Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 10:22 am BST

PDB ID	:	5MDY
EMDB ID	:	EMD-3492
Title	:	Structure of ArfA and TtRF2 bound to the 70S ribosome (pre-accommodated state)
Authors	:	James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on	:	2016-11-13
Resolution	:	3.35 Å(reported)

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

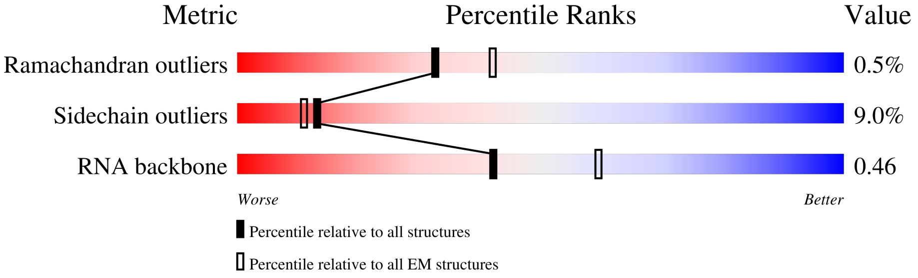
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

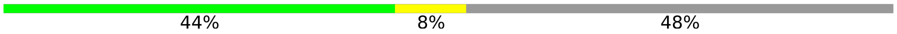
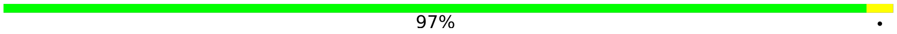
The reported resolution of this entry is 3.35 Å.

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%

Mol	Chain	Length	Quality of chain
1	1	2904	
2	2	1534	
3	3	120	
4	4	18	
5	5	78	
6	6	61	
7	7	378	
8	B	273	
9	C	209	

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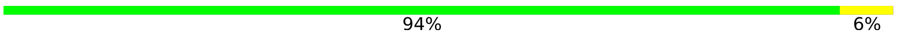
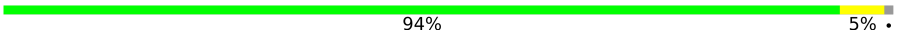
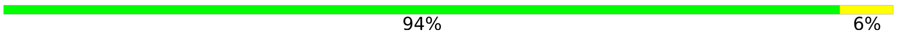
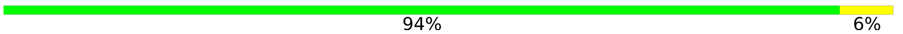
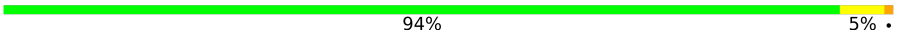
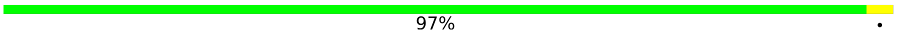
Mol	Chain	Length	Quality of chain
10	D	201	
11	E	179	
12	F	177	
13	G	149	
14	H	165	
15	I	142	
16	J	142	
17	K	123	
18	L	144	
19	M	136	
20	N	127	
21	O	117	
22	P	115	
23	Q	118	
24	R	103	
25	S	110	
26	T	100	
27	U	104	
28	V	94	
29	W	85	
30	X	78	
31	Y	63	
32	Z	59	
33	a	70	
34	b	57	

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Mol	Chain	Length	Quality of chain
35	c	55	87% 7% 5%
36	d	46	85% 15%
37	e	65	89% 9% •
38	f	38	87% 13%
39	g	241	89% 5% 7%
40	h	233	83% 6% 11%
41	i	206	96% •
42	j	167	84% 9% 7%
43	k	135	70% 6% • 23%
44	l	179	74% 10% • 16%
45	m	130	94% 5% •
46	n	130	88% 8% • •
47	o	103	87% 8% • •
48	p	129	84% 6% 9%
49	q	124	91% 8% •
50	r	118	92% 7% •
51	s	101	95% • •
52	t	89	88% 11% •
53	u	82	93% 7%
54	v	84	90% 5% 5%
55	w	75	83% 5% 12%
56	x	92	85% 5% 10%
57	y	87	95% • •
58	z	71	92% 7% •

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 149460 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	887	A	U	conflict	GB 802133627

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	120	2569	1144	468	837	120	0	0

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	5	109	49	22	33	5	0	0

- Molecule 5 is a RNA chain called fMet-NH-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	5	76	1622	725	292	528	76	1	0	0

- Molecule 6 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	32	259	163	53	42	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	0	HIS	-	expression tag	UNP P36675

- Molecule 7 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	324	2597	1630	471	488	8	0	0

- Molecule 8 is a protein called 50S ribosomal protein L2.

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

- Molecule 9 is a protein called 50S ribosomal protein L3.

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

- Molecule 10 is a protein called 50S ribosomal protein L4.

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

- Molecule 11 is a protein called 50S ribosomal protein L5.

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

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	146	Total	C	N	O	S	0	0
			1089	686	194	208	1		

- Molecule 14 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 15 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

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

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called 50S ribosomal protein L16.

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

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	119	Total 951	C 588	N 195	O 163	S 5	0	0

- Molecule 21 is a protein called 50S ribosomal protein L18.

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

- Molecule 22 is a protein called 50S ribosomal protein L19.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L21.

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

- Molecule 25 is a protein called 50S ribosomal protein L22.

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

- Molecule 26 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	T	94	746	470	140	134	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	U	103	788	498	148	142	0	0

- Molecule 28 is a protein called 50S ribosomal protein L25.

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

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	W	76	582	360	117	104	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L28.

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

- Molecule 31 is a protein called 50S ribosomal protein L29.

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

- Molecule 32 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Z	58	448	281	87	78	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	63	Total	C	N	O	S	0	0
			495	304	95	90	6		

- Molecule 34 is a protein called 50S ribosomal protein L32.

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

- Molecule 35 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L35.

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

- Molecule 38 is a protein called 50S ribosomal protein L36.

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

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	208	Total 1636	C 1036	N 307	O 290	S 3	0	0

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	156	Total 1152	C 717	N 217	O 212	S 6	0	0

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	104	Total 848	C 536	N 153	O 152	S 7	0	0

- Molecule 44 is a protein called 30S ribosomal protein S7.

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

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	99	Total 790	C 495	N 151	O 143	S 1	0	0

- Molecule 48 is a protein called 30S ribosomal protein S11.

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

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	116	Total 900	C 558	N 181	O 158	S 3	0	0

- Molecule 51 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	100	Total 805	C 499	N 164	O 139	S 3	0	0

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

- Molecule 54 is a protein called 30S ribosomal protein S17.

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

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	66	Total 544	C 344	N 102	O 97	S 1	0	0

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	83	Total 663	C 424	N 126	O 111	S 2	0	0

- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	86	Total 669	C 414	N 138	O 114	S 3	0	0

- Molecule 58 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	70	Total 589	C 366	N 125	O 97	S 1	0	0

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	1	293	Total 293	Mg 293	0
59	2	143	Total 143	Mg 143	0
59	3	7	Total 7	Mg 7	0
59	5	4	Total 4	Mg 4	0
59	b	1	Total 1	Mg 1	0
59	f	1	Total 1	Mg 1	0

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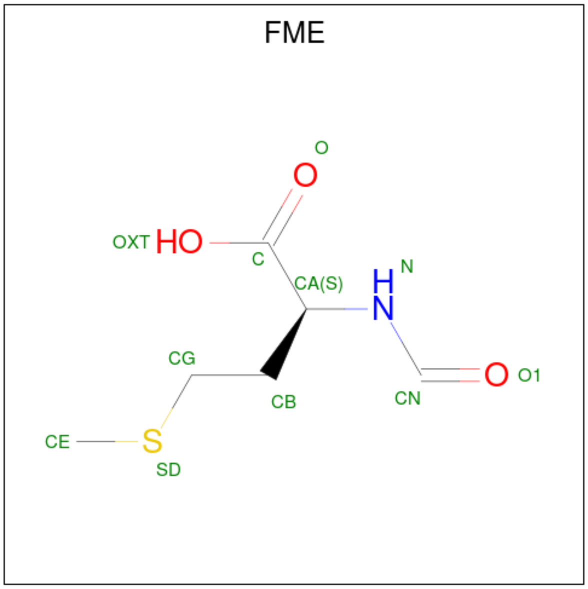
Mol	Chain	Residues	Atoms		AltConf
59	i	1	Total 1	Mg 1	0

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
60	5	1	Total 10	C 6	N 1	O 2	S 1	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	a	1	Total 1	Zn 1	0
61	f	1	Total 1	Zn 1	0

- Molecule 62 is water.

