	112.40	108.20
34	a	800	G	N3-C4-N9	-5.24	122.86	126.00
34	a	1356	G	N3-C4-N9	5.23	129.14	126.00
34	a	1415	G	C5-C6-O6	-5.23	125.46	128.60
8	A	690	G	C4-N9-C1'	-5.22	119.72	126.50
8	A	1093	G	N3-C4-N9	5.21	129.13	126.00
34	a	476	U	N1-C2-O2	5.21	126.44	122.80
34	a	1420	U	C5-C6-N1	5.20	125.30	122.70
55	v	7	G	O4'-C1'-N9	5.20	112.36	108.20
8	A	2186	G	N3-C4-C5	5.20	131.20	128.60
8	A	444	C	C2-N3-C4	-5.19	117.30	119.90
8	A	1251	C	C2-N1-C1'	5.19	124.51	118.80
8	A	1703	G	N7-C8-N9	-5.19	110.51	113.10
8	A	1814	G	N3-C4-N9	-5.18	122.89	126.00
8	A	1638	C	C5-C6-N1	-5.18	118.41	121.00
34	a	1162	C	C6-N1-C2	5.18	122.37	120.30
8	A	1779	U	C2-N3-C4	-5.18	123.89	127.00
8	A	1902	C	C2-N1-C1'	5.18	124.50	118.80
8	A	1145	C	C6-N1-C2	5.18	122.37	120.30
34	a	313	A	C5-C6-N1	5.17	120.29	117.70
34	a	323	U	C5-C6-N1	5.17	125.29	122.70
34	a	843	U	P-O3'-C3'	5.17	125.91	119.70
8	A	1675	C	N3-C2-O2	-5.17	118.28	121.90
8	A	1179	G	N3-C4-N9	5.17	129.10	126.00
34	a	476	U	C6-N1-C1'	-5.16	113.98	121.20
23	P	99	LEU	CA-CB-CG	-5.16	103.43	115.30
34	a	106	C	N1-C2-O2	5.16	122.00	118.90
34	a	824	G	N9-C4-C5	-5.16	103.34	105.40
8	A	974	G	C4-C5-N7	5.16	112.86	110.80
34	a	296	U	C5-C6-N1	-5.15	120.12	122.70
8	A	692	C	C6-N1-C2	5.15	122.36	120.30
8	A	1346	G	C6-C5-N7	-5.15	127.31	130.40
8	A	1425	G	N3-C4-N9	-5.15	122.91	126.00
8	A	2337	G	C8-N9-C4	5.15	108.46	106.40
34	a	404	G	C4-N9-C1'	-5.15	119.81	126.50
8	A	1466	U	C5-C4-O4	5.15	128.99	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1372	U	N3-C2-O2	-5.14	118.60	122.20
8	A	2186	G	C8-N9-C4	5.13	108.45	106.40
8	A	912	C	C2-N1-C1'	5.13	124.44	118.80
8	A	158	U	N3-C2-O2	-5.12	118.61	122.20
8	A	1425	G	C2-N3-C4	-5.12	109.34	111.90
8	A	1968	G	C8-N9-C4	5.12	108.45	106.40
34	a	1417	G	C8-N9-C4	5.12	108.45	106.40
8	A	2579	C	N1-C2-O2	5.12	121.97	118.90
8	A	1639	C	N1-C2-O2	5.12	121.97	118.90
34	a	324	G	N3-C4-C5	5.12	131.16	128.60
8	A	1346	G	N9-C4-C5	-5.11	103.36	105.40
34	a	508	U	C6-N1-C2	5.11	124.07	121.00
8	A	893	C	C6-N1-C1'	5.11	126.93	120.80
55	v	41	C	N1-C2-O2	5.10	121.96	118.90
8	A	2249	U	C4-C5-C6	5.10	122.76	119.70
8	A	293	U	C5-C6-N1	-5.09	120.15	122.70
8	A	1628	G	N1-C6-O6	-5.09	116.84	119.90
34	a	1300	G	P-O3'-C3'	5.09	125.81	119.70
8	A	1398	C	C2-N1-C1'	5.09	124.40	118.80
8	A	2718	G	C6-C5-N7	-5.09	127.35	130.40
8	A	2775	G	C8-N9-C4	5.09	108.44	106.40
34	a	1140	C	N3-C2-O2	-5.09	118.34	121.90
8	A	1244	A	C8-N9-C4	5.08	107.83	105.80
8	A	1894	C	N3-C2-O2	-5.08	118.34	121.90
34	a	679	C	C6-N1-C2	5.08	122.33	120.30
34	a	1103	C	C2-N1-C1'	-5.08	113.21	118.80
8	A	164	C	C2-N1-C1'	5.08	124.39	118.80
8	A	1600	C	C6-N1-C2	-5.08	118.27	120.30
34	a	176	C	C2-N3-C4	-5.07	117.36	119.90
8	A	979	A	C8-N9-C4	5.07	107.83	105.80
34	a	575	G	N3-C4-N9	-5.07	122.96	126.00
8	A	2578	G	N3-C4-C5	5.07	131.13	128.60
34	a	372	C	C2-N1-C1'	-5.07	113.22	118.80
8	A	1413	A	C5-C6-N6	-5.07	119.65	123.70
8	A	708	G	N3-C4-C5	5.06	131.13	128.60
8	A	1228	G	C8-N9-C4	5.06	108.42	106.40
8	A	1047	G	O4'-C1'-N9	5.06	112.25	108.20
8	A	1209	U	C6-N1-C2	5.06	124.03	121.00
8	A	2235	G	C8-N9-C4	5.06	108.42	106.40
56	w	19	G	C8-N9-C4	5.05	108.42	106.40
8	A	617	G	C8-N9-C4	5.05	108.42	106.40
34	a	5	U	C2-N1-C1'	5.05	123.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	343	C	C6-N1-C1'	-5.04	114.75	120.80
8	A	679	C	N1-C2-O2	5.04	121.93	118.90
8	A	951	C	C5-C6-N1	-5.04	118.48	121.00
34	a	1050	G	N3-C4-N9	-5.04	122.98	126.00
8	A	2418	A	C8-N9-C4	5.04	107.81	105.80
8	A	2632	A	C8-N9-C4	5.04	107.81	105.80
8	A	1778	U	C5-C6-N1	-5.03	120.18	122.70
8	A	90	U	N1-C2-N3	5.03	117.92	114.90
34	a	508	U	C5-C6-N1	-5.03	120.18	122.70
8	A	241	A	C8-N9-C4	5.03	107.81	105.80
34	a	215	C	N3-C2-O2	-5.03	118.38	121.90
8	A	883	G	C4-N9-C1'	-5.03	119.96	126.50
8	A	2834	G	N3-C4-C5	5.03	131.11	128.60
34	a	445	G	C4-N9-C1'	-5.03	119.97	126.50
34	a	586	C	C5-C6-N1	-5.02	118.49	121.00
8	A	1130	U	C5-C6-N1	-5.02	120.19	122.70
8	A	2666	C	N1-C2-O2	5.02	121.91	118.90
8	A	248	G	N3-C4-N9	5.02	129.01	126.00
8	A	1395	A	O4'-C1'-N9	5.02	112.21	108.20
8	A	170	U	C6-N1-C1'	-5.01	114.18	121.20
8	A	487	C	N3-C2-O2	-5.01	118.39	121.90
8	A	2222	C	N3-C2-O2	-5.01	118.39	121.90
8	A	2420	C	C6-N1-C1'	-5.01	114.79	120.80
34	a	1415	G	N3-C4-N9	5.01	129.00	126.00
34	a	1043	G	C4-N9-C1'	-5.01	119.99	126.50
34	a	68	G	N3-C4-C5	5.00	131.10	128.60
55	v	13	C	C6-N1-C2	5.00	122.30	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	42 (78%)	12 (22%)	0	100	100
2	1	48/55 (87%)	38 (79%)	10 (21%)	0	100	100
3	2	44/46 (96%)	27 (61%)	17 (39%)	0	100	100
4	3	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
5	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
6	5	129/165 (78%)	100 (78%)	29 (22%)	0	100	100
7	6	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
10	C	269/273 (98%)	213 (79%)	56 (21%)	0	100	100
11	D	207/209 (99%)	172 (83%)	34 (16%)	1 (0%)	29	69
12	E	199/201 (99%)	165 (83%)	34 (17%)	0	100	100
13	F	175/179 (98%)	153 (87%)	22 (13%)	0	100	100
14	G	174/177 (98%)	149 (86%)	25 (14%)	0	100	100
15	H	147/149 (99%)	117 (80%)	30 (20%)	0	100	100
16	I	139/142 (98%)	104 (75%)	35 (25%)	0	100	100
17	J	140/142 (99%)	109 (78%)	31 (22%)	0	100	100
18	K	120/123 (98%)	101 (84%)	19 (16%)	0	100	100
19	L	141/144 (98%)	108 (77%)	33 (23%)	0	100	100
20	M	134/136 (98%)	109 (81%)	24 (18%)	1 (1%)	22	62
21	N	118/127 (93%)	87 (74%)	31 (26%)	0	100	100
22	O	114/117 (97%)	101 (89%)	13 (11%)	0	100	100
23	P	112/115 (97%)	98 (88%)	14 (12%)	0	100	100
24	Q	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
25	R	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
26	S	108/110 (98%)	89 (82%)	19 (18%)	0	100	100
27	T	91/100 (91%)	74 (81%)	17 (19%)	0	100	100
28	U	100/104 (96%)	81 (81%)	19 (19%)	0	100	100
29	V	92/94 (98%)	79 (86%)	13 (14%)	0	100	100
30	W	73/85 (86%)	56 (77%)	17 (23%)	0	100	100
31	X	75/78 (96%)	63 (84%)	12 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	Y	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
33	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
35	b	216/240 (90%)	184 (85%)	32 (15%)	0	100	100
36	c	204/233 (88%)	181 (89%)	23 (11%)	0	100	100
37	d	203/206 (98%)	160 (79%)	42 (21%)	1 (0%)	29	69
38	e	155/167 (93%)	119 (77%)	36 (23%)	0	100	100
39	f	98/135 (73%)	88 (90%)	10 (10%)	0	100	100
40	g	149/179 (83%)	130 (87%)	19 (13%)	0	100	100
41	h	127/130 (98%)	107 (84%)	20 (16%)	0	100	100
42	i	125/130 (96%)	98 (78%)	27 (22%)	0	100	100
43	j	96/103 (93%)	76 (79%)	19 (20%)	1 (1%)	15	54
44	k	114/129 (88%)	92 (81%)	22 (19%)	0	100	100
45	l	121/124 (98%)	96 (79%)	25 (21%)	0	100	100
46	m	112/118 (95%)	99 (88%)	13 (12%)	0	100	100
47	n	99/102 (97%)	87 (88%)	12 (12%)	0	100	100
48	o	86/89 (97%)	74 (86%)	12 (14%)	0	100	100
49	p	80/82 (98%)	61 (76%)	19 (24%)	0	100	100
50	q	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
51	r	63/75 (84%)	49 (78%)	14 (22%)	0	100	100
52	s	80/92 (87%)	70 (88%)	10 (12%)	0	100	100
53	t	83/87 (95%)	66 (80%)	17 (20%)	0	100	100
54	u	63/71 (89%)	50 (79%)	13 (21%)	0	100	100
All	All	5850/6220 (94%)	4809 (82%)	1037 (18%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	j	60	ASP
37	d	144	ILE
11	D	138	LEU
20	M	59	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	45 (96%)	2 (4%)	29	54
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	37 (97%)	1 (3%)	46	67
4	3	51/52 (98%)	45 (88%)	6 (12%)	5	21
5	4	34/34 (100%)	32 (94%)	2 (6%)	19	45
7	6	59/62 (95%)	52 (88%)	7 (12%)	5	20
10	C	216/218 (99%)	214 (99%)	2 (1%)	78	88
11	D	164/164 (100%)	162 (99%)	2 (1%)	71	84
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	141 (95%)	7 (5%)	26	51
14	G	137/138 (99%)	134 (98%)	3 (2%)	52	71
15	H	114/114 (100%)	113 (99%)	1 (1%)	78	88
17	J	116/116 (100%)	112 (97%)	4 (3%)	37	60
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	100 (98%)	2 (2%)	55	74
20	M	109/109 (100%)	108 (99%)	1 (1%)	78	88
21	N	100/103 (97%)	100 (100%)	0	100	100
22	O	86/87 (99%)	81 (94%)	5 (6%)	20	45
23	P	99/100 (99%)	98 (99%)	1 (1%)	76	86
24	Q	89/90 (99%)	87 (98%)	2 (2%)	52	71
25	R	84/84 (100%)	79 (94%)	5 (6%)	19	44
26	S	93/93 (100%)	88 (95%)	5 (5%)	22	47
27	T	80/84 (95%)	78 (98%)	2 (2%)	47	68
28	U	83/85 (98%)	81 (98%)	2 (2%)	49	69
29	V	78/78 (100%)	78 (100%)	0	100	100
30	W	57/63 (90%)	56 (98%)	1 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	X	67/68 (98%)	66 (98%)	1 (2%)	65	80
32	Y	55/55 (100%)	50 (91%)	5 (9%)	9	30
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	178 (99%)	2 (1%)	73	84
36	c	170/190 (90%)	168 (99%)	2 (1%)	71	84
37	d	172/173 (99%)	168 (98%)	4 (2%)	50	71
38	e	114/126 (90%)	113 (99%)	1 (1%)	78	88
39	f	87/116 (75%)	85 (98%)	2 (2%)	50	71
40	g	124/147 (84%)	121 (98%)	3 (2%)	49	69
41	h	104/105 (99%)	102 (98%)	2 (2%)	57	75
42	i	105/107 (98%)	100 (95%)	5 (5%)	25	51
43	j	86/90 (96%)	86 (100%)	0	100	100
44	k	89/99 (90%)	86 (97%)	3 (3%)	37	60
45	l	103/104 (99%)	102 (99%)	1 (1%)	76	86
46	m	92/96 (96%)	90 (98%)	2 (2%)	52	71
47	n	79/84 (94%)	75 (95%)	4 (5%)	24	49
48	o	76/77 (99%)	75 (99%)	1 (1%)	69	82
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/78 (95%)	73 (99%)	1 (1%)	67	80
51	r	56/65 (86%)	55 (98%)	1 (2%)	59	77
52	s	72/79 (91%)	66 (92%)	6 (8%)	11	34
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	44 (96%)	2 (4%)	29	54
57	y	1/1 (100%)	1 (100%)	0	100	100
All	All	4627/4830 (96%)	4516 (98%)	111 (2%)	51	69

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	SER
1	0	38	LEU
3	2	41	ARG
4	3	15	LYS
4	3	29	ARG

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Mol	Chain	Res	Type
4	3	31	ILE
4	3	35	LYS
4	3	42	HIS
4	3	53	ASP
5	4	1	MET
5	4	12	ARG
7	6	37	CYS
7	6	47	LYS
7	6	49	ARG
7	6	50	ASP
7	6	53	THR
7	6	56	ARG
7	6	61	ASN
10	C	264	LYS
10	C	270	ARG
11	D	33	ARG
11	D	138	LEU
13	F	22	ASN
13	F	29	ARG
13	F	48	LEU
13	F	51	ASN
13	F	68	LYS
13	F	79	ARG
13	F	177	ARG
14	G	59	ASP
14	G	94	ARG
14	G	98	LYS
15	H	75	LEU
17	J	12	LYS
17	J	48	VAL
17	J	77	HIS
17	J	116	ARG
19	L	39	LYS
19	L	40	SER
20	M	6	ARG
22	O	30	ARG
22	O	31	THR
22	O	53	THR
22	O	67	ASN
22	O	103	VAL
23	P	88	ARG
24	Q	21	LYS

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Mol	Chain	Res	Type
24	Q	50	ARG
25	R	5	PHE
25	R	49	ILE
25	R	51	VAL
25	R	55	ASP
25	R	85	LYS
26	S	77	ASP
26	S	78	GLU
26	S	83	LYS
26	S	101	SER
26	S	104	THR
27	T	36	LYS
27	T	87	LEU
28	U	72	PHE
28	U	81	ARG
30	W	10	ARG
31	X	76	LYS
32	Y	14	LEU
32	Y	17	GLU
32	Y	18	LEU
32	Y	22	LEU
32	Y	57	LEU
35	b	73	ARG
35	b	131	LYS
36	c	167	TYR
36	c	184	ASN
37	d	44	LYS
37	d	57	LYS
37	d	75	TYR
37	d	150	LYS
38	e	123	LEU
39	f	55	HIS
39	f	76	THR
40	g	21	LEU
40	g	22	LEU
40	g	118	ARG
41	h	68	LYS
41	h	104	SER
42	i	11	ARG
42	i	24	ASN
42	i	26	LYS
42	i	58	GLU

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Mol	Chain	Res	Type
42	i	122	ARG
44	k	12	ARG
44	k	36	ARG
44	k	74	LYS
45	l	45	ASN
46	m	103	THR
46	m	104	ASN
47	n	5	MET
47	n	47	LYS
47	n	61	ARG
47	n	63	ARG
48	o	9	LYS
50	q	27	PHE
51	r	72	ARG
52	s	9	PHE
52	s	28	LYS
52	s	40	PHE
52	s	68	HIS
52	s	78	THR
52	s	80	ARG
54	u	15	LEU
54	u	37	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	6	GLN
3	2	13	ASN
3	2	26	ASN
3	2	29	GLN
5	4	13	ASN
7	6	61	ASN
7	6	65	ASN
10	C	85	ASN
10	C	127	ASN
10	C	133	ASN
10	C	142	ASN
10	C	162	GLN
10	C	196	ASN
10	C	238	ASN
10	C	259	ASN
11	D	32	ASN

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Mol	Chain	Res	Type
11	D	136	ASN
11	D	167	ASN
11	D	173	GLN
12	E	62	GLN
13	F	20	ASN
13	F	62	GLN
14	G	21	GLN
14	G	44	HIS
14	G	110	HIS
14	G	138	GLN
15	H	43	ASN
15	H	73	ASN
15	H	135	HIS
18	K	3	GLN
19	L	99	ASN
19	L	104	GLN
20	M	60	GLN
20	M	97	GLN
21	N	9	GLN
21	N	11	ASN
21	N	16	HIS
21	N	31	HIS
21	N	107	ASN
22	O	116	GLN
23	P	9	GLN
24	Q	36	GLN
24	Q	55	GLN
25	R	18	GLN
25	R	66	HIS
25	R	82	HIS
25	R	86	GLN
26	S	7	HIS
26	S	60	HIS
26	S	61	ASN
27	T	59	ASN
29	V	87	GLN
30	W	46	ASN
31	X	16	ASN
31	X	22	ASN
32	Y	31	GLN
32	Y	36	GLN
32	Y	45	GLN

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Mol	Chain	Res	Type
33	Z	19	HIS
35	b	17	HIS
35	b	119	GLN
37	d	58	GLN
37	d	115	GLN
38	e	72	ASN
38	e	77	ASN
39	f	3	HIS
39	f	68	GLN
40	g	121	ASN
40	g	147	ASN
41	h	37	ASN
41	h	66	GLN
41	h	75	GLN
43	j	58	ASN
44	k	28	ASN
44	k	39	ASN
44	k	80	ASN
45	l	28	GLN
47	n	62	ASN
47	n	66	GLN
48	o	37	HIS
48	o	41	HIS
48	o	45	HIS
49	p	9	HIS
51	r	51	GLN
51	r	53	GLN
52	s	42	ASN
52	s	55	GLN
52	s	56	HIS
52	s	82	HIS
53	t	47	GLN
53	t	51	ASN
53	t	60	GLN
53	t	77	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	575 (37%)	0
55	v	76/77 (98%)	30 (39%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
56	w	74/76 (97%)	32 (43%)	0
58	z	10/33 (30%)	6 (60%)	0
8	A	2897/2903 (99%)	1092 (37%)	86 (2%)
9	B	119/120 (99%)	46 (38%)	2 (1%)
All	All	4712/4751 (99%)	1781 (37%)	88 (1%)

All (1781) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	14	A
8	A	15	G
8	A	16	C
8	A	23	G
8	A	24	G
8	A	27	G
8	A	35	G
8	A	39	G
8	A	44	A
8	A	45	G
8	A	46	G
8	A	50	U
8	A	51	G
8	A	52	A
8	A	55	G
8	A	56	A
8	A	60	G
8	A	62	U
8	A	63	A
8	A	71	A
8	A	73	A
8	A	74	A
8	A	75	G
8	A	76	C
8	A	80	G
8	A	82	U
8	A	84	A
8	A	92	U
8	A	96	C
8	A	101	A
8	A	102	U
8	A	103	A

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Mol	Chain	Res	Type
8	A	106	C
8	A	110	G
8	A	112	U
8	A	114	U
8	A	118	A
8	A	119	A
8	A	120	U
8	A	121	G
8	A	122	G
8	A	124	G
8	A	132	G
8	A	136	G
8	A	137	U
8	A	138	U
8	A	140	C
8	A	141	G
8	A	142	A
8	A	146	A
8	A	158	U
8	A	159	G
8	A	160	A
8	A	161	A
8	A	163	C
8	A	165	A
8	A	166	U
8	A	168	G
8	A	169	G
8	A	170	U
8	A	171	U
8	A	173	A
8	A	178	G
8	A	180	G
8	A	181	A
8	A	188	G
8	A	191	A
8	A	196	A
8	A	199	A
8	A	205	G
8	A	208	C
8	A	209	C
8	A	215	G
8	A	216	A

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Mol	Chain	Res	Type
8	A	217	A
8	A	220	G
8	A	221	A
8	A	223	A
8	A	224	U
8	A	228	C
8	A	229	C
8	A	230	G
8	A	239	C
8	A	241	A
8	A	242	G
8	A	243	U
8	A	248	G
8	A	252	G
8	A	254	G
8	A	255	A
8	A	261	G
8	A	265	A
8	A	266	G
8	A	267	C
8	A	272	A
8	A	275	C
8	A	276	U
8	A	277	G
8	A	278	A
8	A	279	A
8	A	284	U
8	A	286	U
8	A	287	G
8	A	288	U
8	A	291	G
8	A	295	G
8	A	298	G
8	A	299	A
8	A	300	A
8	A	302	C
8	A	305	C
8	A	310	A
8	A	312	G
8	A	323	C
8	A	325	G
8	A	326	G

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Mol	Chain	Res	Type
8	A	329	G
8	A	330	A
8	A	331	C
8	A	332	A
8	A	333	G
8	A	343	C
8	A	345	A
8	A	346	A
8	A	349	U
8	A	359	G
8	A	361	G
8	A	362	A
8	A	363	G
8	A	366	C
8	A	369	U
8	A	371	A
8	A	372	G
8	A	383	C
8	A	384	A
8	A	385	C
8	A	386	G
8	A	387	U
8	A	391	A
8	A	395	U
8	A	399	U
8	A	401	A
8	A	404	A
8	A	405	U
8	A	406	G
8	A	408	G
8	A	411	G
8	A	419	U
8	A	430	A
8	A	434	U
8	A	435	C
8	A	438	G
8	A	442	G
8	A	445	C
8	A	446	G
8	A	449	A
8	A	451	U
8	A	452	G

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Mol	Chain	Res	Type
8	A	453	A
8	A	455	C
8	A	457	A
8	A	458	G
8	A	459	U
8	A	465	G
8	A	473	G
8	A	475	C
8	A	477	A
8	A	478	A
8	A	480	A
8	A	481	G
8	A	482	A
8	A	484	C
8	A	486	C
8	A	489	G
8	A	490	C
8	A	491	G
8	A	504	A
8	A	505	A
8	A	506	G
8	A	508	A
8	A	509	C
8	A	510	C
8	A	511	U
8	A	512	G
8	A	513	A
8	A	514	A
8	A	515	A
8	A	516	C
8	A	525	U
8	A	527	C
8	A	530	G
8	A	531	C
8	A	532	A
8	A	533	G
8	A	534	U
8	A	540	C
8	A	543	G
8	A	544	C
8	A	546	U
8	A	548	G

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Mol	Chain	Res	Type
8	A	549	G
8	A	557	C
8	A	561	G
8	A	562	U
8	A	563	A
8	A	568	U
8	A	573	U
8	A	575	A
8	A	581	C
8	A	586	A
8	A	597	G
8	A	603	A
8	A	609	A
8	A	613	A
8	A	614	A
8	A	615	U
8	A	616	A
8	A	620	G
8	A	621	A
8	A	622	G
8	A	623	C
8	A	627	A
8	A	631	A
8	A	637	A
8	A	642	U
8	A	646	U
8	A	647	G
8	A	653	U
8	A	655	A
8	A	660	C
8	A	664	G
8	A	668	A
8	A	669	G
8	A	670	A
8	A	672	C
8	A	675	A
8	A	677	A
8	A	686	U
8	A	687	C
8	A	689	A
8	A	690	G
8	A	693	A

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Mol	Chain	Res	Type
8	A	703	U
8	A	704	G
8	A	713	G
8	A	714	U
8	A	715	A
8	A	716	A
8	A	717	C
8	A	725	G
8	A	726	G
8	A	730	A
8	A	739	A
8	A	740	C
8	A	744	U
8	A	747	5MC
8	A	748	G
8	A	749	A
8	A	750	A
8	A	757	G
8	A	762	U
8	A	764	A
8	A	766	U
8	A	768	G
8	A	769	U
8	A	774	G
8	A	776	G
8	A	781	A
8	A	782	A
8	A	783	A
8	A	784	G
8	A	785	G
8	A	786	C
8	A	789	A
8	A	790	U
8	A	792	A
8	A	800	A
8	A	801	G
8	A	805	G
8	A	806	C
8	A	808	G
8	A	811	U
8	A	812	C
8	A	819	A

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Mol	Chain	Res	Type
8	A	820	A
8	A	826	U
8	A	827	U
8	A	828	U
8	A	831	G
8	A	834	G
8	A	835	C
8	A	837	C
8	A	841	G
8	A	845	A
8	A	846	U
8	A	847	U
8	A	850	U
8	A	856	G
8	A	858	G
8	A	859	G
8	A	865	C
8	A	868	U
8	A	870	U
8	A	877	A
8	A	878	A
8	A	881	G
8	A	883	G
8	A	884	U
8	A	885	C
8	A	886	A
8	A	887	A
8	A	888	C
8	A	889	C
8	A	890	C
8	A	891	G
8	A	893	C
8	A	894	U
8	A	895	U
8	A	896	A
8	A	897	C
8	A	899	A
8	A	900	A
8	A	902	C
8	A	903	C
8	A	907	G
8	A	910	A

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Mol	Chain	Res	Type
8	A	912	C
8	A	913	U
8	A	915	C
8	A	917	A
8	A	927	A
8	A	931	U
8	A	932	U
8	A	934	U
8	A	941	A
8	A	945	A
8	A	946	C
8	A	957	C
8	A	959	A
8	A	961	C
8	A	973	A
8	A	974	G
8	A	975	A
8	A	976	G
8	A	982	C
8	A	983	A
8	A	985	C
8	A	989	G
8	A	990	A
8	A	995	C
8	A	996	A
8	A	1003	G
8	A	1005	C
8	A	1006	C
8	A	1010	A
8	A	1011	G
8	A	1012	U
8	A	1013	C
8	A	1022	G
8	A	1025	G
8	A	1026	G
8	A	1033	U
8	A	1034	G
8	A	1041	G
8	A	1044	C
8	A	1045	C
8	A	1046	A
8	A	1047	G

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Mol	Chain	Res	Type
8	A	1048	A
8	A	1049	C
8	A	1051	G
8	A	1053	C
8	A	1054	A
8	A	1055	G
8	A	1056	G
8	A	1057	A
8	A	1059	G
8	A	1060	U
8	A	1061	U
8	A	1062	G
8	A	1063	G
8	A	1064	C
8	A	1066	U
8	A	1067	A
8	A	1068	G
8	A	1069	A
8	A	1070	A
8	A	1071	G
8	A	1072	C
8	A	1073	A
8	A	1075	C
8	A	1077	A
8	A	1078	U
8	A	1079	C
8	A	1080	A
8	A	1081	U
8	A	1083	U
8	A	1084	A
8	A	1085	A
8	A	1086	A
8	A	1087	G
8	A	1088	A
8	A	1089	A
8	A	1090	A
8	A	1091	G
8	A	1092	C
8	A	1093	G
8	A	1094	U
8	A	1096	A
8	A	1098	A

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Mol	Chain	Res	Type
8	A	1100	C
8	A	1101	U
8	A	1102	C
8	A	1103	A
8	A	1105	U
8	A	1106	G
8	A	1109	C
8	A	1111	A
8	A	1112	G
8	A	1114	C
8	A	1115	G
8	A	1116	G
8	A	1122	G
8	A	1123	C
8	A	1128	G
8	A	1129	A
8	A	1130	U
8	A	1131	G
8	A	1132	U
8	A	1133	A
8	A	1134	A
8	A	1135	C
8	A	1139	G
8	A	1142	A
8	A	1143	A
8	A	1144	A
8	A	1149	G
8	A	1152	C
8	A	1155	A
8	A	1157	G
8	A	1170	C
8	A	1171	G
8	A	1173	U
8	A	1174	U
8	A	1175	A
8	A	1176	U
8	A	1179	G
8	A	1180	U
8	A	1186	G
8	A	1187	G
8	A	1188	U
8	A	1193	G

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Mol	Chain	Res	Type
8	A	1204	A
8	A	1205	A
8	A	1209	U
8	A	1210	G
8	A	1211	C
8	A	1212	G
8	A	1214	A
8	A	1218	G
8	A	1225	G
8	A	1226	A
8	A	1227	G
8	A	1235	G
8	A	1236	G
8	A	1238	G
8	A	1241	A
8	A	1245	G
8	A	1248	G
8	A	1249	U
8	A	1251	C
8	A	1252	G
8	A	1253	A
8	A	1255	U
8	A	1256	G
8	A	1264	A
8	A	1268	A
8	A	1269	A
8	A	1271	G
8	A	1272	A
8	A	1273	U
8	A	1284	A
8	A	1285	A
8	A	1289	C
8	A	1293	C
8	A	1300	G
8	A	1301	A
8	A	1302	A
8	A	1303	G
8	A	1306	C
8	A	1311	G
8	A	1312	U
8	A	1313	U
8	A	1314	C

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Mol	Chain	Res	Type
8	A	1315	C
8	A	1322	A
8	A	1325	U
8	A	1328	A
8	A	1332	G
8	A	1340	U
8	A	1342	A
8	A	1344	U
8	A	1345	C
8	A	1346	G
8	A	1352	U
8	A	1365	A
8	A	1368	G
8	A	1369	G
8	A	1370	C
8	A	1376	C
8	A	1378	A
8	A	1379	U
8	A	1380	G
8	A	1383	A
8	A	1384	A
8	A	1385	A
8	A	1386	C
8	A	1393	A
8	A	1395	A
8	A	1396	U
8	A	1397	U
8	A	1398	C
8	A	1410	G
8	A	1411	U
8	A	1415	U
8	A	1416	G
8	A	1418	G
8	A	1419	A
8	A	1420	A
8	A	1421	G
8	A	1428	C
8	A	1429	G
8	A	1432	G
8	A	1433	A
8	A	1435	G
8	A	1448	G

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Mol	Chain	Res	Type
8	A	1451	C
8	A	1452	G
8	A	1453	A
8	A	1454	C
8	A	1455	G
8	A	1458	U
8	A	1459	G
8	A	1460	U
8	A	1461	C
8	A	1467	U
8	A	1472	C
8	A	1473	G
8	A	1474	U
8	A	1482	G
8	A	1484	U
8	A	1488	C
8	A	1490	A
8	A	1491	G
8	A	1493	C
8	A	1494	A
8	A	1495	A
8	A	1496	A
8	A	1497	U
8	A	1502	A
8	A	1503	A
8	A	1504	A
8	A	1506	U
8	A	1509	A
8	A	1512	C
8	A	1515	A
8	A	1521	G
8	A	1524	G
8	A	1528	A
8	A	1532	A
8	A	1534	U
8	A	1535	A
8	A	1536	C
8	A	1537	G
8	A	1544	A
8	A	1547	C
8	A	1551	A
8	A	1553	A

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Mol	Chain	Res	Type
8	A	1554	U
8	A	1557	C
8	A	1558	C
8	A	1562	U
8	A	1563	U
8	A	1566	A
8	A	1569	A
8	A	1570	A
8	A	1578	U
8	A	1584	U
8	A	1585	C
8	A	1591	A
8	A	1594	U
8	A	1596	A
8	A	1598	A
8	A	1600	C
8	A	1607	C
8	A	1608	A
8	A	1609	A
8	A	1610	A
8	A	1616	A
8	A	1617	C
8	A	1619	G
8	A	1622	G
8	A	1623	G
8	A	1626	A
8	A	1627	G
8	A	1628	G
8	A	1631	G
8	A	1635	A
8	A	1643	G
8	A	1644	C
8	A	1645	G
8	A	1646	C
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1651	G
8	A	1654	A
8	A	1657	U
8	A	1658	C
8	A	1664	A

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Mol	Chain	Res	Type
8	A	1668	A
8	A	1669	A
8	A	1674	G
8	A	1691	C
8	A	1693	U
8	A	1695	G
8	A	1698	A
8	A	1699	G
8	A	1700	A
8	A	1702	G
8	A	1705	A
8	A	1715	G
8	A	1716	U
8	A	1726	C
8	A	1727	C
8	A	1729	U
8	A	1730	C
8	A	1731	G
8	A	1732	C
8	A	1733	G
8	A	1735	A
8	A	1738	G
8	A	1750	G
8	A	1752	C
8	A	1754	A
8	A	1757	A
8	A	1758	U
8	A	1759	A
8	A	1764	C
8	A	1767	G
8	A	1769	U
8	A	1773	A
8	A	1774	C
8	A	1775	U
8	A	1782	U
8	A	1784	A
8	A	1787	A
8	A	1788	C
8	A	1797	G
8	A	1800	C
8	A	1801	A
8	A	1804	C

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Mol	Chain	Res	Type
8	A	1808	A
8	A	1809	A
8	A	1810	A
8	A	1812	U
8	A	1813	G
8	A	1816	C
8	A	1817	G
8	A	1820	U
8	A	1821	A
8	A	1828	G
8	A	1829	A
8	A	1830	C
8	A	1833	C
8	A	1835	2MG
8	A	1848	A
8	A	1852	U
8	A	1857	G
8	A	1859	U
8	A	1860	G
8	A	1862	G
8	A	1865	U
8	A	1866	A
8	A	1868	C
8	A	1869	G
8	A	1873	G
8	A	1874	C
8	A	1876	A
8	A	1884	G
8	A	1895	C
8	A	1900	A
8	A	1901	A
8	A	1902	C
8	A	1906	G
8	A	1908	C
8	A	1910	G
8	A	1917	PSU
8	A	1918	A
8	A	1919	A
8	A	1921	G
8	A	1922	G
8	A	1923	U
8	A	1925	C

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Mol	Chain	Res	Type
8	A	1926	U
8	A	1928	A
8	A	1930	G
8	A	1932	A
8	A	1935	G
8	A	1938	A
8	A	1939	5MU
8	A	1940	U
8	A	1941	C
8	A	1944	U
8	A	1946	U
8	A	1955	U
8	A	1956	U
8	A	1962	5MC
8	A	1963	U
8	A	1964	G
8	A	1965	C
8	A	1967	C
8	A	1970	A
8	A	1972	G
8	A	1977	A
8	A	1979	U
8	A	1982	U
8	A	1991	U
8	A	1992	G
8	A	1993	U
8	A	1997	C
8	A	2001	C
8	A	2002	G
8	A	2003	A
8	A	2007	U
8	A	2009	A
8	A	2012	G
8	A	2013	A
8	A	2015	A
8	A	2016	U
8	A	2019	A
8	A	2021	C
8	A	2022	U
8	A	2023	C
8	A	2027	G
8	A	2028	U