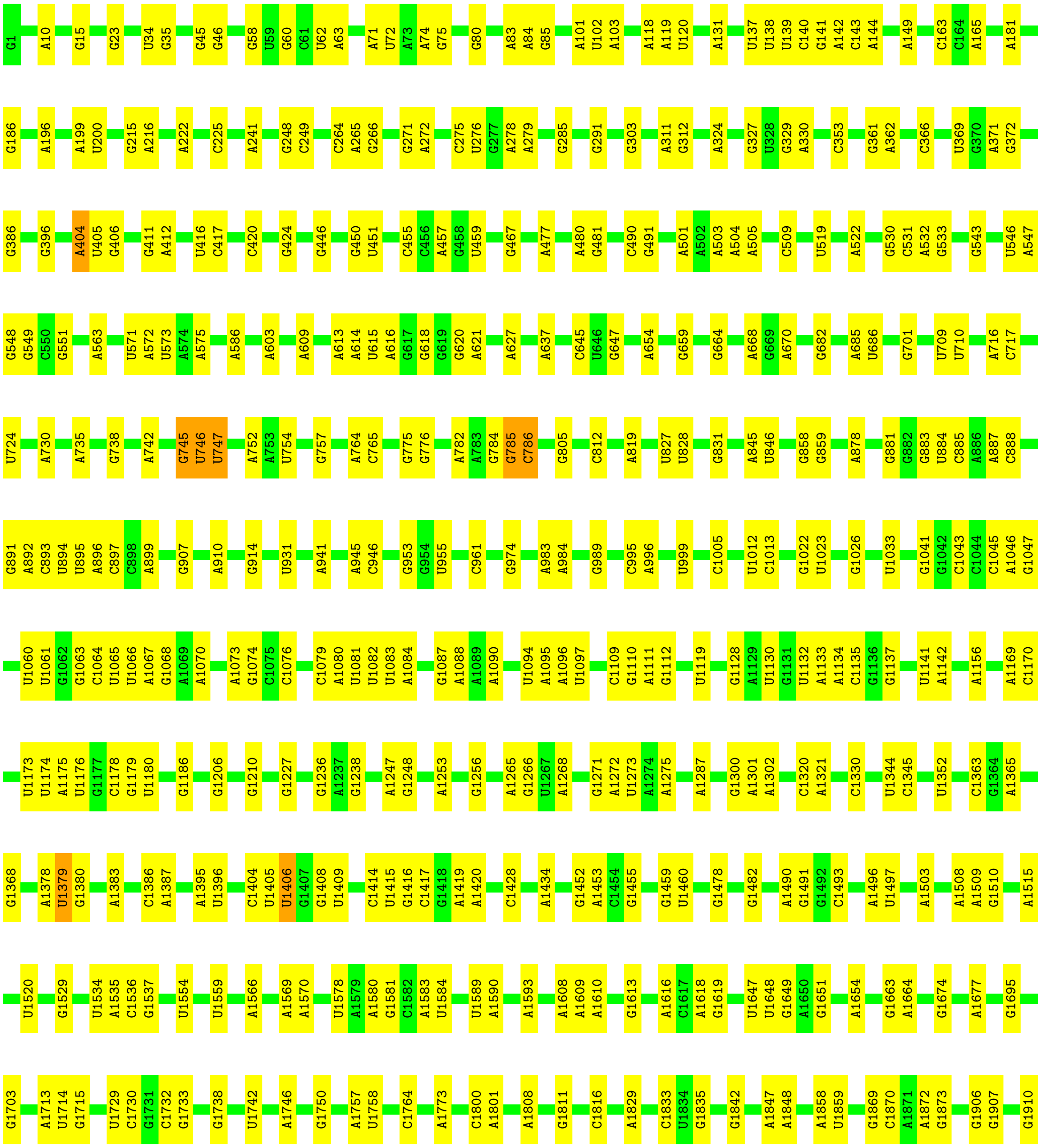
Mol	Chain	Residues	Atoms		AltConf
62	B	2	Total 2	O 2	0
62	O	1	Total 1	O 1	0

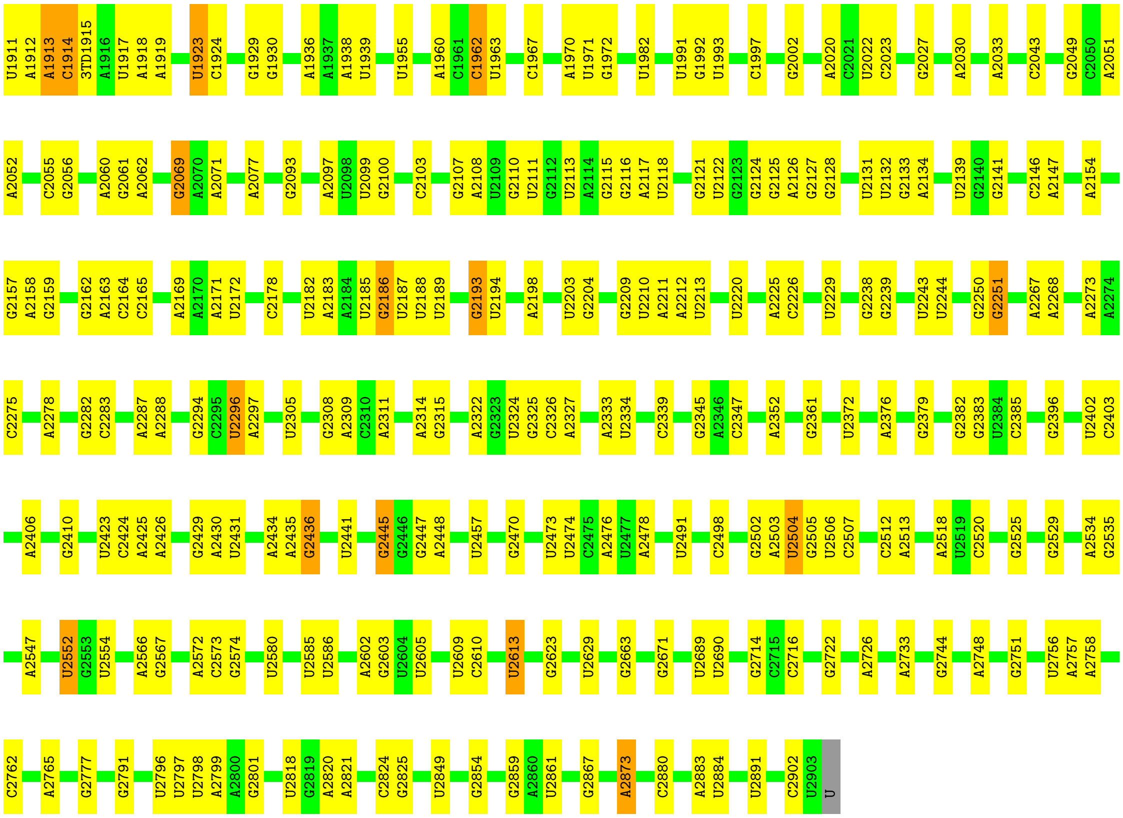
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal RNA