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Mol	Chain	Res	Type
8	A	2029	G
8	A	2031	A
8	A	2032	G
8	A	2033	A
8	A	2034	U
8	A	2036	C
8	A	2042	A
8	A	2043	C
8	A	2044	C
8	A	2049	G
8	A	2051	A
8	A	2052	A
8	A	2055	C
8	A	2056	G
8	A	2057	G
8	A	2060	A
8	A	2061	G
8	A	2062	A
8	A	2063	C
8	A	2067	G
8	A	2068	U
8	A	2069	G7M
8	A	2073	C
8	A	2076	U
8	A	2077	A
8	A	2081	U
8	A	2089	C
8	A	2091	C
8	A	2092	U
8	A	2093	G
8	A	2097	A
8	A	2101	A
8	A	2102	G
8	A	2103	C
8	A	2104	C
8	A	2109	U
8	A	2110	G
8	A	2111	U
8	A	2112	G
8	A	2114	A
8	A	2115	G
8	A	2116	G

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Mol	Chain	Res	Type
8	A	2118	U
8	A	2119	A
8	A	2124	G
8	A	2125	G
8	A	2126	A
8	A	2127	G
8	A	2128	G
8	A	2129	C
8	A	2130	U
8	A	2131	U
8	A	2132	U
8	A	2133	G
8	A	2134	A
8	A	2135	A
8	A	2136	G
8	A	2138	G
8	A	2139	U
8	A	2143	C
8	A	2144	G
8	A	2145	C
8	A	2146	C
8	A	2147	A
8	A	2148	G
8	A	2150	C
8	A	2151	U
8	A	2152	G
8	A	2153	C
8	A	2155	U
8	A	2156	G
8	A	2157	G
8	A	2158	A
8	A	2159	G
8	A	2160	C
8	A	2161	C
8	A	2162	G
8	A	2163	A
8	A	2164	C
8	A	2166	U
8	A	2169	A
8	A	2170	A
8	A	2171	A
8	A	2172	U

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Mol	Chain	Res	Type
8	A	2173	A
8	A	2175	C
8	A	2176	A
8	A	2180	U
8	A	2181	U
8	A	2183	A
8	A	2186	G
8	A	2190	G
8	A	2193	G
8	A	2198	A
8	A	2199	A
8	A	2200	C
8	A	2203	U
8	A	2204	G
8	A	2208	C
8	A	2210	U
8	A	2211	A
8	A	2212	A
8	A	2214	C
8	A	2225	A
8	A	2226	C
8	A	2232	C
8	A	2238	G
8	A	2239	G
8	A	2248	C
8	A	2251	OMG
8	A	2259	U
8	A	2262	U
8	A	2265	U
8	A	2266	A
8	A	2267	A
8	A	2269	G
8	A	2273	A
8	A	2274	A
8	A	2279	G
8	A	2281	A
8	A	2283	C
8	A	2285	C
8	A	2286	G
8	A	2287	A
8	A	2288	A
8	A	2297	A

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Mol	Chain	Res	Type
8	A	2300	C
8	A	2305	U
8	A	2307	G
8	A	2308	G
8	A	2309	A
8	A	2310	C
8	A	2318	G
8	A	2320	U
8	A	2321	U
8	A	2322	A
8	A	2325	G
8	A	2327	A
8	A	2333	A
8	A	2334	U
8	A	2335	A
8	A	2336	A
8	A	2337	G
8	A	2343	U
8	A	2344	U
8	A	2345	G
8	A	2347	C
8	A	2349	G
8	A	2350	C
8	A	2358	A
8	A	2361	G
8	A	2373	G
8	A	2374	C
8	A	2379	G
8	A	2380	C
8	A	2382	G
8	A	2383	G
8	A	2384	U
8	A	2385	C
8	A	2388	A
8	A	2392	A
8	A	2396	G
8	A	2402	U
8	A	2403	C
8	A	2406	A
8	A	2422	C
8	A	2423	U
8	A	2424	C

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Mol	Chain	Res	Type
8	A	2425	A
8	A	2426	A
8	A	2427	C
8	A	2428	G
8	A	2429	G
8	A	2430	A
8	A	2432	A
8	A	2433	A
8	A	2434	A
8	A	2435	A
8	A	2437	G
8	A	2439	A
8	A	2441	U
8	A	2442	C
8	A	2445	2MG
8	A	2447	G
8	A	2448	A
8	A	2449	U
8	A	2456	C
8	A	2458	G
8	A	2459	A
8	A	2462	C
8	A	2467	C
8	A	2469	A
8	A	2474	U
8	A	2475	C
8	A	2476	A
8	A	2480	C
8	A	2482	A
8	A	2484	G
8	A	2490	G
8	A	2491	U
8	A	2494	G
8	A	2496	C
8	A	2498	OMC
8	A	2499	C
8	A	2500	U
8	A	2502	G
8	A	2505	G
8	A	2513	A
8	A	2518	A
8	A	2520	C

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Mol	Chain	Res	Type
8	A	2524	G
8	A	2528	U
8	A	2529	G
8	A	2532	G
8	A	2534	A
8	A	2535	G
8	A	2536	G
8	A	2543	G
8	A	2547	A
8	A	2553	G
8	A	2554	U
8	A	2555	U
8	A	2560	A
8	A	2564	A
8	A	2566	A
8	A	2567	G
8	A	2572	A
8	A	2573	C
8	A	2574	G
8	A	2576	G
8	A	2577	A
8	A	2578	G
8	A	2579	C
8	A	2581	G
8	A	2582	G
8	A	2583	G
8	A	2584	U
8	A	2585	U
8	A	2595	G
8	A	2599	G
8	A	2600	A
8	A	2602	A
8	A	2603	G
8	A	2606	C
8	A	2609	U
8	A	2610	C
8	A	2613	U
8	A	2618	G
8	A	2623	G
8	A	2627	G
8	A	2629	U
8	A	2633	G

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Mol	Chain	Res	Type
8	A	2634	A
8	A	2635	A
8	A	2636	C
8	A	2644	G
8	A	2646	C
8	A	2648	G
8	A	2650	U
8	A	2651	C
8	A	2654	A
8	A	2656	U
8	A	2660	A
8	A	2661	G
8	A	2663	G
8	A	2671	G
8	A	2682	A
8	A	2683	C
8	A	2684	U
8	A	2688	G
8	A	2690	U
8	A	2694	G
8	A	2699	C
8	A	2702	G
8	A	2707	U
8	A	2710	C
8	A	2711	A
8	A	2712	C
8	A	2714	G
8	A	2718	G
8	A	2719	G
8	A	2720	U
8	A	2721	A
8	A	2729	G
8	A	2732	G
8	A	2733	A
8	A	2739	U
8	A	2744	G
8	A	2748	A
8	A	2750	A
8	A	2751	G
8	A	2752	C
8	A	2755	C
8	A	2757	A

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Mol	Chain	Res	Type
8	A	2758	A
8	A	2761	A
8	A	2764	A
8	A	2765	A
8	A	2767	C
8	A	2778	A
8	A	2779	U
8	A	2780	G
8	A	2782	G
8	A	2787	C
8	A	2790	U
8	A	2791	G
8	A	2793	C
8	A	2796	U
8	A	2797	U
8	A	2798	U
8	A	2799	A
8	A	2800	A
8	A	2801	G
8	A	2803	G
8	A	2804	U
8	A	2809	A
8	A	2812	G
8	A	2813	A
8	A	2820	A
8	A	2821	A
8	A	2823	A
8	A	2824	C
8	A	2825	G
8	A	2831	G
8	A	2833	U
8	A	2834	G
8	A	2835	A
8	A	2849	U
8	A	2850	A
8	A	2861	U
8	A	2867	G
8	A	2868	A
8	A	2869	G
8	A	2872	A
8	A	2879	A
8	A	2883	A

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Mol	Chain	Res	Type
8	A	2884	U
8	A	2886	A
8	A	2889	C
8	A	2891	U
8	A	2892	G
8	A	2893	A
8	A	2895	G
8	A	2900	A
8	A	2901	C
9	B	3	C
9	B	7	G
9	B	9	G
9	B	10	G
9	B	13	G
9	B	14	U
9	B	16	G
9	B	17	C
9	B	18	G
9	B	19	C
9	B	22	U
9	B	25	U
9	B	30	C
9	B	32	U
9	B	34	A
9	B	35	C
9	B	37	C
9	B	40	U
9	B	41	G
9	B	42	C
9	B	44	G
9	B	46	A
9	B	47	C
9	B	51	G
9	B	53	A
9	B	56	G
9	B	57	A
9	B	58	A
9	B	62	C
9	B	65	U
9	B	66	A
9	B	67	G
9	B	73	A

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Mol	Chain	Res	Type
9	B	80	U
9	B	84	G
9	B	88	C
9	B	89	U
9	B	90	C
9	B	91	C
9	B	101	A
9	B	102	G
9	B	108	A
9	B	109	A
9	B	116	G
9	B	119	A
9	B	120	U
34	a	3	A
34	a	6	G
34	a	7	A
34	a	9	G
34	a	12	U
34	a	16	A
34	a	18	C
34	a	30	U
34	a	31	G
34	a	32	A
34	a	33	A
34	a	34	C
34	a	39	G
34	a	46	G
34	a	47	C
34	a	48	C
34	a	49	U
34	a	50	A
34	a	51	A
34	a	53	A
34	a	60	A
34	a	61	G
34	a	66	A
34	a	70	U
34	a	71	A
34	a	76	G
34	a	78	A
34	a	80	A
34	a	81	A

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Mol	Chain	Res	Type
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	87	C
34	a	89	U
34	a	94	G
34	a	95	C
34	a	96	U
34	a	99	C
34	a	107	G
34	a	108	G
34	a	109	A
34	a	110	C
34	a	117	G
34	a	121	U
34	a	122	G
34	a	130	A
34	a	131	A
34	a	144	G
34	a	145	G
34	a	149	A
34	a	153	C
34	a	159	G
34	a	160	A
34	a	161	A
34	a	163	C
34	a	165	G
34	a	166	U
34	a	169	C
34	a	171	A
34	a	173	U
34	a	174	A
34	a	175	C
34	a	179	A
34	a	180	U
34	a	182	A
34	a	183	C
34	a	184	G
34	a	185	U
34	a	196	A
34	a	197	A

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Mol	Chain	Res	Type
34	a	198	G
34	a	200	G
34	a	205	A
34	a	208	U
34	a	210	C
34	a	211	G
34	a	214	C
34	a	216	U
34	a	217	C
34	a	220	G
34	a	223	A
34	a	226	G
34	a	228	A
34	a	230	G
34	a	240	G
34	a	245	U
34	a	246	A
34	a	247	G
34	a	251	G
34	a	253	A
34	a	262	A
34	a	263	A
34	a	266	G
34	a	267	C
34	a	270	A
34	a	271	C
34	a	274	A
34	a	275	G
34	a	280	C
34	a	281	G
34	a	289	G
34	a	293	G
34	a	294	U
34	a	298	A
34	a	301	G
34	a	306	A
34	a	317	U
34	a	321	A
34	a	322	C
34	a	323	U
34	a	324	G
34	a	326	G

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Mol	Chain	Res	Type
34	a	328	C
34	a	329	A
34	a	330	C
34	a	338	A
34	a	344	A
34	a	345	C
34	a	351	G
34	a	352	C
34	a	353	A
34	a	354	G
34	a	356	A
34	a	361	G
34	a	363	A
34	a	364	A
34	a	365	U
34	a	366	A
34	a	367	U
34	a	371	A
34	a	372	C
34	a	374	A
34	a	375	U
34	a	376	G
34	a	377	G
34	a	382	A
34	a	387	U
34	a	388	G
34	a	390	U
34	a	397	A
34	a	398	U
34	a	404	G
34	a	406	G
34	a	407	U
34	a	411	A
34	a	413	G
34	a	414	A
34	a	421	U
34	a	423	G
34	a	429	U
34	a	431	A
34	a	439	U
34	a	443	C
34	a	446	G

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Mol	Chain	Res	Type
34	a	448	A
34	a	449	G
34	a	456	A
34	a	458	U
34	a	461	A
34	a	462	G
34	a	464	U
34	a	465	A
34	a	466	A
34	a	468	A
34	a	469	C
34	a	470	C
34	a	473	U
34	a	479	U
34	a	480	U
34	a	483	C
34	a	484	G
34	a	485	U
34	a	486	U
34	a	493	A
34	a	495	A
34	a	496	A
34	a	505	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	516	PSU
34	a	517	G
34	a	518	C
34	a	519	C
34	a	521	G
34	a	525	C
34	a	530	G
34	a	531	U
34	a	532	A
34	a	533	A
34	a	534	U
34	a	535	A
34	a	536	C
34	a	537	G
34	a	541	G
34	a	547	A

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Mol	Chain	Res	Type
34	a	548	G
34	a	554	A
34	a	560	A
34	a	561	U
34	a	562	U
34	a	563	A
34	a	564	C
34	a	567	G
34	a	570	G
34	a	572	A
34	a	574	A
34	a	576	C
34	a	577	G
34	a	582	C
34	a	583	A
34	a	589	U
34	a	592	G
34	a	595	A
34	a	596	A
34	a	597	G
34	a	599	C
34	a	607	A
34	a	614	C
34	a	615	G
34	a	618	C
34	a	626	G
34	a	629	A
34	a	631	C
34	a	633	G
34	a	645	G
34	a	650	G
34	a	656	G
34	a	659	U
34	a	665	A
34	a	666	G
34	a	680	C
34	a	681	A
34	a	687	A
34	a	692	U
34	a	698	G
34	a	701	U
34	a	703	G

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Mol	Chain	Res	Type
34	a	704	A
34	a	708	C
34	a	711	G
34	a	714	G
34	a	718	A
34	a	721	G
34	a	722	G
34	a	723	U
34	a	724	G
34	a	729	A
34	a	732	C
34	a	733	G
34	a	734	G
34	a	735	C
34	a	746	A
34	a	748	G
34	a	751	U
34	a	753	A
34	a	755	G
34	a	756	C
34	a	759	A
34	a	765	G
34	a	773	G
34	a	774	G
34	a	777	A
34	a	781	A
34	a	782	A
34	a	787	A
34	a	788	U
34	a	790	A
34	a	792	A
34	a	793	U
34	a	794	A
34	a	796	C
34	a	805	C
34	a	808	C
34	a	810	C
34	a	811	C
34	a	812	G
34	a	814	A
34	a	815	A
34	a	816	A

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Mol	Chain	Res	Type
34	a	817	C
34	a	820	U
34	a	821	G
34	a	822	U
34	a	828	U
34	a	832	G
34	a	838	G
34	a	841	C
34	a	843	U
34	a	844	G
34	a	846	G
34	a	848	C
34	a	849	G
34	a	851	G
34	a	854	U
34	a	858	G
34	a	862	C
34	a	864	A
34	a	867	G
34	a	872	A
34	a	874	G
34	a	876	C
34	a	884	U
34	a	885	G
34	a	889	A
34	a	890	G
34	a	891	U
34	a	898	G
34	a	902	G
34	a	910	C
34	a	916	U
34	a	919	A
34	a	920	U
34	a	926	G
34	a	927	G
34	a	934	C
34	a	935	A
34	a	938	A
34	a	939	G
34	a	945	G
34	a	946	A
34	a	957	U

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Mol	Chain	Res	Type
34	a	960	U
34	a	964	A
34	a	966	2MG
34	a	967	5MC
34	a	968	A
34	a	969	A
34	a	971	G
34	a	973	G
34	a	975	A
34	a	976	G
34	a	977	A
34	a	980	C
34	a	982	U
34	a	984	C
34	a	986	U
34	a	992	U
34	a	993	G
34	a	994	A
34	a	996	A
34	a	997	U
34	a	998	C
34	a	1003	G
34	a	1004	A
34	a	1005	A
34	a	1006	G
34	a	1009	U
34	a	1010	U
34	a	1014	A
34	a	1020	G
34	a	1021	A
34	a	1022	A
34	a	1023	U
34	a	1024	G
34	a	1025	U
34	a	1026	G
34	a	1027	C
34	a	1028	C
34	a	1029	U
34	a	1030	U
34	a	1031	C
34	a	1032	G
34	a	1035	A

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Mol	Chain	Res	Type
34	a	1042	A
34	a	1043	G
34	a	1044	A
34	a	1045	C
34	a	1050	G
34	a	1053	G
34	a	1054	C
34	a	1055	A
34	a	1056	U
34	a	1060	U
34	a	1064	G
34	a	1065	U
34	a	1066	C
34	a	1071	C
34	a	1079	G
34	a	1081	A
34	a	1085	U
34	a	1088	G
34	a	1092	A
34	a	1094	G
34	a	1095	U
34	a	1101	A
34	a	1103	C
34	a	1108	G
34	a	1109	C
34	a	1111	A
34	a	1113	C
34	a	1120	C
34	a	1124	G
34	a	1125	U
34	a	1126	U
34	a	1127	G
34	a	1129	C
34	a	1130	A
34	a	1131	G
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1139	G
34	a	1140	C
34	a	1143	G
34	a	1145	A

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Mol	Chain	Res	Type
34	a	1147	C
34	a	1150	A
34	a	1151	A
34	a	1152	A
34	a	1157	A
34	a	1158	C
34	a	1159	U
34	a	1160	G
34	a	1161	C
34	a	1167	A
34	a	1168	U
34	a	1169	A
34	a	1179	A
34	a	1184	G
34	a	1190	G
34	a	1191	A
34	a	1193	G
34	a	1194	U
34	a	1196	A
34	a	1197	A
34	a	1198	G
34	a	1200	C
34	a	1206	G
34	a	1210	C
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1219	A
34	a	1222	G
34	a	1224	U
34	a	1225	A
34	a	1226	C
34	a	1237	C
34	a	1238	A
34	a	1239	A
34	a	1240	U
34	a	1241	G
34	a	1248	A
34	a	1250	A
34	a	1252	A
34	a	1253	G
34	a	1254	A