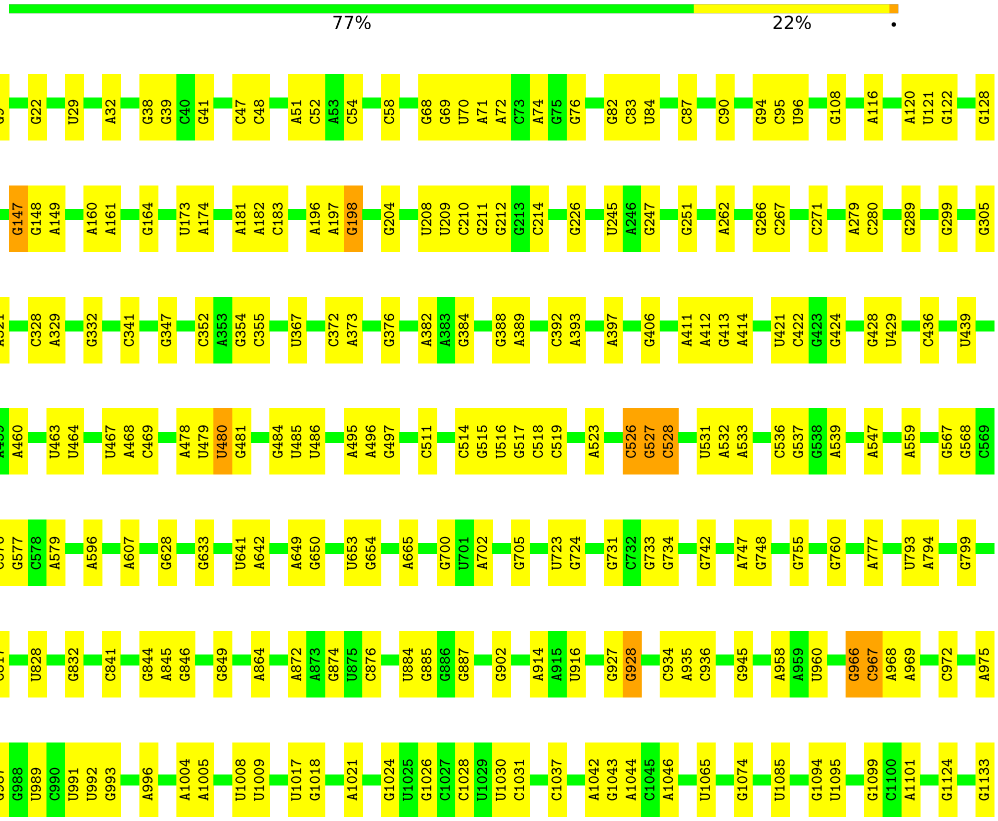
Chain 1:

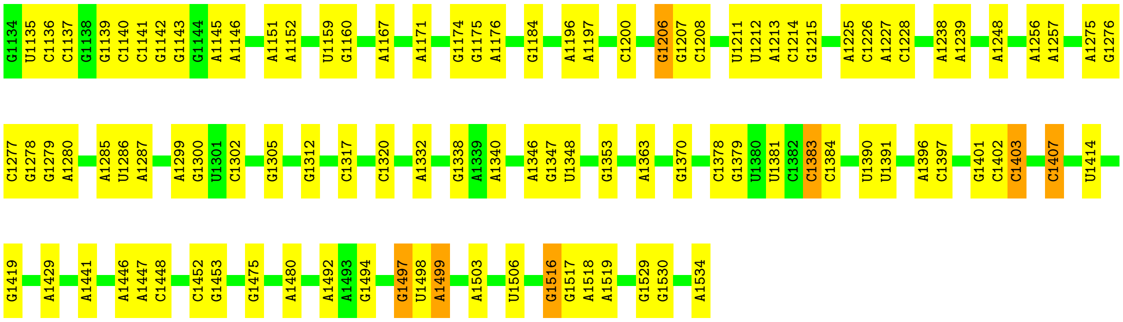




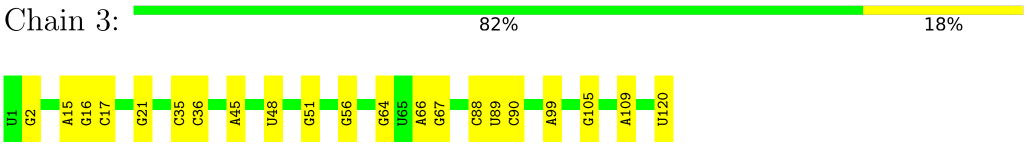
- Molecule 2: 16S ribosomal RNA

Chain 2:



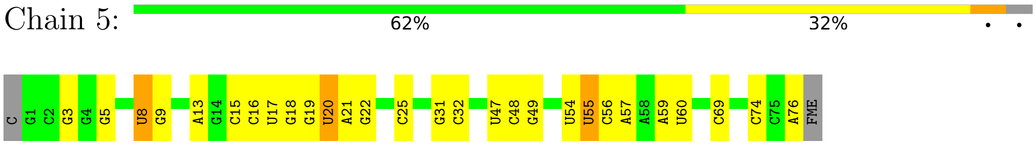


- Molecule 3: 5S ribosomal RNA

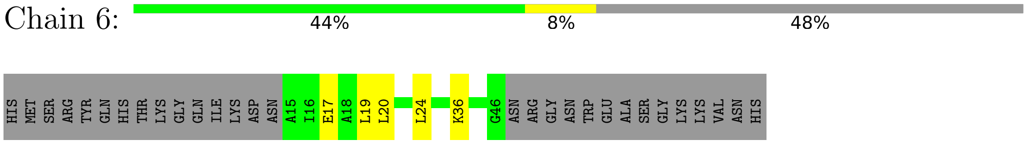


- Molecule 4: mRNA

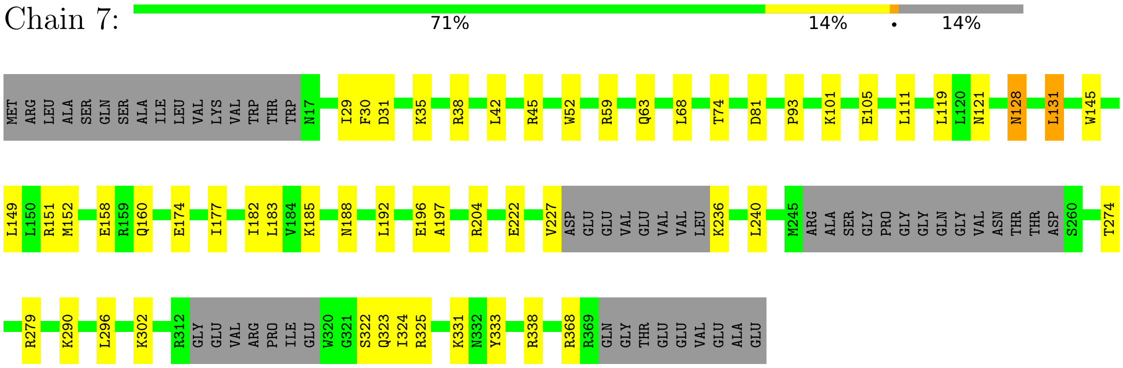
- Molecule 5: fMet-NH-tRNA(fMet)



- Molecule 6: Alternative ribosome-rescue factor A

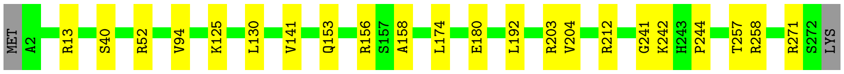


- Molecule 7: Peptide chain release factor 2



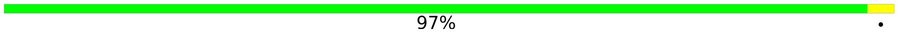
- Molecule 8: 50S ribosomal protein L2

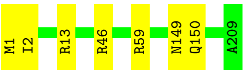
Chain B:



- Molecule 9: 50S ribosomal protein L3

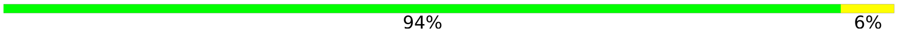
Chain C:

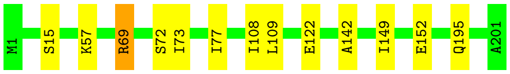




- Molecule 10: 50S ribosomal protein L4

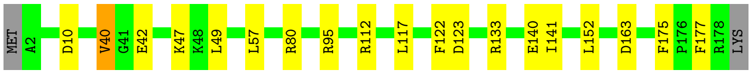
Chain D:





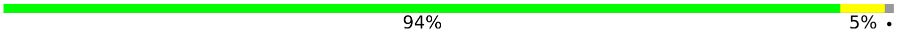
- Molecule 11: 50S ribosomal protein L5

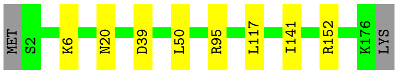
Chain E:



- Molecule 12: 50S ribosomal protein L6

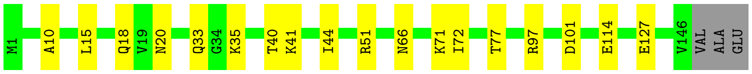
Chain F:





- Molecule 13: 50S ribosomal protein L9

Chain G:

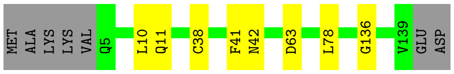


- Molecule 14: 50S ribosomal protein L10

Chain H:

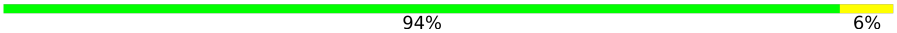
- Molecule 15: 50S ribosomal protein L11

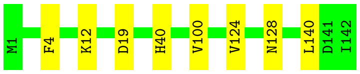
Chain I:



- Molecule 16: 50S ribosomal protein L13

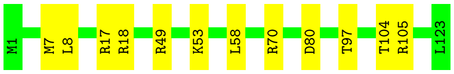
Chain J:





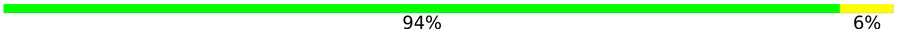
- Molecule 17: 50S ribosomal protein L14

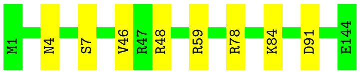
Chain K:



- Molecule 18: 50S ribosomal protein L15

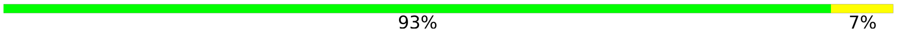
Chain L:

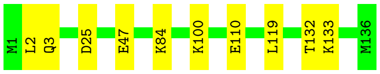




- Molecule 19: 50S ribosomal protein L16

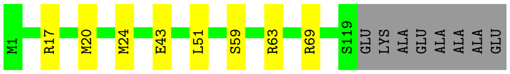
Chain M:





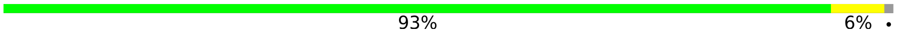
- Molecule 20: 50S ribosomal protein L17

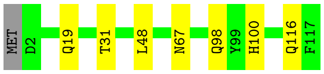
Chain N:



- Molecule 21: 50S ribosomal protein L18

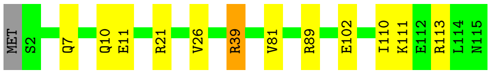
Chain O:





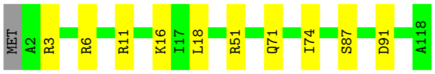
- Molecule 22: 50S ribosomal protein L19

Chain P:

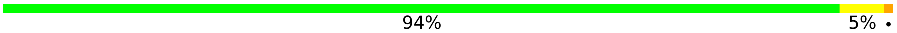



- Molecule 23: 50S ribosomal protein L20

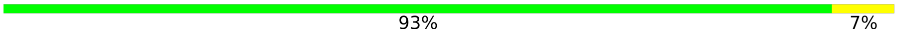
Chain Q:

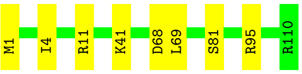



- Molecule 24: 50S ribosomal protein L21

Chain R:


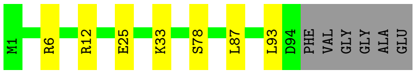
- Molecule 25: 50S ribosomal protein L22

Chain S:




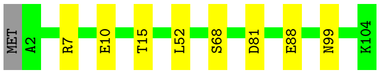
- Molecule 26: 50S ribosomal protein L23

Chain T:

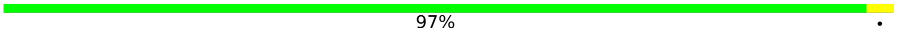



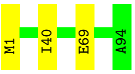
- Molecule 27: 50S ribosomal protein L24

Chain U:

- Molecule 28: 50S ribosomal protein L25

Chain V:


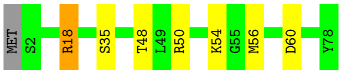


- Molecule 29: 50S ribosomal protein L27

Chain W:

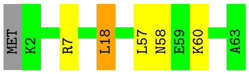
- Molecule 30: 50S ribosomal protein L28

Chain X:



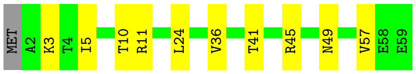
- Molecule 31: 50S ribosomal protein L29

Chain Y:



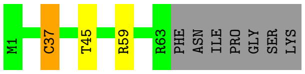
- Molecule 32: 50S ribosomal protein L30

Chain Z:



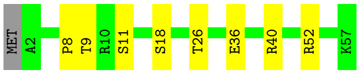
- Molecule 33: 50S ribosomal protein L31

Chain a:



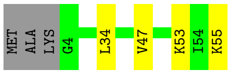
- Molecule 34: 50S ribosomal protein L32

Chain b:

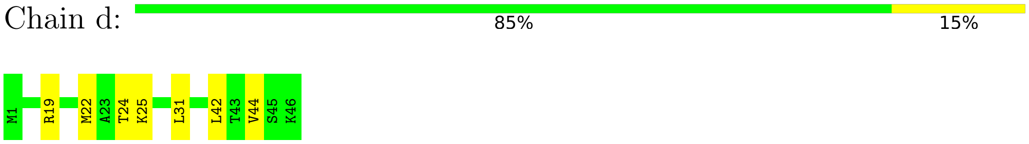


- Molecule 35: 50S ribosomal protein L33

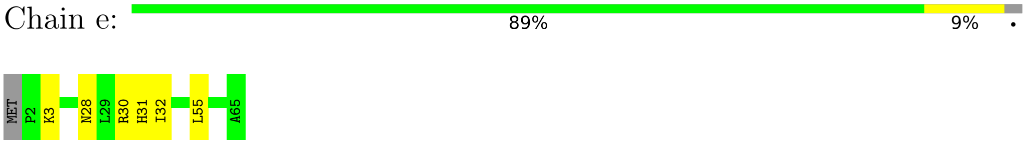
Chain c:



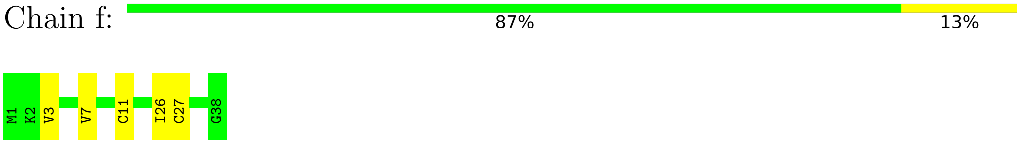
- Molecule 36: 50S ribosomal protein L34



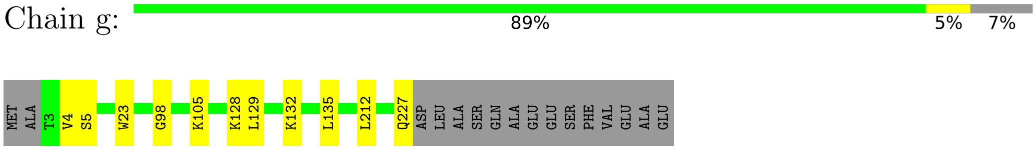
- Molecule 37: 50S ribosomal protein L35



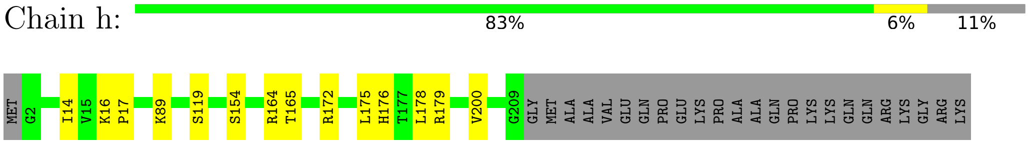
- Molecule 38: 50S ribosomal protein L36