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Mol	Chain	Res	Type
34	a	1256	A
34	a	1257	A
34	a	1258	G
34	a	1260	G
34	a	1261	A
34	a	1262	C
34	a	1267	C
34	a	1270	G
34	a	1274	A
34	a	1275	A
34	a	1278	G
34	a	1279	G
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1294	G
34	a	1295	U
34	a	1297	G
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1303	C
34	a	1304	G
34	a	1305	G
34	a	1307	U
34	a	1317	C
34	a	1320	C
34	a	1325	C
34	a	1328	C
34	a	1330	U
34	a	1331	G
34	a	1332	A
34	a	1338	G
34	a	1340	A
34	a	1345	U
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1350	A

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Mol	Chain	Res	Type
34	a	1351	U
34	a	1358	U
34	a	1361	G
34	a	1363	A
34	a	1364	U
34	a	1370	G
34	a	1372	U
34	a	1374	A
34	a	1375	A
34	a	1378	C
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1386	G
34	a	1387	G
34	a	1388	C
34	a	1394	A
34	a	1395	C
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1403	C
34	a	1408	A
34	a	1413	A
34	a	1416	G
34	a	1417	G
34	a	1418	A
34	a	1419	G
34	a	1420	U
34	a	1421	G
34	a	1423	G
34	a	1426	G
34	a	1427	C
34	a	1429	A
34	a	1430	A
34	a	1432	G
34	a	1433	A
34	a	1436	U
34	a	1437	A
34	a	1440	U
34	a	1441	A
34	a	1442	G

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Mol	Chain	Res	Type
34	a	1446	A
34	a	1448	C
34	a	1451	U
34	a	1452	C
34	a	1457	G
34	a	1459	G
34	a	1467	C
34	a	1472	U
34	a	1474	U
34	a	1475	G
34	a	1476	A
34	a	1483	A
34	a	1484	C
34	a	1485	U
34	a	1486	G
34	a	1489	G
34	a	1491	G
34	a	1492	A
34	a	1494	G
34	a	1497	G
34	a	1498	UR3
34	a	1499	A
34	a	1500	A
34	a	1503	A
34	a	1504	G
34	a	1506	U
34	a	1507	A
34	a	1508	A
34	a	1515	G
34	a	1517	G
34	a	1520	C
34	a	1524	C
34	a	1526	G
34	a	1527	U
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1538	C
34	a	1539	C
34	a	1540	U

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Mol	Chain	Res	Type
55	v	2	G
55	v	7	G
55	v	14	A
55	v	16	C
55	v	17	C
55	v	17(A)	U
55	v	18	G
55	v	19	G
55	v	20	H2U
55	v	21	A
55	v	24	U
55	v	33	U
55	v	34	C
55	v	35	A
55	v	38	A
55	v	42	G
55	v	43	A
55	v	44	A
55	v	47	U
55	v	48	C
55	v	52	G
55	v	55	PSU
55	v	56	C
55	v	59	A
55	v	63	G
55	v	69	C
55	v	72	A
55	v	73	A
55	v	75	C
55	v	76	A
56	w	8	4SU
56	w	13	C
56	w	16	U
56	w	17	C
56	w	18	G
56	w	19	G
56	w	20	U
56	w	21	A
56	w	22	G
56	w	31	A
56	w	33	U
56	w	40	C

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Mol	Chain	Res	Type
56	w	45	U
56	w	46	G7M
56	w	47	U
56	w	49	C
56	w	50	U
56	w	52	G
56	w	53	G
56	w	54	5MU
56	w	57	G
56	w	58	A
56	w	59	U
56	w	60	U
56	w	61	C
56	w	64	A
56	w	67	C
56	w	68	C
56	w	73	A
56	w	74	C
56	w	75	C
56	w	76	A
58	z	-1	C
58	z	0	U
58	z	2	U
58	z	4	U
58	z	5	U
58	z	8	U

All (88) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	73	A
8	A	141	G
8	A	242	G
8	A	361	G
8	A	444	C
8	A	457	A
8	A	458	G
8	A	479	A
8	A	481	G
8	A	504	A
8	A	510	C
8	A	545	U

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Mol	Chain	Res	Type
8	A	562	U
8	A	580	U
8	A	619	G
8	A	671	C
8	A	686	U
8	A	715	A
8	A	746	PSU
8	A	758	C
8	A	784	G
8	A	819	A
8	A	827	U
8	A	830	G
8	A	846	U
8	A	883	G
8	A	884	U
8	A	885	C
8	A	894	U
8	A	926	G
8	A	958	U
8	A	960	A
8	A	982	C
8	A	1024	G
8	A	1062	G
8	A	1082	U
8	A	1090	A
8	A	1093	G
8	A	1143	A
8	A	1183	U
8	A	1224	U
8	A	1300	G
8	A	1331	G
8	A	1385	A
8	A	1432	G
8	A	1552	A
8	A	1607	C
8	A	1643	G
8	A	1663	G
8	A	1715	G
8	A	1808	A
8	A	1816	C
8	A	1847	G
8	A	1875	G

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Mol	Chain	Res	Type
8	A	1899	A
8	A	1907	G
8	A	1920	C
8	A	1921	G
8	A	1981	A
8	A	2015	A
8	A	2031	A
8	A	2149	U
8	A	2150	C
8	A	2158	A
8	A	2159	G
8	A	2192	U
8	A	2287	A
8	A	2319	G
8	A	2324	U
8	A	2343	U
8	A	2344	U
8	A	2405	G
8	A	2426	A
8	A	2445	2MG
8	A	2468	A
8	A	2474	U
8	A	2481	G
8	A	2572	A
8	A	2655	G
8	A	2706	A
8	A	2728	U
8	A	2732	G
8	A	2756	U
8	A	2796	U
8	A	2808	G
8	A	2848	G
9	B	66	A
9	B	89	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	OMC	A	2498	8	15,22,23	1.04	2 (13%)	17,31,34	1.53	2 (11%)
34	MA6	a	1519	34	19,26,27	1.07	1 (5%)	18,38,41	2.72	2 (11%)
56	PSU	w	32	56	17,21,22	1.00	1 (5%)	20,30,33	3.28	7 (35%)
8	PSU	A	746	8	17,21,22	1.09	2 (11%)	20,30,33	3.08	6 (30%)
55	4SU	v	8	55	14,21,22	3.18	5 (35%)	15,30,33	1.57	2 (13%)
8	G7M	A	2069	8	20,26,27	3.25	8 (40%)	20,39,42	3.03	6 (30%)
8	1MG	A	745	8	18,26,27	3.39	7 (38%)	19,39,42	2.44	3 (15%)
55	5MU	v	54	55	15,22,23	2.84	3 (20%)	16,32,35	2.70	2 (12%)
34	PSU	a	516	34	17,21,22	1.07	2 (11%)	20,30,33	3.37	7 (35%)
56	MIA	w	37	56	24,31,32	2.44	4 (16%)	26,44,47	3.10	9 (34%)
34	G7M	a	527	34	20,26,27	3.23	8 (40%)	20,39,42	2.06	3 (15%)
8	PSU	A	2604	8	17,21,22	1.11	2 (11%)	20,30,33	3.06	7 (35%)
8	6MZ	A	1618	8	18,25,26	4.09	8 (44%)	16,36,39	2.40	6 (37%)
8	OMU	A	2552	8	14,22,23	3.33	5 (35%)	14,31,34	0.78	0
34	2MG	a	1516	34	19,26,27	4.64	8 (42%)	21,38,41	2.28	7 (33%)
56	G7M	w	46	56	20,26,27	3.28	8 (40%)	20,39,42	2.33	5 (25%)
8	PSU	A	2605	8	17,21,22	0.95	1 (5%)	20,30,33	2.89	6 (30%)
8	5MU	A	1939	8	15,22,23	2.84	3 (20%)	16,32,35	2.71	2 (12%)
8	5MC	A	747	8	15,22,23	3.10	5 (33%)	19,32,35	1.33	1 (5%)
56	5MU	w	54	56	15,22,23	1.17	2 (13%)	16,32,35	2.15	3 (18%)
8	OMG	A	2251	56,8	18,26,27	3.50	7 (38%)	20,38,41	1.79	3 (15%)
34	5MC	a	967	34	15,22,23	3.18	5 (33%)	19,32,35	1.18	2 (10%)
8	PSU	A	2580	8	17,21,22	1.71	2 (11%)	20,30,33	3.24	9 (45%)
56	4SU	w	8	56	14,21,22	3.36	5 (35%)	15,30,33	1.18	2 (13%)
34	4OC	a	1402	34	16,23,24	3.02	6 (37%)	17,32,35	0.97	1 (5%)
55	PSU	v	55	55	17,21,22	0.97	1 (5%)	20,30,33	3.03	6 (30%)
8	PSU	A	1911	8	17,21,22	1.47	3 (17%)	20,30,33	3.12	6 (30%)
8	5MC	A	1962	8	15,22,23	3.05	5 (33%)	19,32,35	1.37	3 (15%)
34	MA6	a	1518	34	19,26,27	1.10	1 (5%)	18,38,41	1.94	2 (11%)
8	PSU	A	2457	8	17,21,22	1.19	3 (17%)	20,30,33	2.93	6 (30%)
8	2MG	A	2445	8	19,26,27	4.57	8 (42%)	21,38,41	2.20	7 (33%)
34	5MC	a	1407	34	15,22,23	2.87	5 (33%)	19,32,35	1.18	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	PSU	A	955	8	17,21,22	1.43	2 (11%)	20,30,33	3.33	7 (35%)
8	2MG	A	1835	8	19,26,27	4.73	8 (42%)	21,38,41	2.37	6 (28%)
8	6MZ	A	2030	8	18,25,26	4.06	8 (44%)	16,36,39	2.60	4 (25%)
56	PSU	w	39	56	17,21,22	0.92	1 (5%)	20,30,33	3.11	7 (35%)
34	2MG	a	1207	34	19,26,27	4.47	8 (42%)	21,38,41	2.13	7 (33%)
34	UR3	a	1498	34	14,22,23	2.63	4 (28%)	15,32,35	0.77	0
8	PSU	A	1917	8	17,21,22	1.05	2 (11%)	20,30,33	2.85	6 (30%)
56	PSU	w	55	56	17,21,22	1.97	5 (29%)	20,30,33	3.38	6 (30%)
57	FME	y	101	57	8,9,10	0.90	0	7,9,11	1.14	0
8	2MA	A	2503	8	17,25,26	3.35	6 (35%)	19,37,40	1.97	5 (26%)
34	2MG	a	966	34	19,26,27	4.73	8 (42%)	21,38,41	2.29	6 (28%)
8	PSU	A	2504	8	17,21,22	1.59	3 (17%)	20,30,33	3.31	7 (35%)
55	H2U	v	20	55	18,21,22	2.95	5 (27%)	21,30,33	2.17	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OMC	A	2498	8	-	3/7/27/28	0/2/2/2
34	MA6	a	1519	34	-	4/7/29/30	0/3/3/3
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
8	PSU	A	746	8	-	4/7/25/26	0/2/2/2
55	4SU	v	8	55	-	1/5/25/26	0/2/2/2
8	G7M	A	2069	8	-	2/3/25/26	0/3/3/3
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
55	5MU	v	54	55	-	2/5/25/26	0/2/2/2
34	PSU	a	516	34	-	1/7/25/26	0/2/2/2
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
34	G7M	a	527	34	-	1/3/25/26	0/3/3/3
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	5/5/27/28	0/3/3/3
8	OMU	A	2552	8	-	4/7/27/28	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
56	G7M	w	46	56	-	3/3/25/26	0/3/3/3
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	5MU	A	1939	8	-	1/5/25/26	0/2/2/2
8	5MC	A	747	8	-	2/5/25/26	0/2/2/2
56	5MU	w	54	56	-	5/5/25/26	0/2/2/2
8	OMG	A	2251	56,8	-	3/5/27/28	0/3/3/3
34	5MC	a	967	34	-	1/5/25/26	0/2/2/2
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
56	4SU	w	8	56	-	4/5/25/26	0/2/2/2
34	4OC	a	1402	34	-	3/9/29/30	0/2/2/2
55	PSU	v	55	55	-	6/7/25/26	0/2/2/2
8	PSU	A	1911	8	-	1/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	5/5/25/26	0/2/2/2
34	MA6	a	1518	34	-	3/7/29/30	0/3/3/3
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
34	5MC	a	1407	34	-	0/5/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3
56	PSU	w	39	56	-	4/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	UR3	a	1498	34	-	2/5/25/26	0/2/2/2
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
56	PSU	w	55	56	-	1/7/25/26	0/2/2/2
57	FME	y	101	57	-	6/7/9/11	-
8	2MA	A	2503	8	-	3/3/25/26	0/3/3/3
34	2MG	a	966	34	-	1/5/27/28	0/3/3/3
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1516	2MG	C2-N2	15.45	1.47	1.34
34	a	966	2MG	C2-N2	15.38	1.47	1.34
8	A	1835	2MG	C2-N2	15.31	1.47	1.34
8	A	2445	2MG	C2-N2	15.15	1.46	1.34
34	a	1207	2MG	C2-N2	14.80	1.46	1.34
55	v	54	5MU	C4-C5	9.24	1.61	1.41
55	v	20	H2U	C2-N1	9.01	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1835	2MG	C4-N3	8.88	1.49	1.35
8	A	2030	6MZ	C3'-C4'	-8.88	1.30	1.53
8	A	1618	6MZ	C3'-C4'	-8.75	1.30	1.53
34	a	1516	2MG	C4-N3	8.62	1.49	1.35
34	a	966	2MG	C4-N3	8.60	1.49	1.35
8	A	1939	5MU	C4-C5	8.57	1.59	1.41
8	A	745	1MG	C4-N3	8.45	1.48	1.35
8	A	2251	OMG	C4-N3	8.30	1.48	1.35
8	A	2445	2MG	C4-N3	8.24	1.48	1.35
34	a	527	G7M	C4-N3	8.09	1.48	1.35
8	A	2030	6MZ	O4'-C4'	8.07	1.63	1.45
34	a	1207	2MG	C4-N3	7.86	1.48	1.35
8	A	2069	G7M	C4-N3	7.72	1.47	1.35
56	w	46	G7M	C4-N3	7.70	1.47	1.35
8	A	1618	6MZ	O4'-C1'	-7.62	1.30	1.41
8	A	1618	6MZ	O4'-C4'	7.61	1.62	1.45
8	A	1618	6MZ	C6-N6	7.56	1.47	1.35
8	A	2503	2MA	C4-N3	7.51	1.47	1.35
34	a	967	5MC	C4-N3	7.51	1.45	1.35
8	A	2030	6MZ	O4'-C1'	-7.49	1.30	1.41
8	A	2030	6MZ	C6-N6	7.37	1.47	1.35
8	A	1962	5MC	C4-N3	7.29	1.45	1.35
56	w	46	G7M	C6-C5	7.09	1.53	1.41
56	w	8	4SU	C5-C4	7.05	1.46	1.38
8	A	2552	OMU	C4-N3	7.03	1.45	1.33
56	w	37	MIA	C13-C14	7.03	1.52	1.32
8	A	747	5MC	C4-N3	7.02	1.45	1.35
8	A	2069	G7M	C6-C5	7.00	1.53	1.41
34	a	527	G7M	C6-C5	6.95	1.53	1.41
34	a	1498	UR3	C6-N1	6.75	1.44	1.35
34	a	966	2MG	C6-C5	6.73	1.53	1.41
55	v	8	4SU	C5-C4	6.72	1.46	1.38
8	A	2503	2MA	C6-C5	6.72	1.51	1.41
8	A	1835	2MG	C6-C5	6.70	1.52	1.41
8	A	2251	OMG	C6-C5	6.69	1.52	1.41
56	w	37	MIA	C2-S10	6.64	1.81	1.75
8	A	745	1MG	C2-N2	6.64	1.47	1.33
34	a	1402	4OC	C6-N1	6.56	1.43	1.35
8	A	2552	OMU	C6-N1	6.50	1.43	1.35
34	a	1207	2MG	C6-C5	6.29	1.52	1.41
34	a	1407	5MC	C4-N3	6.24	1.44	1.35
55	v	20	H2U	C2-N3	6.12	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	745	1MG	C2-N3	6.09	1.43	1.34
8	A	2445	2MG	C6-C5	6.00	1.51	1.41
8	A	745	1MG	C6-C5	5.99	1.50	1.41
34	a	1516	2MG	C6-C5	5.89	1.51	1.41
8	A	1939	5MU	C4-N3	-5.86	1.22	1.33
8	A	2552	OMU	C2-N3	5.84	1.49	1.38
8	A	2251	OMG	C2-N2	5.74	1.45	1.33
56	w	8	4SU	C6-N1	5.68	1.42	1.35
56	w	46	G7M	C6-N1	5.66	1.42	1.33
8	A	2503	2MA	C2-N3	5.65	1.44	1.34
8	A	2503	2MA	C2-N1	5.64	1.44	1.34
8	A	747	5MC	C5-C4	5.57	1.50	1.41
8	A	2251	OMG	C6-N1	5.52	1.42	1.33
8	A	1962	5MC	C2-N3	5.50	1.49	1.38
34	a	967	5MC	C2-N3	5.42	1.48	1.38
56	w	37	MIA	C6-N6	5.41	1.44	1.34
34	a	966	2MG	C6-N1	5.40	1.42	1.33
56	w	8	4SU	C4-S4	-5.40	1.57	1.67
55	v	8	4SU	C6-N1	5.26	1.42	1.35
34	a	967	5MC	C5-C4	5.20	1.49	1.41
34	a	1402	4OC	C4-N3	5.20	1.44	1.34
8	A	2069	G7M	C6-N1	5.19	1.42	1.33
56	w	46	G7M	C2-N2	5.06	1.44	1.33
8	A	1835	2MG	C6-N1	5.01	1.41	1.33
8	A	2580	PSU	C5-C1’	-4.99	1.48	1.52
55	v	8	4SU	C2-N3	4.97	1.48	1.38
34	a	1207	2MG	C6-N1	4.95	1.41	1.33
8	A	2504	PSU	C5-C1’	-4.94	1.48	1.52
34	a	1498	UR3	C6-C5	4.94	1.49	1.38
34	a	1516	2MG	C6-N1	4.93	1.41	1.33
34	a	527	G7M	C6-N1	4.92	1.41	1.33
8	A	2069	G7M	C2-N2	4.90	1.43	1.33
55	v	54	5MU	C4-N3	-4.90	1.24	1.33
8	A	1962	5MC	C4-N4	4.89	1.46	1.34
56	w	46	G7M	C2-N1	4.86	1.44	1.35
34	a	527	G7M	C2-N2	4.86	1.43	1.33
8	A	747	5MC	C4-N4	4.85	1.46	1.34
56	w	8	4SU	C2-N3	4.85	1.47	1.38
34	a	1407	5MC	C2-N3	4.84	1.47	1.38
8	A	2251	OMG	C2-N1	4.83	1.44	1.35
34	a	967	5MC	C4-N4	4.83	1.46	1.34
34	a	1407	5MC	C4-N4	4.79	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	747	5MC	C2-N3	4.77	1.47	1.38
34	a	1407	5MC	C5-C4	4.72	1.48	1.41
8	A	2445	2MG	C6-N1	4.67	1.41	1.33
55	v	20	H2U	C4-N3	4.66	1.45	1.37
55	v	8	4SU	C4-S4	-4.65	1.59	1.67
34	a	1402	4OC	C2-N3	4.63	1.47	1.38
56	w	8	4SU	C6-C5	4.62	1.48	1.38
55	v	8	4SU	C6-C5	4.57	1.48	1.38
8	A	1962	5MC	C5-C4	4.45	1.48	1.41
8	A	955	PSU	C5-C1’	-4.45	1.48	1.52
56	w	55	PSU	C5-C1’	-4.45	1.48	1.52
34	a	1402	4OC	C6-C5	4.43	1.47	1.38
8	A	1911	PSU	C5-C1’	-4.35	1.48	1.52
8	A	2552	OMU	C6-C5	4.29	1.47	1.38
34	a	527	G7M	C2-N1	4.21	1.42	1.35
8	A	2069	G7M	C2-N1	4.18	1.42	1.35
34	a	1402	4OC	C4-N4	4.11	1.45	1.36
34	a	1498	UR3	C4-N3	4.07	1.44	1.38
8	A	1618	6MZ	O3’-C3’	4.06	1.52	1.43
56	w	55	PSU	C2’-C1’	-4.03	1.49	1.54
8	A	1835	2MG	C2-N3	4.00	1.46	1.34
8	A	2503	2MA	C6-N1	3.97	1.42	1.35
8	A	2069	G7M	C5-C4	-3.90	1.34	1.39
34	a	1402	4OC	C5-C4	3.86	1.48	1.39
34	a	966	2MG	C2-N3	3.80	1.46	1.34
8	A	2445	2MG	C2-N3	3.80	1.46	1.34
34	a	1516	2MG	C2-N3	3.70	1.45	1.34
8	A	747	5MC	C6-C5	3.44	1.49	1.40
34	a	1207	2MG	C2-N3	3.40	1.45	1.34
8	A	2580	PSU	O4’-C1’	-3.39	1.39	1.44
34	a	967	5MC	C6-C5	3.36	1.49	1.40
8	A	2445	2MG	O6-C6	-3.31	1.16	1.24
56	w	54	5MU	C4-C5	3.19	1.48	1.41
34	a	1407	5MC	C6-C5	3.17	1.48	1.40
34	a	1516	2MG	O6-C6	-3.14	1.16	1.24
8	A	2030	6MZ	O3’-C3’	3.09	1.50	1.43
34	a	966	2MG	O6-C6	-3.07	1.16	1.24
8	A	1835	2MG	O6-C6	-3.07	1.16	1.24
34	a	1207	2MG	O6-C6	-3.06	1.16	1.24
8	A	1962	5MC	C6-C5	3.06	1.48	1.40
8	A	2030	6MZ	O2’-C2’	-3.04	1.35	1.43
34	a	527	G7M	C5-C4	-3.04	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1518	MA6	C5-C4	-3.00	1.33	1.40
8	A	1618	6MZ	O2'-C2'	-2.99	1.35	1.43
8	A	1618	6MZ	C5-C4	-2.97	1.33	1.40
56	w	37	MIA	C5-C4	-2.94	1.33	1.40
8	A	2030	6MZ	C5-C4	-2.92	1.33	1.40
34	a	527	G7M	O6-C6	-2.89	1.17	1.24
56	w	32	PSU	C4-N3	2.87	1.38	1.33
34	a	966	2MG	C2-N1	2.83	1.43	1.34
8	A	1618	6MZ	C2-N3	2.82	1.36	1.32
34	a	1519	MA6	C5-C4	-2.81	1.33	1.40
56	w	55	PSU	C2-N1	-2.76	1.32	1.38
34	a	1207	2MG	C2-N1	2.76	1.43	1.34
8	A	2030	6MZ	C2-N3	2.76	1.36	1.32
55	v	55	PSU	C4-N3	2.73	1.37	1.33
8	A	2069	G7M	O6-C6	-2.73	1.17	1.24
8	A	2552	OMU	O4-C4	-2.73	1.17	1.24
8	A	1939	5MU	O4-C4	-2.69	1.17	1.24
8	A	2457	PSU	C5-C1'	-2.66	1.50	1.52
8	A	1917	PSU	C4-N3	2.65	1.37	1.33
8	A	2251	OMG	O6-C6	-2.64	1.17	1.24
34	a	527	G7M	C2-N3	2.64	1.47	1.34
8	A	745	1MG	C6-N1	2.62	1.42	1.38
8	A	746	PSU	C4-N3	2.60	1.37	1.33
56	w	46	G7M	O6-C6	-2.58	1.18	1.24
34	a	1516	2MG	C2-N1	2.58	1.42	1.34
8	A	2445	2MG	C2-N1	2.57	1.42	1.34
34	a	516	PSU	C4-N3	2.57	1.37	1.33
8	A	2604	PSU	O4'-C1'	-2.56	1.40	1.44
8	A	1911	PSU	C4-N3	2.56	1.37	1.33
56	w	46	G7M	C5-C4	-2.55	1.36	1.39
56	w	39	PSU	C4-N3	2.50	1.37	1.33
8	A	2503	2MA	C5-C4	-2.50	1.34	1.40
56	w	46	G7M	C2-N3	2.49	1.46	1.34
8	A	2504	PSU	C4-N3	2.48	1.37	1.33
8	A	2251	OMG	C2-N3	2.48	1.46	1.34
8	A	2504	PSU	O4'-C1'	-2.45	1.41	1.44
8	A	1835	2MG	C2-N1	2.45	1.42	1.34
8	A	2604	PSU	C4-N3	2.44	1.37	1.33
8	A	2445	2MG	C5-C4	-2.43	1.34	1.40
8	A	2457	PSU	O4'-C1'	-2.43	1.41	1.44
34	a	1498	UR3	O4-C4	-2.41	1.18	1.24
55	v	20	H2U	O4-C4	-2.40	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2605	PSU	C4-N3	2.40	1.37	1.33
55	v	54	5MU	O4-C4	-2.38	1.18	1.24
55	v	20	H2U	O2-C2	-2.37	1.18	1.23
34	a	966	2MG	C5-C4	-2.36	1.34	1.40
8	A	2069	G7M	C2-N3	2.32	1.45	1.34
8	A	2457	PSU	C4-N3	2.29	1.37	1.33
8	A	1835	2MG	C5-C4	-2.29	1.34	1.40
8	A	1911	PSU	O4'-C1'	-2.28	1.41	1.44
34	a	1516	2MG	C5-C4	-2.27	1.34	1.40
34	a	516	PSU	O4'-C1'	-2.26	1.41	1.44
56	w	55	PSU	C2-N3	-2.24	1.33	1.38
56	w	55	PSU	C6-C5	-2.22	1.35	1.38
8	A	746	PSU	O4'-C1'	-2.21	1.41	1.44
34	a	1207	2MG	C5-C4	-2.15	1.35	1.40
8	A	745	1MG	C5-C4	-2.14	1.35	1.40
8	A	2498	OMC	C6-N1	-2.09	1.33	1.35
56	w	54	5MU	C2-N3	-2.08	1.34	1.38
8	A	955	PSU	O4'-C1'	-2.07	1.41	1.44
8	A	1917	PSU	O4'-C1'	-2.07	1.41	1.44
8	A	2498	OMC	O4'-C1'	2.06	1.44	1.41
8	A	745	1MG	O6-C6	-2.01	1.19	1.24