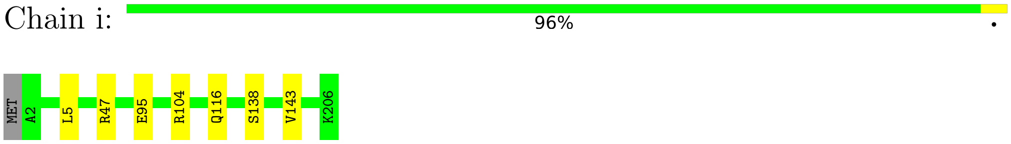
- Molecule 39: 30S ribosomal protein S2



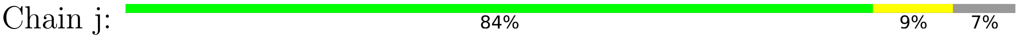
- Molecule 40: 30S ribosomal protein S3

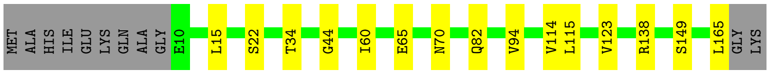


- Molecule 41: 30S ribosomal protein S4

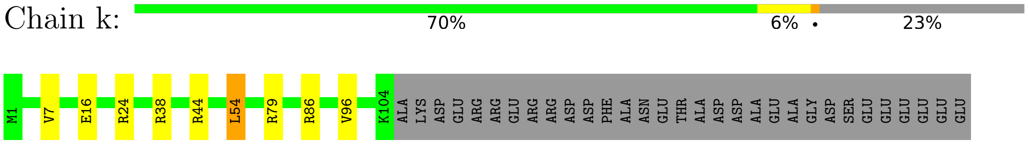


- Molecule 42: 30S ribosomal protein S5

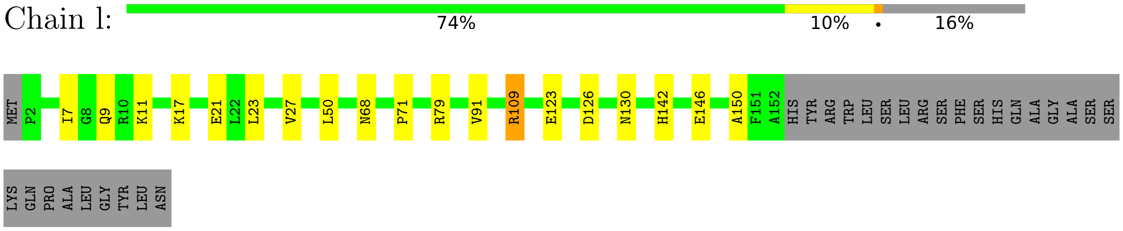




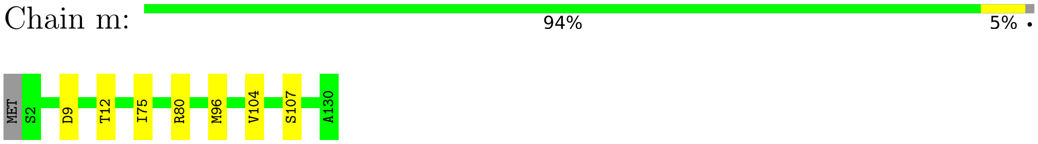
- Molecule 43: 30S ribosomal protein S6



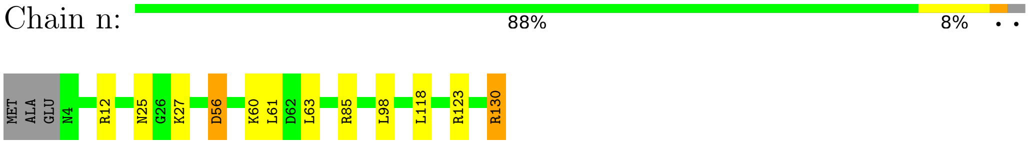
- Molecule 44: 30S ribosomal protein S7



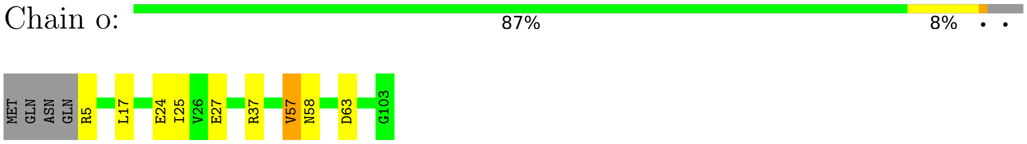
- Molecule 45: 30S ribosomal protein S8



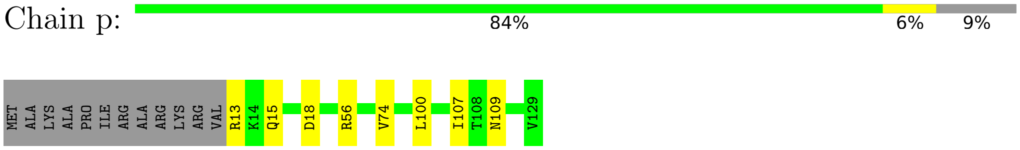
- Molecule 46: 30S ribosomal protein S9



- Molecule 47: 30S ribosomal protein S10

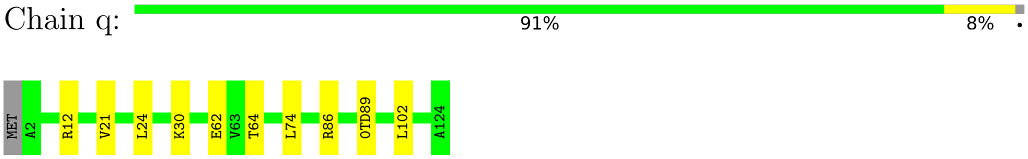


- Molecule 48: 30S ribosomal protein S11



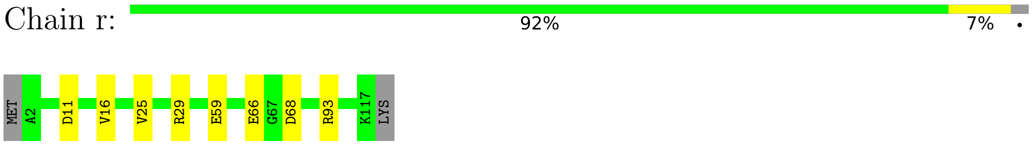
- Molecule 49: 30S ribosomal protein S12

Chain q:



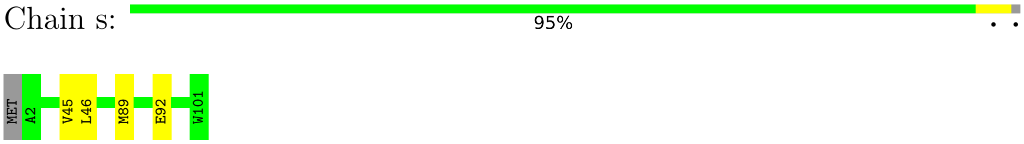
- Molecule 50: 30S ribosomal protein S13

Chain r:



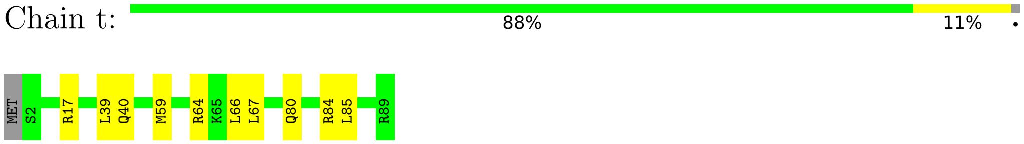
- Molecule 51: 30S ribosomal protein S14

Chain s:



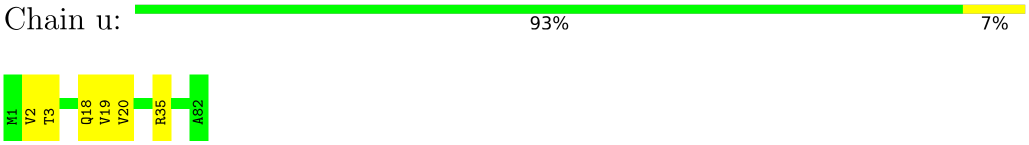
- Molecule 52: 30S ribosomal protein S15

Chain t:



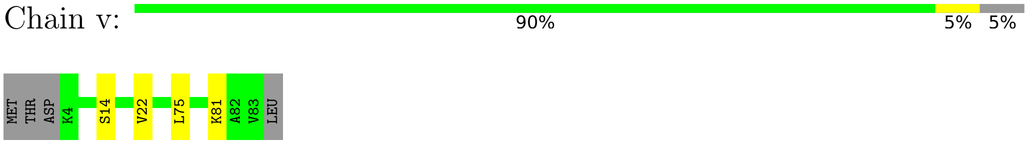
- Molecule 53: 30S ribosomal protein S16

Chain u:



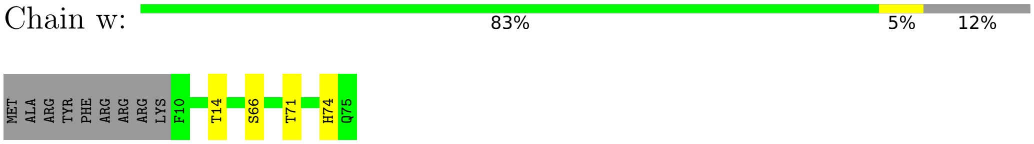
- Molecule 54: 30S ribosomal protein S17

Chain v:



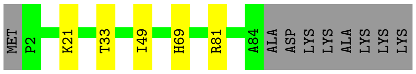
- Molecule 55: 30S ribosomal protein S18

Chain w:



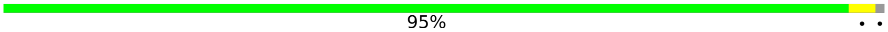
- Molecule 56: 30S ribosomal protein S19