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	516	PSU	N1-C2-N3	-11.42	119.35	128.43
56	w	32	PSU	N1-C2-N3	-11.34	119.41	128.43
8	A	2069	G7M	C1'-N9-C4	-10.93	107.44	126.64
56	w	55	PSU	N1-C2-N3	-10.65	119.97	128.43
8	A	746	PSU	N1-C2-N3	-10.34	120.21	128.43
8	A	2604	PSU	N1-C2-N3	-10.04	120.44	128.43
8	A	955	PSU	N1-C2-N3	-10.01	120.48	128.43
56	w	39	PSU	N1-C2-N3	-9.96	120.51	128.43
8	A	2457	PSU	N1-C2-N3	-9.96	120.51	128.43
8	A	1917	PSU	N1-C2-N3	-9.84	120.61	128.43
55	v	55	PSU	N1-C2-N3	-9.77	120.66	128.43
34	a	1519	MA6	N1-C6-N6	-9.77	106.78	117.06
8	A	2605	PSU	N1-C2-N3	-9.52	120.86	128.43
8	A	2504	PSU	N1-C2-N3	-9.50	120.88	128.43
8	A	1911	PSU	N1-C2-N3	-9.46	120.91	128.43
8	A	2580	PSU	N1-C2-N3	-9.39	120.97	128.43
8	A	745	1MG	C1'-N9-C4	-9.20	110.48	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	w	37	MIA	C12-C13-C14	-8.92	109.78	127.14
56	w	37	MIA	C11-S10-C2	8.85	108.87	102.27
8	A	1939	5MU	C5-C6-N1	-8.63	112.89	122.19
55	v	20	H2U	C4-N3-C2	-7.71	119.39	125.79
55	v	54	5MU	C5-C6-N1	-7.54	114.07	122.19
56	w	55	PSU	C4-N3-C2	7.28	121.29	115.14
55	v	54	5MU	C4-N3-C2	7.26	121.27	115.14
8	A	2504	PSU	C5-C1'-C2'	-7.25	102.39	115.32
8	A	2030	6MZ	C9-N6-C6	-7.18	116.69	122.87
56	w	46	G7M	C1'-N9-C4	-7.03	114.28	126.64
8	A	955	PSU	C4-N3-C2	6.77	120.86	115.14
8	A	1835	2MG	N2-C2-N3	6.65	123.35	116.96
8	A	1939	5MU	C4-N3-C2	6.26	120.43	115.14
34	a	1516	2MG	N2-C2-N3	6.20	122.92	116.96
56	w	54	5MU	C4-N3-C2	6.15	120.34	115.14
34	a	966	2MG	C1'-N9-C4	-6.04	116.03	126.64
56	w	39	PSU	C4-N3-C2	5.90	120.12	115.14
55	v	55	PSU	C4-N3-C2	5.89	120.12	115.14
34	a	527	G7M	C1'-N9-C4	-5.81	116.42	126.64
8	A	955	PSU	C5-C4-N3	-5.71	118.01	125.36
34	a	516	PSU	C4-N3-C2	5.60	119.87	115.14
34	a	1518	MA6	N1-C6-N6	-5.55	111.21	117.06
8	A	2030	6MZ	N3-C2-N1	-5.51	120.06	128.68
8	A	1618	6MZ	N3-C2-N1	-5.45	120.17	128.68
56	w	32	PSU	C4-N3-C2	5.44	119.73	115.14
34	a	1519	MA6	N3-C2-N1	-5.44	120.18	128.68
34	a	1518	MA6	N3-C2-N1	-5.37	120.29	128.68
8	A	2580	PSU	C5-C6-N1	-5.29	117.93	124.44
8	A	746	PSU	C4-N3-C2	5.25	119.57	115.14
8	A	2445	2MG	C1'-N9-C4	-5.23	117.45	126.64
8	A	2251	OMG	N3-C2-N1	-5.17	120.32	127.22
8	A	2069	G7M	N3-C2-N1	-5.09	120.43	127.22
8	A	1618	6MZ	C9-N6-C6	-5.05	118.53	122.87
8	A	2604	PSU	C5-C6-N1	-4.97	118.33	124.44
56	w	37	MIA	C15-C14-C13	-4.95	108.35	122.65
56	w	55	PSU	C5-C4-N3	-4.94	119.00	125.36
34	a	1207	2MG	CM2-N2-C2	-4.91	117.67	123.59
8	A	1911	PSU	C5-C1'-C2'	-4.90	106.58	115.32
8	A	2504	PSU	C5-C6-N1	-4.90	118.42	124.44
8	A	2503	2MA	C1'-N9-C4	-4.90	118.04	126.64
8	A	2445	2MG	N2-C2-N3	4.78	121.55	116.96
56	w	37	MIA	C16-C14-C13	-4.77	108.86	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2457	PSU	C5-C6-N1	-4.74	118.61	124.44
56	w	46	G7M	N3-C2-N1	-4.64	121.03	127.22
34	a	1516	2MG	C1'-N9-C4	-4.64	118.49	126.64
8	A	1835	2MG	C1'-N9-C4	-4.63	118.50	126.64
34	a	527	G7M	C2-N3-C4	4.62	120.63	115.36
55	v	55	PSU	C5-C4-N3	-4.60	119.44	125.36
8	A	2580	PSU	C4-N3-C2	4.58	119.01	115.14
8	A	1917	PSU	C4-N3-C2	4.58	119.01	115.14
8	A	747	5MC	C5-C6-N1	-4.57	117.27	122.19
56	w	54	5MU	C3'-C2'-C1'	4.56	107.84	100.98
8	A	1911	PSU	C5-C4-N3	-4.55	119.50	125.36
8	A	2605	PSU	C5-C6-N1	-4.54	118.86	124.44
8	A	1911	PSU	C4-N3-C2	4.42	118.87	115.14
8	A	2251	OMG	C2-N3-C4	4.41	120.39	115.36
34	a	1207	2MG	C1'-N9-C4	-4.41	118.90	126.64
56	w	46	G7M	C2-N3-C4	4.40	120.38	115.36
8	A	1911	PSU	C5-C6-N1	-4.34	119.10	124.44
8	A	2580	PSU	C5-C4-N3	-4.23	119.92	125.36
34	a	527	G7M	N3-C2-N1	-4.23	121.58	127.22
8	A	2503	2MA	C2-N3-C4	4.23	118.96	115.52
55	v	8	4SU	C2-N3-C4	4.22	121.27	115.15
56	w	39	PSU	C5-C4-N3	-4.22	119.93	125.36
34	a	966	2MG	N2-C2-N3	4.21	121.00	116.96
56	w	32	PSU	O4'-C1'-C5	4.13	116.33	109.93
8	A	1835	2MG	C2-N3-C4	4.07	119.90	115.28
8	A	2498	OMC	C2-N3-C4	4.06	120.45	116.34
34	a	516	PSU	O4'-C1'-C5	4.02	116.15	109.93
8	A	2604	PSU	C6-N1-C2	4.01	121.98	115.36
8	A	2580	PSU	O4'-C1'-C5	-3.96	103.79	109.93
8	A	746	PSU	C5-C4-N3	-3.96	120.26	125.36
8	A	745	1MG	C2-N3-C4	3.96	119.88	115.36
34	a	1516	2MG	N3-C2-N1	-3.91	120.05	126.23
55	v	8	4SU	C5-C4-N3	-3.76	118.80	123.83
8	A	2504	PSU	C5-C4-N3	-3.76	120.51	125.36
34	a	966	2MG	C2-N3-C4	3.76	119.54	115.28
8	A	2457	PSU	C6-N1-C2	3.74	121.53	115.36
34	a	966	2MG	N3-C2-N1	-3.73	120.34	126.23
34	a	1516	2MG	C2-N3-C4	3.70	119.48	115.28
8	A	2605	PSU	C6-N1-C2	3.69	121.44	115.36
8	A	1835	2MG	N3-C2-N1	-3.65	120.45	126.23
8	A	2604	PSU	O4'-C1'-C5	3.63	115.56	109.93
34	a	516	PSU	C5-C4-N3	-3.63	120.69	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1917	PSU	C5-C4-N3	-3.61	120.71	125.36
8	A	2030	6MZ	C1'-N9-C4	-3.60	120.31	126.64
8	A	2069	G7M	C2-N3-C4	3.58	119.45	115.36
8	A	2457	PSU	C4-N3-C2	3.57	118.16	115.14
8	A	1618	6MZ	C1'-N9-C4	-3.51	120.47	126.64
8	A	2504	PSU	C4-N3-C2	3.50	118.10	115.14
8	A	955	PSU	C5-C6-N1	-3.50	120.14	124.44
8	A	2504	PSU	C6-N1-C2	3.49	121.12	115.36
34	a	1407	5MC	C2-N3-C4	3.49	120.23	116.02
56	w	55	PSU	C6-N1-C2	3.43	121.02	115.36
34	a	516	PSU	C5-C6-N1	-3.40	120.27	124.44
8	A	2604	PSU	C4-N3-C2	3.39	118.01	115.14
8	A	746	PSU	C5-C6-N1	-3.37	120.29	124.44
34	a	516	PSU	C6-N1-C2	3.37	120.92	115.36
56	w	37	MIA	C2-N3-C4	3.33	119.92	115.32
8	A	2445	2MG	C2-N3-C4	3.33	119.06	115.28
34	a	966	2MG	CM2-N2-C2	-3.31	119.59	123.59
56	w	32	PSU	C6-N1-C2	3.31	120.82	115.36
8	A	2580	PSU	C6-N1-C2	3.31	120.82	115.36
56	w	32	PSU	C5-C4-N3	-3.30	121.11	125.36
8	A	2605	PSU	C4-N3-C2	3.29	117.92	115.14
55	v	20	H2U	N3-C2-N1	3.29	120.13	116.65
8	A	746	PSU	C5-C1'-C2'	-3.28	109.46	115.32
56	w	37	MIA	N3-C2-N1	-3.27	120.97	126.98
34	a	1207	2MG	C2-N3-C4	3.20	118.91	115.28
56	w	8	4SU	C2-N3-C4	3.19	119.77	115.15
8	A	955	PSU	C5-C1'-C2'	-3.16	109.68	115.32
55	v	20	H2U	C5-C4-N3	3.15	120.19	116.65
8	A	2503	2MA	C5-C6-N1	-3.15	119.76	123.06
8	A	746	PSU	C6-N1-C2	3.12	120.50	115.36
8	A	2503	2MA	N3-C2-N1	-3.12	119.99	125.72
8	A	1962	5MC	C2-N3-C4	3.11	119.77	116.02
8	A	2445	2MG	N3-C2-N1	-3.10	121.32	126.23
8	A	1911	PSU	C6-N1-C2	3.09	120.46	115.36
8	A	2605	PSU	O4'-C1'-C5	3.09	114.71	109.93
34	a	1207	2MG	N2-C2-N1	3.07	119.91	116.96
56	w	39	PSU	C5-C1'-C2'	-3.04	109.89	115.32
56	w	55	PSU	C5-C1'-C2'	-3.04	109.89	115.32
34	a	967	5MC	C2-N3-C4	3.03	119.67	116.02
34	a	1207	2MG	N3-C2-N1	-3.01	121.47	126.23
8	A	2457	PSU	C5-C4-N3	-2.99	121.51	125.36
8	A	1835	2MG	CM2-N2-C2	-2.99	119.98	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2445	2MG	CM2-N2-C2	-2.95	120.03	123.59
8	A	2580	PSU	C5-C1'-C2'	2.92	120.52	115.32
34	a	1207	2MG	C5-C6-N1	-2.87	119.51	123.43
8	A	2604	PSU	C5-C4-N3	-2.87	121.67	125.36
8	A	2605	PSU	C5-C4-N3	-2.86	121.68	125.36
8	A	1917	PSU	O4'-C1'-C5	2.82	114.30	109.93
8	A	1962	5MC	N4-C4-N3	2.81	121.00	117.03
8	A	2503	2MA	CM2-C2-N1	2.81	121.53	117.15
56	w	39	PSU	O4'-C1'-C5	2.78	114.24	109.93
8	A	2030	6MZ	O4'-C1'-C2'	-2.78	102.86	106.93
8	A	2498	OMC	N4-C4-N3	2.78	120.88	116.49
8	A	1962	5MC	C5-C6-N1	-2.76	119.22	122.19
8	A	1917	PSU	C6-N1-C2	2.76	119.91	115.36
56	w	39	PSU	C6-N1-C2	2.74	119.88	115.36
56	w	39	PSU	C5-C6-N1	-2.72	121.09	124.44
55	v	20	H2U	O2-C2-N1	-2.70	119.71	123.11
8	A	1618	6MZ	C2'-C3'-C4'	2.69	107.88	102.64
8	A	955	PSU	C6-N1-C2	2.66	119.74	115.36
34	a	1516	2MG	C6-N1-C2	2.65	119.92	115.18
56	w	32	PSU	C5-C6-N1	-2.65	121.19	124.44
55	v	55	PSU	C5-C6-N1	-2.62	121.22	124.44
56	w	37	MIA	C1'-N9-C4	2.61	131.23	126.64
56	w	54	5MU	C5-C6-N1	-2.58	119.41	122.19
55	v	55	PSU	O4'-C1'-C5	2.57	113.91	109.93
55	v	55	PSU	C6-N1-C2	2.57	119.59	115.36
8	A	1917	PSU	C5-C6-N1	-2.51	121.35	124.44
8	A	1618	6MZ	O3'-C3'-C2'	2.47	119.80	111.82
34	a	1516	2MG	C5-C6-N1	-2.45	120.08	123.43
34	a	967	5MC	C5-C6-N1	-2.41	119.60	122.19
56	w	8	4SU	C5-C4-N3	-2.37	120.65	123.83
55	v	20	H2U	C5-C6-N1	2.37	119.43	111.61
8	A	2580	PSU	O4'-C1'-C2'	2.33	108.43	104.66
8	A	2445	2MG	C5-C6-N1	-2.30	120.28	123.43
8	A	2445	2MG	C3'-C2'-C1'	2.29	104.43	100.98
56	w	46	G7M	N2-C2-N1	2.29	120.81	117.25
56	w	37	MIA	C16-C14-C15	-2.28	109.56	114.60
56	w	46	G7M	C5-C6-N1	-2.26	120.34	123.43
8	A	2604	PSU	O4'-C1'-C2'	2.22	108.25	104.66
8	A	2504	PSU	C4-C5-C1'	-2.21	116.94	121.12
56	w	55	PSU	O3'-C3'-C4'	2.21	117.44	111.05
8	A	955	PSU	O4'-C1'-C5	-2.20	106.52	109.93
8	A	1835	2MG	C6-N1-C2	2.20	119.11	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	w	37	MIA	S10-C2-N1	2.19	123.58	116.01
34	a	1207	2MG	C6-N1-C2	2.18	119.08	115.18
34	a	516	PSU	O4'-C1'-C2'	2.17	108.17	104.66
34	a	966	2MG	C6-N1-C2	2.17	119.06	115.18
8	A	1618	6MZ	C3'-C2'-C1'	2.16	104.23	100.98
8	A	2069	G7M	C5-C6-N1	-2.08	120.58	123.43
8	A	2251	OMG	C5-C6-N1	-2.08	120.59	123.43
8	A	745	1MG	N2-C2-N1	2.07	121.07	118.47
56	w	32	PSU	O4'-C1'-C2'	2.06	108.00	104.66
34	a	1516	2MG	CM2-N2-C2	-2.04	121.13	123.59
8	A	2580	PSU	O2'-C2'-C1'	-2.03	107.12	111.94
8	A	2457	PSU	O4'-C1'-C2'	2.02	107.93	104.66
8	A	2069	G7M	C6-N1-C2	2.02	119.13	115.93
8	A	2069	G7M	C6-C5-C4	-2.01	118.88	120.80
34	a	1402	4OC	N4-C4-N3	2.01	121.51	116.37

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	8	4SU	O4'-C1'-N1-C6
55	v	20	H2U	O4'-C1'-N1-C6
55	v	20	H2U	C2'-C1'-N1-C2
55	v	20	H2U	C2'-C1'-N1-C6
8	A	746	PSU	C2'-C1'-C5-C4
8	A	746	PSU	C2'-C1'-C5-C6
8	A	746	PSU	O4'-C1'-C5-C6
8	A	747	5MC	C3'-C4'-C5'-O5'
8	A	1618	6MZ	C5-C6-N6-C9
8	A	1618	6MZ	N1-C6-N6-C9
8	A	1962	5MC	O4'-C1'-N1-C6
8	A	1962	5MC	C2'-C1'-N1-C6
8	A	2251	OMG	O4'-C4'-C5'-O5'
8	A	2251	OMG	C3'-C4'-C5'-O5'
8	A	2498	OMC	C1'-C2'-O2'-CM2
8	A	2503	2MA	O4'-C4'-C5'-O5'
8	A	2552	OMU	C1'-C2'-O2'-CM2
34	a	1402	4OC	C1'-C2'-O2'-CM2
34	a	1498	UR3	O4'-C4'-C5'-O5'
34	a	1518	MA6	C5-C6-N6-C10
34	a	1518	MA6	N1-C6-N6-C10
34	a	1519	MA6	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
34	a	1519	MA6	C5-C6-N6-C10
56	w	8	4SU	C2'-C1'-N1-C6
56	w	8	4SU	O4'-C1'-N1-C6
56	w	32	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C6
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
56	w	39	PSU	O4'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C6
56	w	46	G7M	C3'-C4'-C5'-O5'
56	w	54	5MU	C2'-C1'-N1-C6
56	w	54	5MU	O4'-C1'-N1-C6
56	w	54	5MU	O4'-C4'-C5'-O5'
57	y	101	FME	O1-CN-N-CA
57	y	101	FME	N-CA-CB-CG
57	y	101	FME	O-C-CA-CB
8	A	1618	6MZ	O4'-C4'-C5'-O5'
8	A	1618	6MZ	C3'-C4'-C5'-O5'
8	A	1962	5MC	O4'-C4'-C5'-O5'
8	A	2069	G7M	O4'-C4'-C5'-O5'
8	A	2445	2MG	O4'-C4'-C5'-O5'
8	A	2445	2MG	C3'-C4'-C5'-O5'
8	A	2498	OMC	O4'-C4'-C5'-O5'
34	a	1498	UR3	C3'-C4'-C5'-O5'
34	a	1519	MA6	C4'-C5'-O5'-P
8	A	747	5MC	O4'-C4'-C5'-O5'
8	A	1835	2MG	C3'-C4'-C5'-O5'
8	A	1962	5MC	C3'-C4'-C5'-O5'
8	A	2069	G7M	C3'-C4'-C5'-O5'
8	A	2503	2MA	C3'-C4'-C5'-O5'
34	a	1402	4OC	O4'-C4'-C5'-O5'
56	w	54	5MU	C3'-C4'-C5'-O5'
34	a	1519	MA6	N1-C6-N6-C9
57	y	101	FME	CB-CG-SD-CE
55	v	55	PSU	C3'-C4'-C5'-O5'
8	A	1835	2MG	O4'-C4'-C5'-O5'
8	A	2498	OMC	C3'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
56	w	39	PSU	C3'-C4'-C5'-O5'
55	v	54	5MU	O4'-C4'-C5'-O5'
55	v	55	PSU	O4'-C4'-C5'-O5'
56	w	46	G7M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	v	54	5MU	C3'-C4'-C5'-O5'
8	A	2552	OMU	O4'-C4'-C5'-O5'
8	A	2251	OMG	C4'-C5'-O5'-P
56	w	39	PSU	O4'-C4'-C5'-O5'
8	A	746	PSU	O4'-C1'-C5-C4
34	a	966	2MG	C4'-C5'-O5'-P
55	v	55	PSU	C4'-C5'-O5'-P
8	A	2552	OMU	C4'-C5'-O5'-P
34	a	527	G7M	C4'-C5'-O5'-P
8	A	1962	5MC	C4'-C5'-O5'-P
34	a	1518	MA6	C5-C6-N6-C9
56	w	46	G7M	C4'-C5'-O5'-P
56	w	54	5MU	C4'-C5'-O5'-P
8	A	2030	6MZ	C3'-C4'-C5'-O5'
57	y	101	FME	C-CA-CB-CG
8	A	1618	6MZ	C4'-C5'-O5'-P
8	A	2030	6MZ	C4'-C5'-O5'-P
8	A	2503	2MA	C4'-C5'-O5'-P
55	v	20	H2U	C4'-C5'-O5'-P
8	A	1939	5MU	O4'-C4'-C5'-O5'
34	a	967	5MC	C3'-C4'-C5'-O5'
55	v	55	PSU	O4'-C1'-C5-C6
55	v	55	PSU	O4'-C1'-C5-C4
56	w	8	4SU	C4'-C5'-O5'-P
55	v	55	PSU	C2'-C1'-C5-C6
8	A	2552	OMU	C3'-C4'-C5'-O5'
56	w	8	4SU	O4'-C4'-C5'-O5'
56	w	55	PSU	O4'-C4'-C5'-O5'
55	v	20	H2U	O4'-C1'-N1-C2
56	w	37	MIA	N1-C2-S10-C11
34	a	516	PSU	C3'-C4'-C5'-O5'
57	y	101	FME	CB-CA-N-CN
8	A	1911	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	AM2	a	2001	-	40,40,40	1.66	10 (25%)	53,60,60	1.71	11 (20%)

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
60	AM2	a	2001	-	-	8/12/84/84	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	a	2001	AM2	OA4-CA1	4.04	1.52	1.41
60	a	2001	AM2	CB3-CB4	-3.69	1.48	1.53
60	a	2001	AM2	OA5-CA8	3.20	1.50	1.41
60	a	2001	AM2	OA5-CA4	3.08	1.51	1.44
60	a	2001	AM2	OB1-CB1	2.89	1.49	1.41
60	a	2001	AM2	OA8-CA8	-2.63	1.34	1.41
60	a	2001	AM2	OA8-CB1	-2.58	1.34	1.41
60	a	2001	AM2	OA4-CA5	2.57	1.48	1.44
60	a	2001	AM2	OA1-CA1	-2.50	1.34	1.41
60	a	2001	AM2	CA7-NA7	-2.27	1.43	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	a	2001	AM2	CA1-OA1-CC1	-5.36	104.71	117.96
60	a	2001	AM2	CA8-CA7-NA7	-3.99	103.86	111.00
60	a	2001	AM2	CB1-OA8-CA8	-3.84	107.56	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	a	2001	AM2	CA9-NA7-CA7	-3.31	109.57	114.38
60	a	2001	AM2	OA1-CA1-CA2	3.21	113.61	108.23
60	a	2001	AM2	CA8-OA5-CA4	-2.69	108.41	113.69
60	a	2001	AM2	CB1-OB1-CB5	-2.46	108.87	113.69
60	a	2001	AM2	OA5-CA4-CA3	2.41	113.38	108.39
60	a	2001	AM2	OA8-CB1-OB1	-2.38	104.03	110.67
60	a	2001	AM2	OA8-CA8-CA7	-2.11	104.60	108.24
60	a	2001	AM2	CA6-CA5-CA4	2.01	115.53	110.93

There are no chirality outliers.

All (8) torsion outliers are listed below:

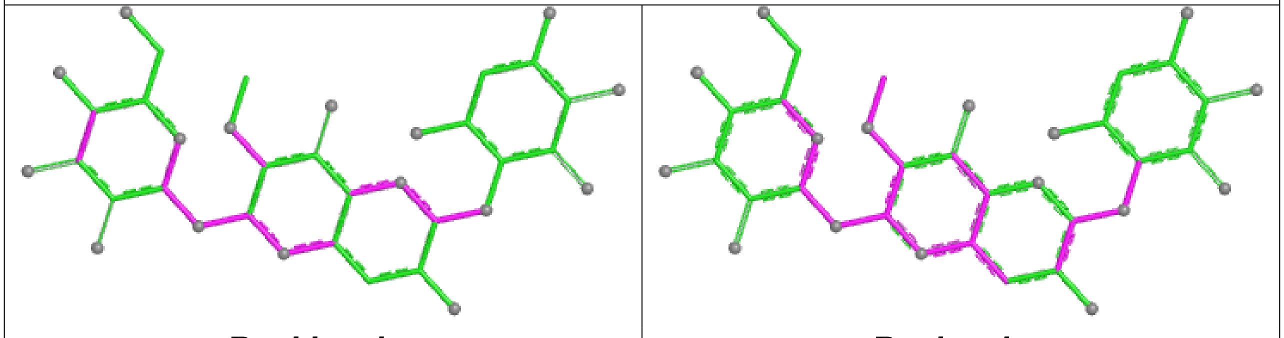
Mol	Chain	Res	Type	Atoms
60	a	2001	AM2	CA7-CA8-OA8-CB1
60	a	2001	AM2	OA5-CA8-OA8-CB1
60	a	2001	AM2	OB1-CB5-CB6-OB6
60	a	2001	AM2	CB4-CB5-CB6-OB6
60	a	2001	AM2	OB1-CB1-OA8-CA8
60	a	2001	AM2	CB2-CB1-OA8-CA8
60	a	2001	AM2	CA6-CA7-NA7-CA9
60	a	2001	AM2	OA4-CA1-OA1-CC1

There are no ring outliers.

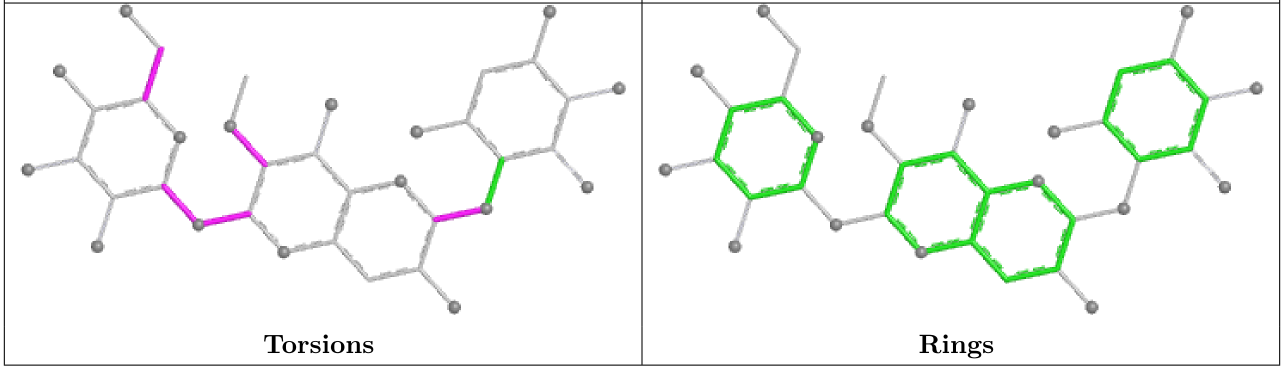
No monomer is involved in short contacts.