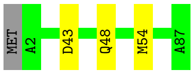
Chain x:



- Molecule 57: 30S ribosomal protein S20

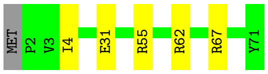
Chain y:





- Molecule 58: 30S ribosomal protein S21

Chain z:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54465	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 $(e^{-}/\text{Å}^{2})$	48	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	134615	Depositor
Image detector	FEI FALCON II (4k x 4k)	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: 1MG, H2U, 5MC, 0TD, 3TD, OMC, 4SU, FME, 2MG, ZN, MA6, OMG, 5MU, 4OC, PSU, 7MG, 8AN, 2MA, OMU, G7M, MG, UR3, 6MZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1	0.39	0/69285	0.75	25/108083 (0.0%)
2	2	0.33	0/36590	0.76	35/57074 (0.1%)
3	3	0.29	0/2872	0.71	0/4478
4	4	0.39	0/122	0.70	0/188
5	5	0.28	0/1672	0.72	0/2603
6	6	0.41	0/263	0.78	0/345
7	7	0.55	0/2642	0.85	1/3563 (0.0%)
8	B	0.52	0/2121	0.85	2/2852 (0.1%)
9	C	0.52	0/1586	0.76	0/2134
10	D	0.52	0/1571	0.83	2/2113 (0.1%)
11	E	0.48	0/1434	0.80	0/1926
12	F	0.41	0/1333	0.72	0/1805
13	G	0.45	0/1100	0.72	0/1486
14	H	0.50	0/993	0.75	1/1340 (0.1%)
15	I	0.45	0/998	0.71	0/1348
16	J	0.52	0/1152	0.82	0/1551
17	K	0.50	0/955	0.87	1/1279 (0.1%)
18	L	0.49	0/1062	0.83	0/1413
19	M	0.53	0/1093	0.86	0/1460
20	N	0.57	0/964	0.90	0/1289
21	O	0.54	0/902	0.86	0/1209
22	P	0.49	0/929	0.84	1/1242 (0.1%)
23	Q	0.69	0/960	0.99	1/1278 (0.1%)
24	R	0.46	0/829	0.74	1/1107 (0.1%)
25	S	0.56	0/864	0.87	0/1156
26	T	0.49	0/752	0.78	0/1005
27	U	0.40	0/796	0.69	0/1062
28	V	0.43	0/766	0.68	0/1025
29	W	0.52	0/589	0.84	0/779
30	X	0.53	0/635	0.92	1/848 (0.1%)
31	Y	0.56	0/502	0.90	1/667 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Z	0.45	0/452	0.78	0/605
33	a	0.42	0/503	0.78	1/671 (0.1%)
34	b	0.49	0/450	0.83	0/599
35	c	0.44	0/433	0.70	0/576
36	d	0.60	0/380	0.99	0/498
37	e	0.52	0/513	0.86	0/676
38	f	0.45	0/303	0.89	0/397
39	g	0.47	0/1791	0.73	0/2413
40	h	0.48	0/1663	0.76	0/2241
41	i	0.50	0/1665	0.79	0/2227
42	j	0.52	0/1165	0.84	0/1568
43	k	0.47	0/867	0.78	1/1171 (0.1%)
44	l	0.52	0/1195	0.89	1/1602 (0.1%)
45	m	0.47	0/989	0.75	0/1326
46	n	0.46	0/1034	0.84	1/1375 (0.1%)
47	o	0.43	0/800	0.83	1/1082 (0.1%)
48	p	0.44	0/893	0.75	0/1205
49	q	0.46	0/960	0.83	0/1286
50	r	0.50	0/909	0.89	0/1215
51	s	0.51	0/817	0.80	0/1088
52	t	0.56	0/722	0.88	1/964 (0.1%)
53	u	0.50	0/659	0.82	0/884
54	v	0.41	0/657	0.70	0/881
55	w	0.50	0/553	0.84	0/743
56	x	0.41	0/680	0.70	0/915
57	y	0.59	0/675	0.87	0/895
58	z	0.55	0/597	0.91	0/792
All	All	0.42	0/160657	0.77	78/239603 (0.0%)