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 AM2 a 2001



Bond lengths **Bond angles**



Torsions **Rings**

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

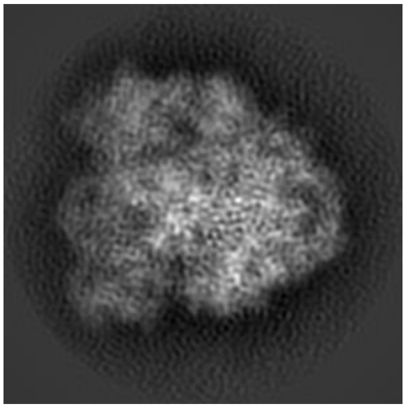
6 Map visualisation

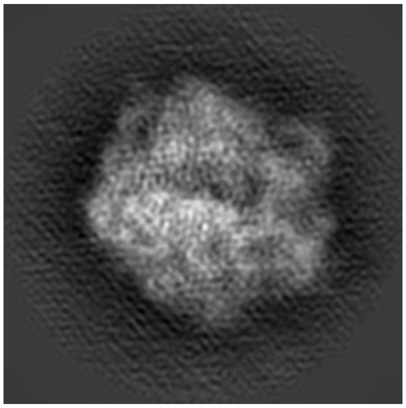
This section contains visualisations of the EMDB entry EMD-13459. These allow visual inspection of the internal detail of the map and identification of artifacts.

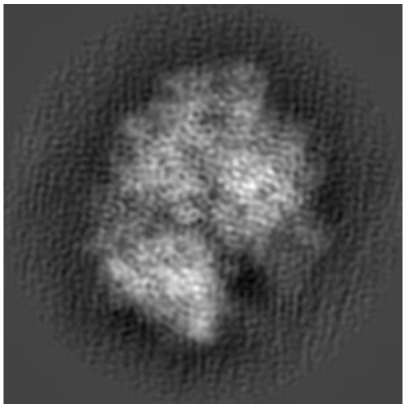
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

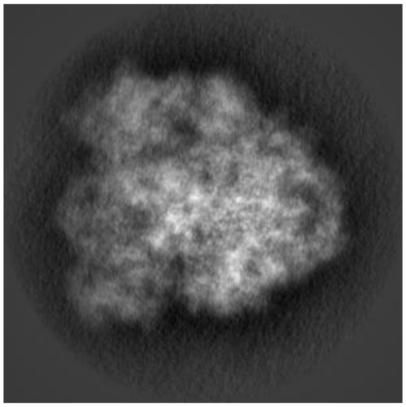
6.1.1 Primary map

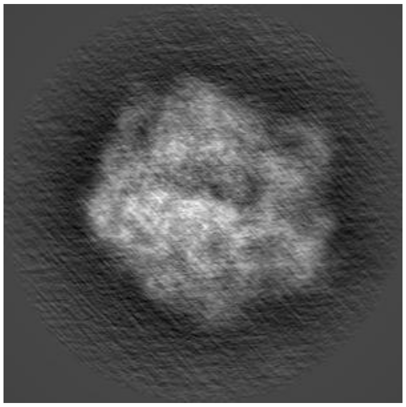

X

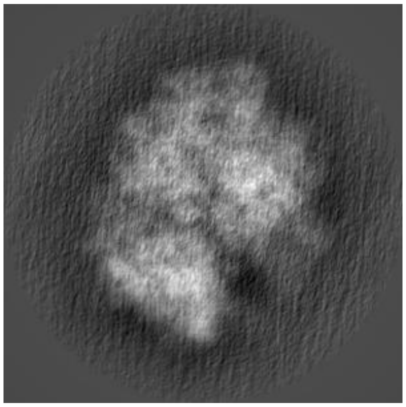

Y


Z

6.1.2 Raw map


X

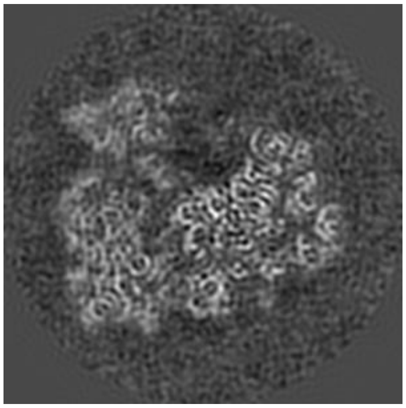

Y

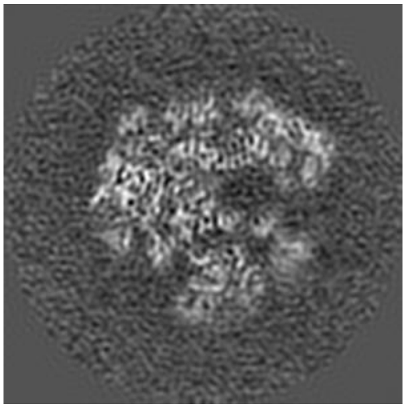

Z

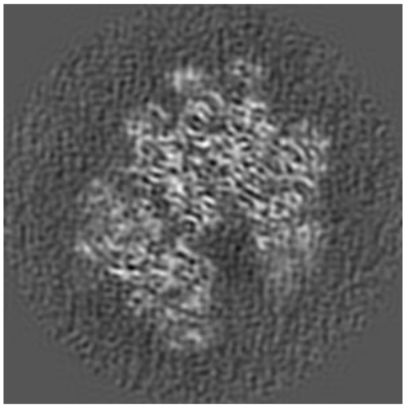
The images above show the map projected in three orthogonal directions.

6.2 Central slices

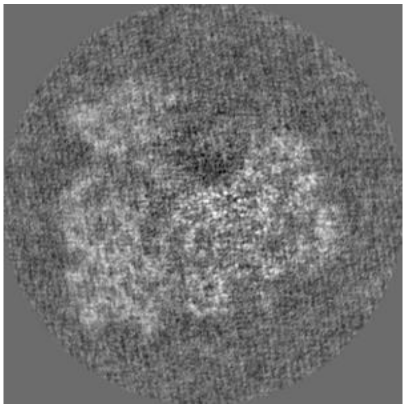
6.2.1 Primary map

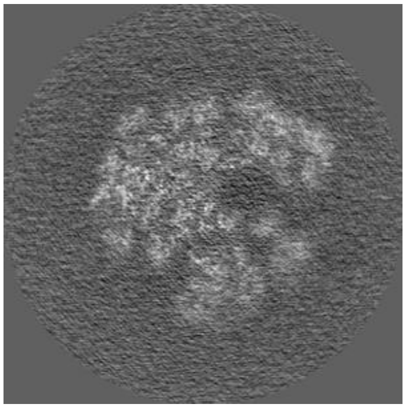

X Index: 144

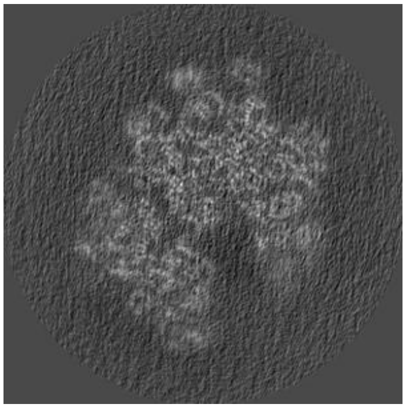

Y Index: 144


Z Index: 144

6.2.2 Raw map


X Index: 144

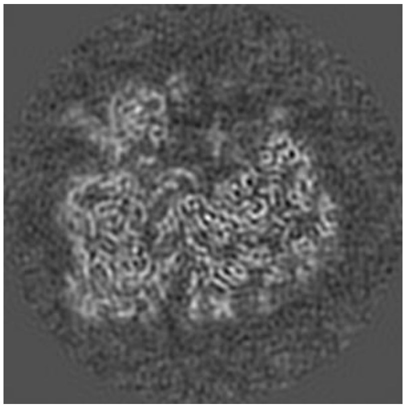

Y Index: 144

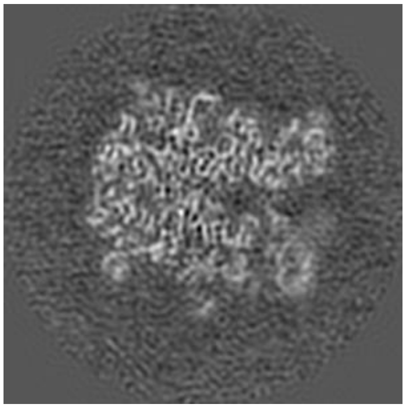

Z Index: 144

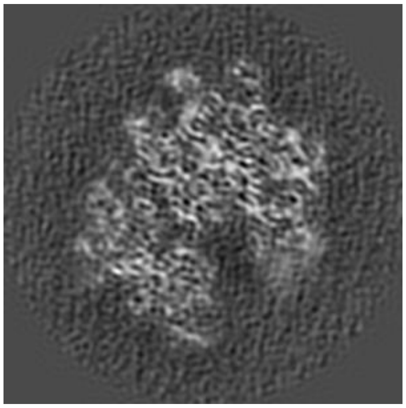
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

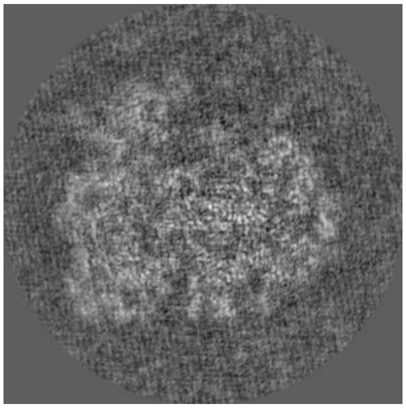
6.3.1 Primary map

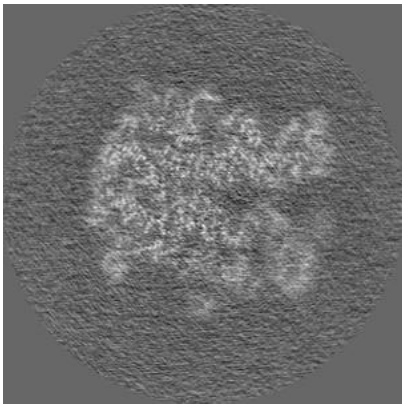

X Index: 139

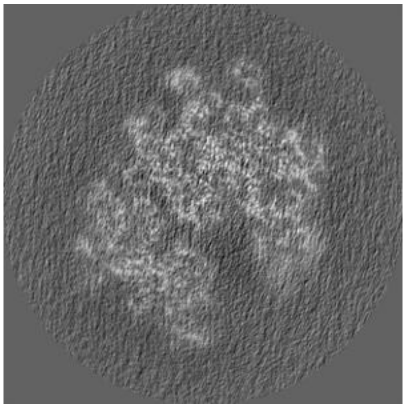

Y Index: 158


Z Index: 146

6.3.2 Raw map


X Index: 138

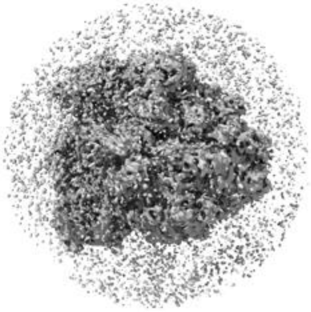

Y Index: 157


Z Index: 146

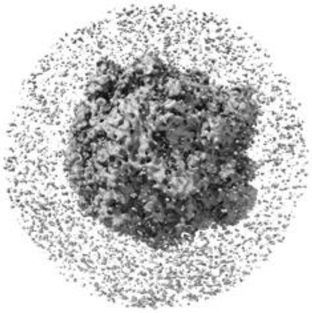
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

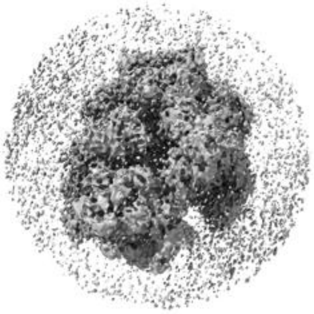
6.4.1 Primary map



X



Y

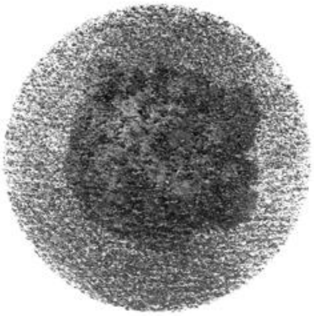


Z

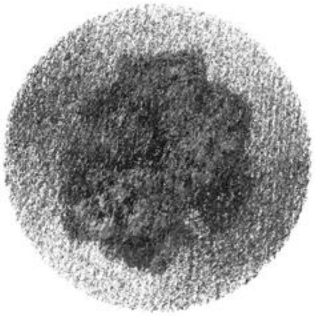
The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X



Y



Z

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

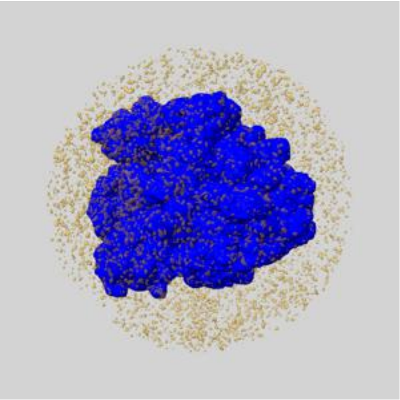
6.5 Mask visualisation ⓘ

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

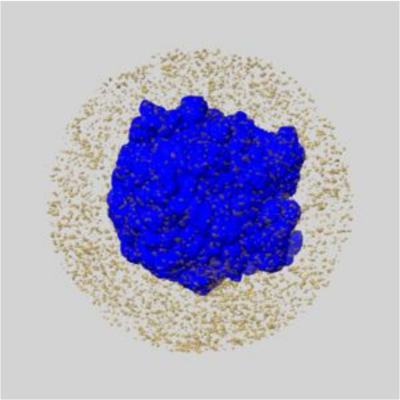
A mask typically either:

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

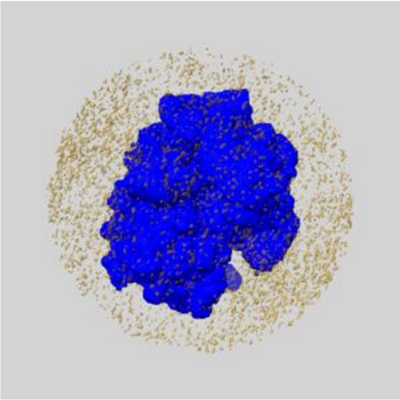
6.5.1 emd_13459_msk_1.map ⓘ



X



Y

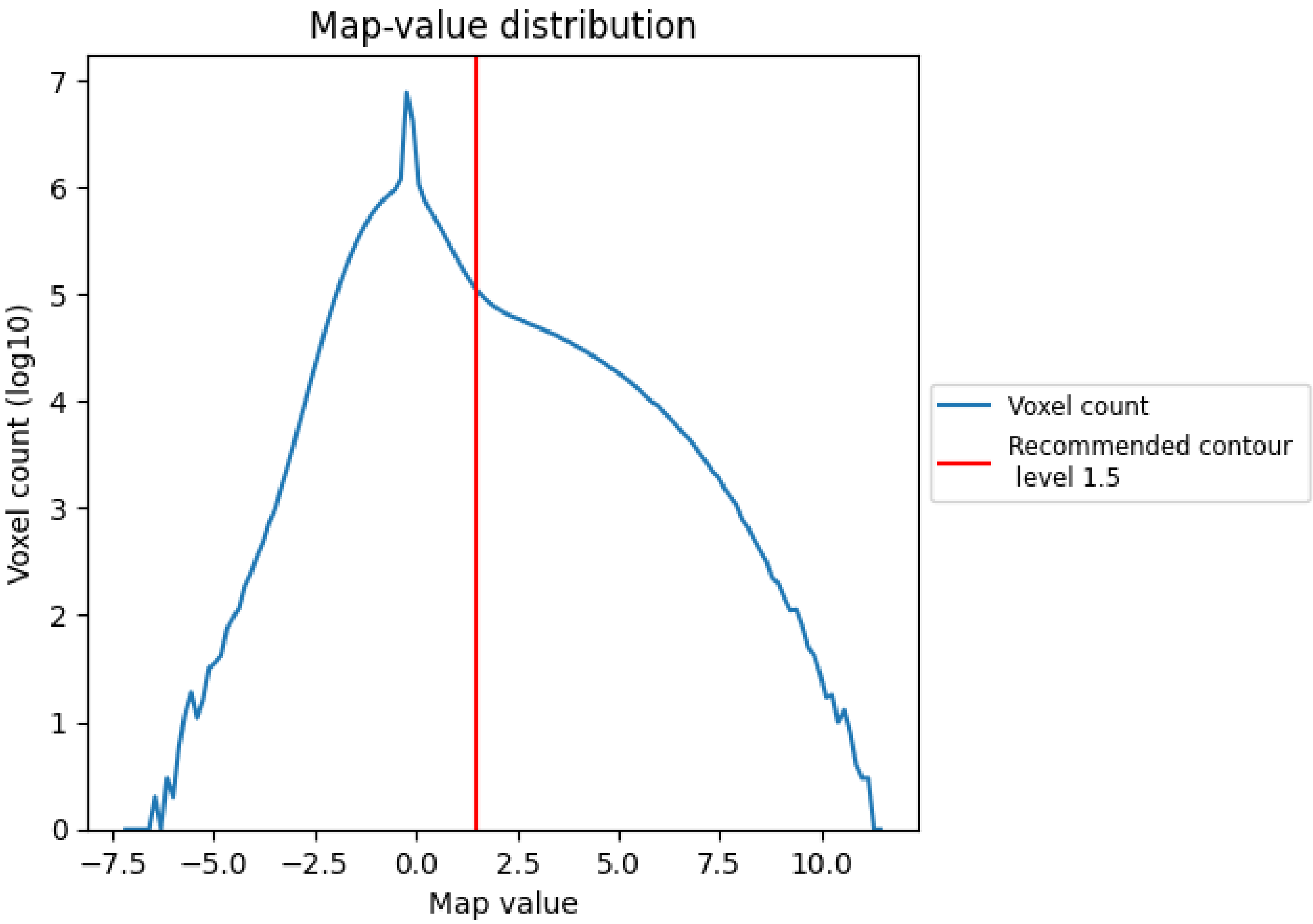


Z

7 Map analysis ⓘ

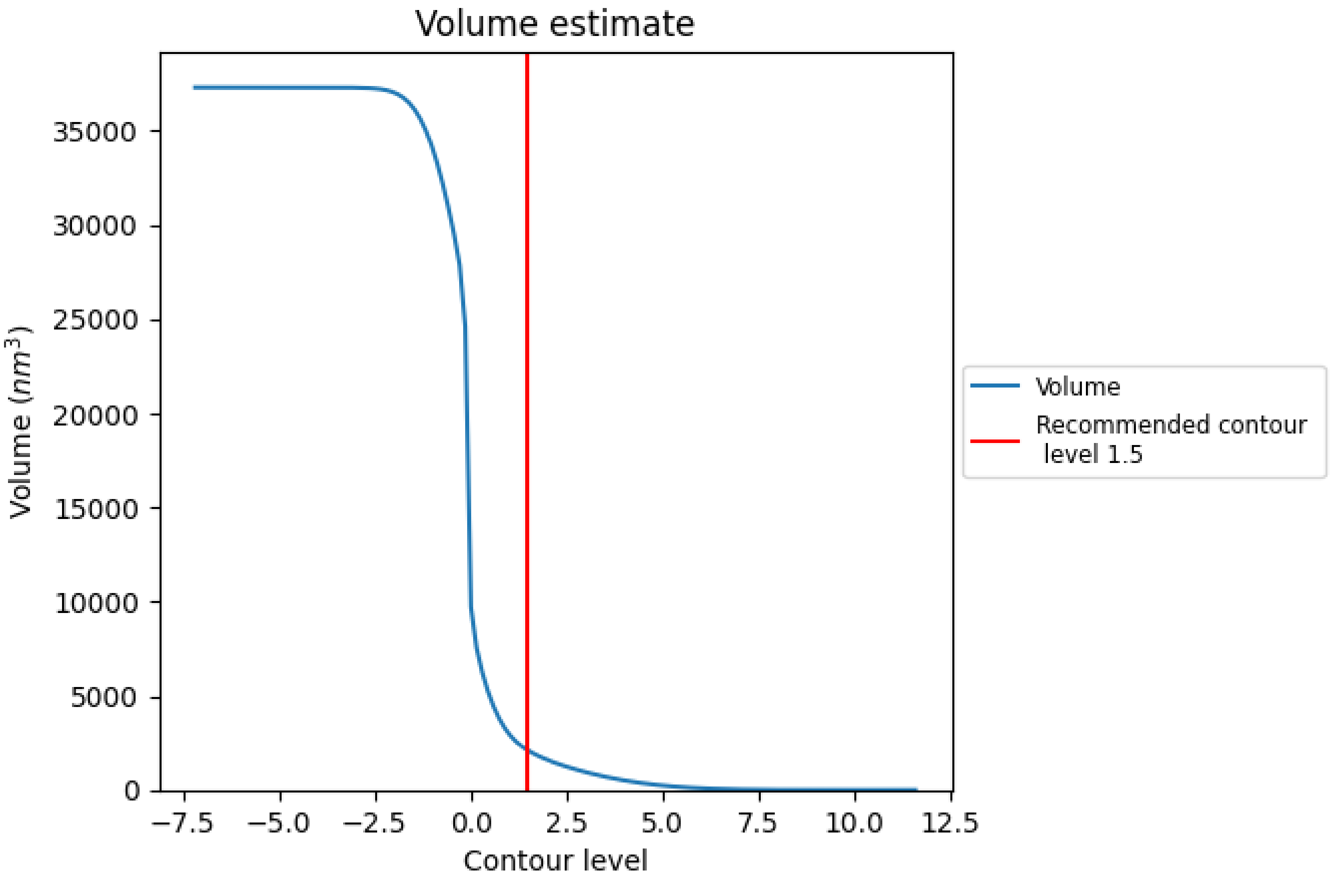
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

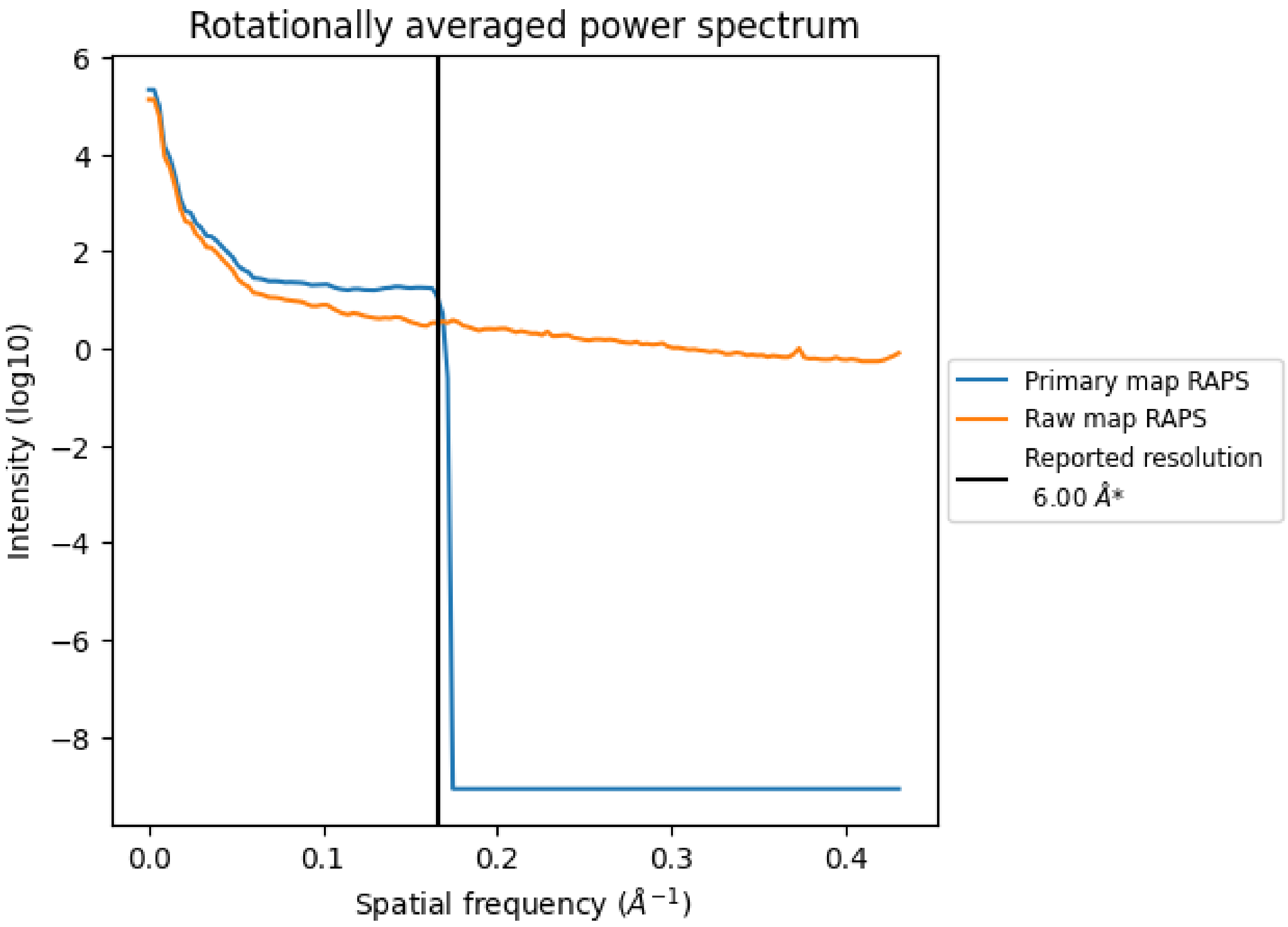
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2098 nm^3; this corresponds to an approximate mass of 1895 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

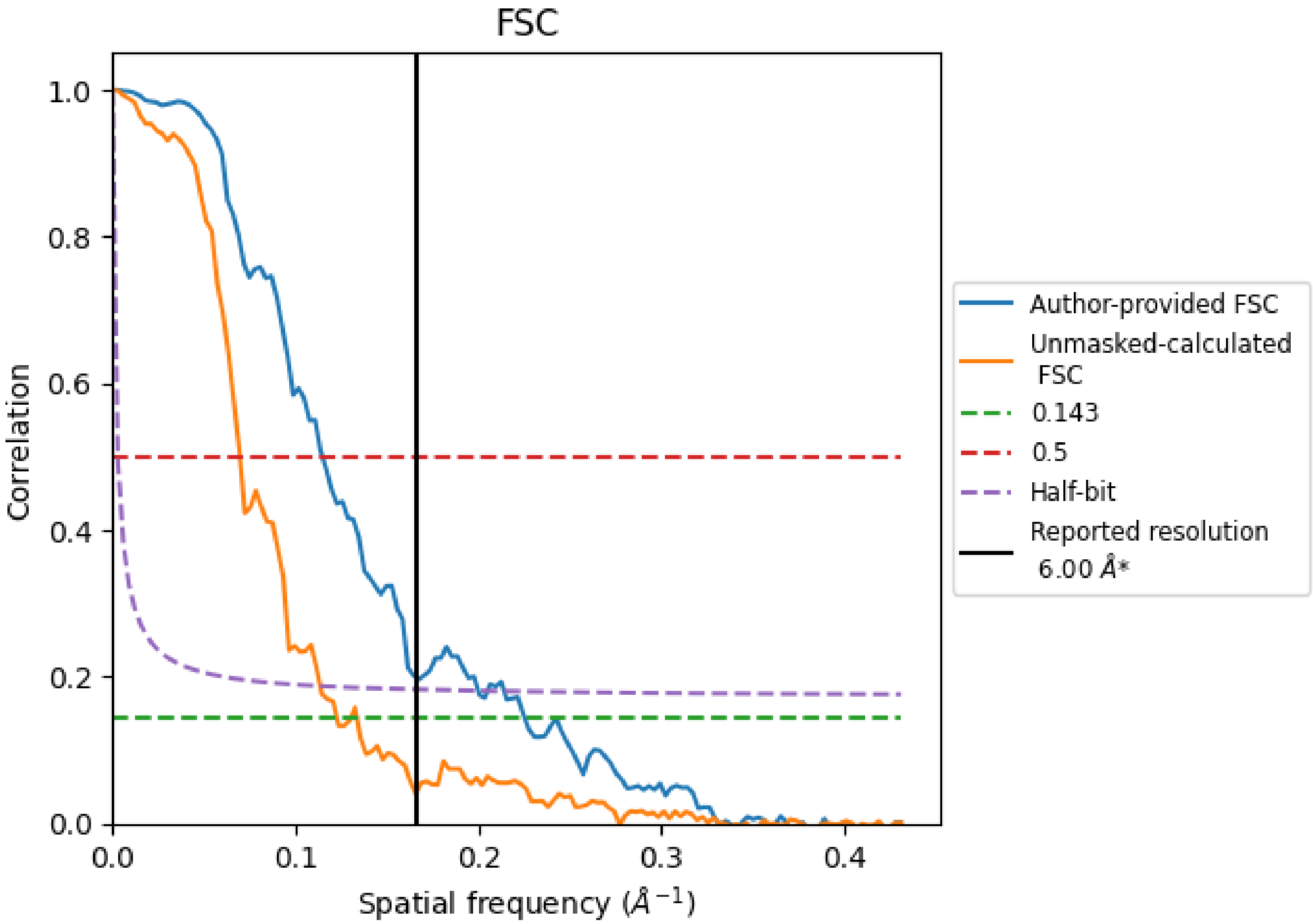


*Reported resolution corresponds to spatial frequency of 0.167 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.167 $Å^{-1}$

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	4.44	8.72	5.00
Unmasked-calculated*	8.15	14.37	8.80

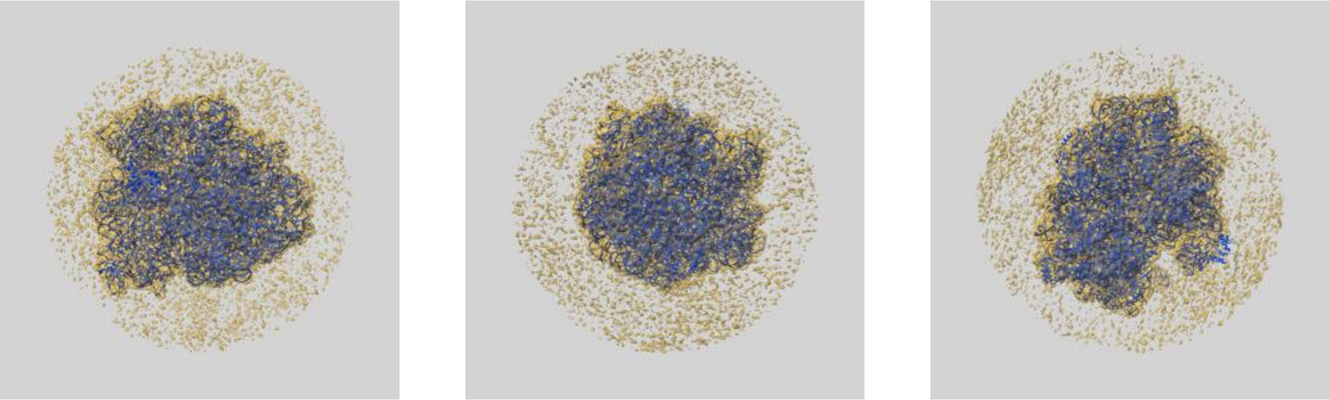
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 6.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.15 differs from the reported value 6.0 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13459 and PDB model 7PJT. Per-residue inclusion information can be found in section 3 on page 15.

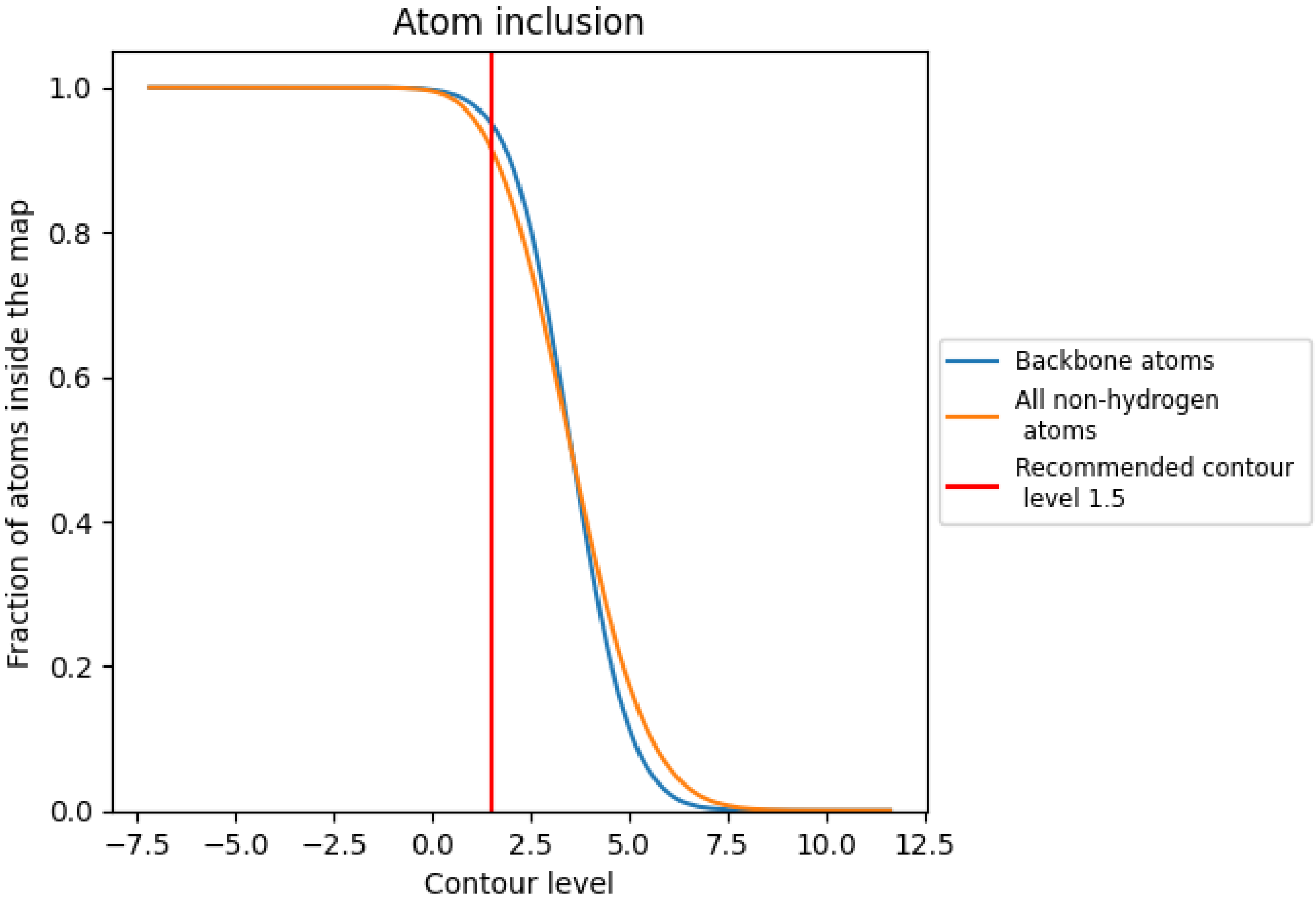
9.1 Map-model overlay (i)



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.