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	786	C	N1-C1'-C2'	-13.18	96.86	114.00
2	2	1277	C	N1-C1'-C2'	-12.59	97.64	114.00
2	2	928	G	N9-C1'-C2'	-12.13	98.23	114.00
2	2	198	G	N9-C1'-C2'	-10.73	100.05	114.00
2	2	1401	G	N9-C1'-C2'	-10.71	100.08	114.00
2	2	1391	U	N1-C1'-C2'	-10.59	100.23	114.00
2	2	528	C	N1-C1'-C2'	-10.52	100.33	114.00
2	2	927	G	N9-C1'-C2'	-10.26	100.67	114.00
2	2	1384	C	N1-C1'-C2'	-10.10	100.87	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1406	U	N1-C1'-C2'	-10.07	100.91	114.00
2	2	1499	A	N9-C1'-C2'	-10.06	100.92	114.00
2	2	1206	G	N9-C1'-C2'	-9.57	101.47	112.00
1	1	1914	C	C4'-C3'-O3'	9.42	131.84	113.00
2	2	1208	C	N1-C1'-C2'	-9.17	101.92	112.00
2	2	1383	C	N1-C1'-C2'	-9.03	102.07	112.00
2	2	148	G	N9-C1'-C2'	-9.00	102.10	112.00
1	1	2315	G	N9-C1'-C2'	-8.43	102.73	112.00
2	2	526	C	N1-C1'-C2'	-8.16	103.02	112.00
2	2	1276	G	N9-C1'-C2'	-7.92	103.29	112.00
46	n	130	ARG	NE-CZ-NH2	7.83	124.21	120.30
1	1	2436	G	N9-C1'-C2'	-7.79	103.43	112.00
44	l	109	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	1	2193	G	C2'-C3'-O3'	7.30	125.56	109.50
2	2	928	G	C4'-C3'-O3'	7.20	127.41	113.00
1	1	1913	A	C4'-C3'-O3'	7.15	127.30	113.00
33	a	37	CYS	CA-CB-SG	-7.15	101.14	114.00
2	2	1276	G	C1'-C2'-O2'	-7.11	89.28	110.60
2	2	1497	G	N9-C1'-C2'	-6.98	104.32	112.00
1	1	1910	G	N9-C1'-C2'	-6.80	104.52	112.00
7	7	131	LEU	CA-CB-CG	6.80	130.93	115.30
2	2	1403	C	N1-C1'-C2'	-6.70	104.63	112.00
1	1	785	G	N9-C1'-C2'	-6.65	104.69	112.00
1	1	1923	U	C4'-C3'-O3'	6.62	126.24	113.00
2	2	864	A	N9-C1'-C2'	6.54	122.51	114.00
2	2	927	G	C4'-C3'-O3'	6.54	126.08	113.00
1	1	1404	C	N1-C1'-C2'	-6.42	104.93	112.00
2	2	515	G	N9-C1'-C2'	-6.38	104.98	112.00
2	2	480	U	N1-C1'-C2'	-6.34	105.02	112.00
2	2	198	G	C4'-C3'-O3'	6.33	125.66	113.00
1	1	1141	U	N1-C1'-C2'	6.29	122.17	114.00
2	2	1206	G	C4'-C3'-O3'	6.29	125.57	113.00
2	2	1401	G	C4'-C3'-O3'	6.16	125.33	113.00
2	2	147	G	N9-C1'-C2'	-6.15	105.23	112.00
2	2	864	A	C8-N9-C1'	-6.14	116.66	127.70
2	2	1390	U	N1-C1'-C2'	-6.04	105.36	112.00
1	1	1379	U	C2'-C3'-O3'	5.95	123.22	113.70
1	1	2613	U	O4'-C1'-N1	5.93	112.94	108.20
22	P	39	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	1	2186	G	C4'-C3'-O3'	5.91	124.81	113.00
2	2	884	U	N1-C1'-C2'	5.81	121.55	114.00
1	1	754	U	N1-C1'-C2'	5.81	121.55	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1276	G	C4'-C3'-O3'	5.64	124.28	113.00
2	2	1391	U	C4'-C3'-O3'	5.56	124.11	113.00
24	R	78	ARG	NE-CZ-NH2	5.49	123.05	120.30
2	2	927	G	C1'-C2'-O2'	-5.48	94.16	110.60
1	1	2296	U	C4'-C3'-O3'	5.42	123.84	113.00
1	1	786	C	C4'-C3'-O3'	5.36	123.72	113.00
47	o	57	VAL	N-CA-C	5.36	125.47	111.00
2	2	864	A	C4-N9-C1'	5.28	135.81	126.30
1	1	742	A	C8-N9-C1'	-5.28	118.19	127.70
30	X	18	ARG	NE-CZ-NH2	5.28	122.94	120.30
52	t	59	MET	CA-CB-CG	5.27	122.25	113.30
1	1	2071	A	C4'-C3'-O3'	-5.26	98.36	109.40
1	1	742	A	C4-N9-C1'	5.22	135.70	126.30
2	2	515	G	C4'-C3'-O3'	5.20	123.39	113.00
1	1	2873	A	C1'-O4'-C4'	-5.19	105.75	109.90
1	1	1404	C	C4'-C3'-O3'	5.19	123.38	113.00
1	1	404	A	C2'-C3'-O3'	5.18	122.00	113.70
8	B	212	ARG	NE-CZ-NH2	5.18	122.89	120.30
8	B	212	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	1	1405	U	C1'-C2'-O2'	-5.12	95.23	110.60
10	D	69	ARG	NE-CZ-NH2	-5.10	117.75	120.30
43	k	54	LEU	CA-CB-CG	5.10	127.02	115.30
14	H	81	LEU	CA-CB-CG	5.05	126.91	115.30
23	Q	6	ARG	NE-CZ-NH2	5.03	122.81	120.30
31	Y	18	LEU	CA-CB-CG	5.02	126.85	115.30
10	D	69	ARG	NE-CZ-NH1	5.00	122.80	120.30
17	K	18	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	30/61 (49%)	27 (90%)	3 (10%)	0	100	100
7	7	316/378 (84%)	287 (91%)	26 (8%)	3 (1%)	17	51
8	B	269/273 (98%)	252 (94%)	15 (6%)	2 (1%)	22	56
9	C	207/209 (99%)	191 (92%)	15 (7%)	1 (0%)	29	63
10	D	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	29	63
11	E	175/179 (98%)	160 (91%)	12 (7%)	3 (2%)	9	36
12	F	173/177 (98%)	162 (94%)	11 (6%)	0	100	100
13	G	144/149 (97%)	133 (92%)	10 (7%)	1 (1%)	22	56
14	H	128/165 (78%)	107 (84%)	18 (14%)	3 (2%)	6	31
15	I	133/142 (94%)	116 (87%)	16 (12%)	1 (1%)	19	53
16	J	140/142 (99%)	132 (94%)	7 (5%)	1 (1%)	22	56
17	K	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
18	L	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
19	M	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
20	N	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
21	O	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	17	51
22	P	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
23	Q	115/118 (98%)	110 (96%)	3 (3%)	2 (2%)	9	36
24	R	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
25	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
26	T	92/100 (92%)	88 (96%)	4 (4%)	0	100	100
27	U	101/104 (97%)	91 (90%)	9 (9%)	1 (1%)	15	49
28	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
29	W	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
31	Y	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
32	Z	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	8	35
33	a	61/70 (87%)	56 (92%)	5 (8%)	0	100	100
34	b	54/57 (95%)	49 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	c	50/55 (91%)	44 (88%)	6 (12%)	0	100	100
36	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
37	e	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	24
38	f	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
39	g	223/241 (92%)	207 (93%)	15 (7%)	1 (0%)	34	68
40	h	206/233 (88%)	191 (93%)	14 (7%)	1 (0%)	29	63
41	i	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
42	j	154/167 (92%)	148 (96%)	5 (3%)	1 (1%)	25	59
43	k	102/135 (76%)	94 (92%)	7 (7%)	1 (1%)	15	49
44	l	149/179 (83%)	143 (96%)	3 (2%)	3 (2%)	7	33
45	m	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
46	n	125/130 (96%)	117 (94%)	7 (6%)	1 (1%)	19	53
47	o	97/103 (94%)	92 (95%)	5 (5%)	0	100	100
48	p	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	17	51
49	q	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
50	r	114/118 (97%)	106 (93%)	7 (6%)	1 (1%)	17	51
51	s	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
52	t	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
53	u	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
54	v	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
55	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
56	x	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
57	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
58	z	68/71 (96%)	68 (100%)	0	0	100	100
All	All	6209/6659 (93%)	5804 (94%)	371 (6%)	34 (0%)	32	63

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	7	128	ASN
9	C	150	GLN
14	H	117	LEU
46	n	56	ASP
7	7	93	PRO

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Mol	Chain	Res	Type
8	B	241	GLY
11	E	177	PHE
21	O	100	HIS
23	Q	3	ARG
37	e	28	ASN
7	7	197	ALA
8	B	158	ALA
10	D	142	ALA
16	J	100	VAL
32	Z	3	LYS
27	U	99	ASN
40	h	17	PRO
42	j	44	GLY
43	k	96	VAL
44	l	130	ASN
44	l	150	ALA
50	r	66	GLU
11	E	42	GLU
14	H	109	LYS
11	E	40	VAL
13	G	10	ALA
14	H	51	TYR
37	e	32	ILE
45	m	75	ILE
15	I	136	GLY
23	Q	74	ILE
39	g	98	GLY
48	p	74	VAL
44	l	71	PRO

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
6	6	26/51 (51%)	21 (81%)	5 (19%)	1 5
7	7	275/319 (86%)	223 (81%)	52 (19%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	B	216/218 (99%)	197 (91%)	19 (9%)	10	34
9	C	164/164 (100%)	158 (96%)	6 (4%)	34	63
10	D	165/165 (100%)	153 (93%)	12 (7%)	14	43
11	E	148/150 (99%)	131 (88%)	17 (12%)	5	22
12	F	136/138 (99%)	128 (94%)	8 (6%)	19	51
13	G	112/114 (98%)	95 (85%)	17 (15%)	3	12
14	H	99/123 (80%)	89 (90%)	10 (10%)	7	28
15	I	104/110 (94%)	97 (93%)	7 (7%)	16	47
16	J	116/116 (100%)	109 (94%)	7 (6%)	19	50
17	K	104/104 (100%)	93 (89%)	11 (11%)	6	26
18	L	103/103 (100%)	95 (92%)	8 (8%)	12	40
19	M	109/109 (100%)	99 (91%)	10 (9%)	9	32
20	N	99/103 (96%)	91 (92%)	8 (8%)	11	38
21	O	86/87 (99%)	80 (93%)	6 (7%)	15	45
22	P	99/100 (99%)	87 (88%)	12 (12%)	5	20
23	Q	89/90 (99%)	82 (92%)	7 (8%)	12	40
24	R	84/84 (100%)	78 (93%)	6 (7%)	14	45
25	S	93/93 (100%)	85 (91%)	8 (9%)	10	36
26	T	81/84 (96%)	74 (91%)	7 (9%)	10	36
27	U	84/85 (99%)	77 (92%)	7 (8%)	11	37
28	V	78/78 (100%)	75 (96%)	3 (4%)	33	63
29	W	58/63 (92%)	56 (97%)	2 (3%)	37	66
30	X	67/68 (98%)	60 (90%)	7 (10%)	7	27
31	Y	54/55 (98%)	49 (91%)	5 (9%)	9	32
32	Z	48/49 (98%)	39 (81%)	9 (19%)	1	6
33	a	56/62 (90%)	53 (95%)	3 (5%)	22	54
34	b	47/48 (98%)	39 (83%)	8 (17%)	2	9
35	c	47/49 (96%)	43 (92%)	4 (8%)	10	36
36	d	38/38 (100%)	31 (82%)	7 (18%)	1	6
37	e	51/52 (98%)	47 (92%)	4 (8%)	12	40
38	f	34/34 (100%)	29 (85%)	5 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	g	187/199 (94%)	177 (95%)	10 (5%)	22	54
40	h	171/190 (90%)	158 (92%)	13 (8%)	13	41
41	i	172/173 (99%)	165 (96%)	7 (4%)	30	61
42	j	119/126 (94%)	105 (88%)	14 (12%)	5	21
43	k	91/116 (78%)	83 (91%)	8 (9%)	10	34
44	l	124/147 (84%)	108 (87%)	16 (13%)	4	17
45	m	104/105 (99%)	98 (94%)	6 (6%)	20	52
46	n	105/107 (98%)	93 (89%)	12 (11%)	5	22
47	o	86/90 (96%)	77 (90%)	9 (10%)	7	26
48	p	90/99 (91%)	83 (92%)	7 (8%)	12	40
49	q	102/103 (99%)	93 (91%)	9 (9%)	10	34
50	r	94/96 (98%)	87 (93%)	7 (7%)	13	42
51	s	83/84 (99%)	79 (95%)	4 (5%)	25	57
52	t	76/77 (99%)	67 (88%)	9 (12%)	5	21
53	u	65/65 (100%)	59 (91%)	6 (9%)	9	32
54	v	74/78 (95%)	70 (95%)	4 (5%)	22	54
55	w	57/65 (88%)	53 (93%)	4 (7%)	15	45
56	x	72/79 (91%)	67 (93%)	5 (7%)	15	46
57	y	65/66 (98%)	62 (95%)	3 (5%)	27	59
58	z	60/61 (98%)	55 (92%)	5 (8%)	11	37
All	All	5167/5432 (95%)	4702 (91%)	465 (9%)	13	33

All (465) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	17	GLU
6	6	19	LEU
6	6	20	LEU
6	6	24	LEU
6	6	36	LYS
7	7	29	ILE
7	7	30	PHE
7	7	31	ASP
7	7	35	LYS
7	7	38	ARG

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Mol	Chain	Res	Type
7	7	42	LEU
7	7	45	ARG
7	7	52	TRP
7	7	59	ARG
7	7	63	GLN
7	7	68	LEU
7	7	74	THR
7	7	81	ASP
7	7	101	LYS
7	7	105	GLU
7	7	111	LEU
7	7	119	LEU
7	7	121	ASN
7	7	128	ASN
7	7	131	LEU
7	7	145	TRP
7	7	149	LEU
7	7	151	ARG
7	7	152	MET
7	7	158	GLU
7	7	160	GLN
7	7	174	GLU
7	7	177	ILE
7	7	182	ILE
7	7	183	LEU
7	7	185	LYS
7	7	188	ASN
7	7	192	LEU
7	7	196	GLU
7	7	204	ARG
7	7	222	GLU
7	7	227	VAL
7	7	236	LYS
7	7	240	LEU
7	7	274	THR
7	7	279	ARG
7	7	290	LYS
7	7	296	LEU
7	7	302	LYS
7	7	322	SER
7	7	323	GLN
7	7	324	ILE

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Mol	Chain	Res	Type
7	7	325	ARG
7	7	331	LYS
7	7	333	TYR
7	7	338	ARG
7	7	368	ARG
8	B	13	ARG
8	B	40	SER
8	B	52	ARG
8	B	94	VAL
8	B	125	LYS
8	B	130	LEU
8	B	141	VAL
8	B	153	GLN
8	B	156	ARG
8	B	174	LEU
8	B	180	GLU
8	B	192	LEU
8	B	203	ARG
8	B	204	VAL
8	B	242	LYS
8	B	244	PRO
8	B	257	THR
8	B	258	ARG
8	B	271	ARG
9	C	1	MET
9	C	2	ILE
9	C	13	ARG
9	C	46	ARG
9	C	59	ARG
9	C	149	ASN
10	D	15	SER
10	D	57	LYS
10	D	69	ARG
10	D	72	SER
10	D	73	ILE
10	D	77	ILE
10	D	108	ILE
10	D	109	LEU
10	D	122	GLU
10	D	149	ILE
10	D	152	GLU
10	D	195	GLN

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Mol	Chain	Res	Type
11	E	10	ASP
11	E	40	VAL
11	E	47	LYS
11	E	49	LEU
11	E	57	LEU
11	E	80	ARG
11	E	95	ARG
11	E	112	ARG
11	E	117	LEU
11	E	122	PHE
11	E	123	ASP
11	E	133	ARG
11	E	140	GLU
11	E	141	ILE
11	E	152	LEU
11	E	163	ASP
11	E	175	PHE
12	F	6	LYS
12	F	20	ASN
12	F	39	ASP
12	F	50	LEU
12	F	95	ARG
12	F	117	LEU
12	F	141	ILE
12	F	152	ARG
13	G	15	LEU
13	G	18	GLN
13	G	20	ASN
13	G	33	GLN
13	G	35	LYS
13	G	40	THR
13	G	41	LYS
13	G	44	ILE
13	G	51	ARG
13	G	66	ASN
13	G	71	LYS
13	G	72	ILE
13	G	77	THR
13	G	97	ARG
13	G	101	ASP
13	G	114	GLU
13	G	127	GLU

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Mol	Chain	Res	Type
14	H	3	LEU
14	H	31	ARG
14	H	34	THR
14	H	37	LYS
14	H	40	GLU
14	H	54	VAL
14	H	57	ASN
14	H	109	LYS
14	H	122	GLN
14	H	123	ILE
15	I	10	LEU
15	I	11	GLN
15	I	38	CYS
15	I	41	PHE
15	I	42	ASN
15	I	63	ASP
15	I	78	LEU
16	J	4	PHE
16	J	12	LYS
16	J	19	ASP
16	J	40	HIS
16	J	124	VAL
16	J	128	ASN
16	J	140	LEU
17	K	7	MET
17	K	8	LEU
17	K	17	ARG
17	K	49	ARG
17	K	53	LYS
17	K	58	LEU
17	K	70	ARG
17	K	80	ASP
17	K	97	THR
17	K	104	THR
17	K	105	ARG
18	L	4	ASN
18	L	7	SER
18	L	46	VAL
18	L	48	ARG
18	L	59	ARG
18	L	78	ARG
18	L	84	LYS

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Mol	Chain	Res	Type
18	L	91	ASP
19	M	2	LEU
19	M	3	GLN
19	M	25	ASP
19	M	47	GLU
19	M	84	LYS
19	M	100	LYS
19	M	110	GLU
19	M	119	LEU
19	M	132	THR
19	M	133	LYS
20	N	17	ARG
20	N	20	MET
20	N	24	MET
20	N	43	GLU
20	N	51	LEU
20	N	59	SER
20	N	63	ARG
20	N	69	ARG
21	O	19	GLN
21	O	31	THR
21	O	48	LEU
21	O	67	ASN
21	O	98	GLN
21	O	116	GLN
22	P	7	GLN
22	P	10	GLN
22	P	11	GLU
22	P	21	ARG
22	P	26	VAL
22	P	39	ARG
22	P	81	VAL
22	P	89	ARG
22	P	102	GLU
22	P	110	ILE
22	P	111	LYS
22	P	113	ARG
23	Q	11	ARG
23	Q	16	LYS
23	Q	18	LEU
23	Q	51	ARG
23	Q	71	GLN

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Mol	Chain	Res	Type
23	Q	87	SER
23	Q	91	ASP
24	R	6	GLN
24	R	10	LYS
24	R	14	VAL
24	R	78	ARG
24	R	86	GLN
24	R	95	ASP
25	S	1	MET
25	S	4	ILE
25	S	11	ARG
25	S	41	LYS
25	S	68	ASP
25	S	69	LEU
25	S	81	SER
25	S	95	ARG
26	T	6	ARG
26	T	12	ARG
26	T	25	GLU
26	T	33	LYS
26	T	78	SER
26	T	87	LEU
26	T	93	LEU
27	U	7	ARG
27	U	10	GLU
27	U	15	THR
27	U	52	LEU
27	U	68	SER
27	U	81	ASP
27	U	88	GLU
28	V	1	MET
28	V	40	ILE
28	V	69	GLU
29	W	10	THR
29	W	77	ARG
30	X	18	ARG
30	X	35	SER
30	X	48	THR
30	X	50	ARG
30	X	54	LYS
30	X	56	MET
30	X	60	ASP

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Mol	Chain	Res	Type
31	Y	7	ARG
31	Y	18	LEU
31	Y	57	LEU
31	Y	58	ASN
31	Y	60	LYS
32	Z	5	ILE
32	Z	10	THR
32	Z	11	ARG
32	Z	24	LEU
32	Z	36	VAL
32	Z	41	THR
32	Z	45	ARG
32	Z	49	ASN
32	Z	57	VAL
33	a	37	CYS
33	a	45	THR
33	a	59	ARG
34	b	8	PRO
34	b	9	THR
34	b	11	SER
34	b	18	SER
34	b	26	THR
34	b	36	GLU
34	b	40	ARG
34	b	52	ARG
35	c	34	LEU
35	c	47	VAL
35	c	53	LYS
35	c	55	LYS
36	d	19	ARG
36	d	22	MET
36	d	24	THR
36	d	25	LYS
36	d	31	LEU
36	d	42	LEU
36	d	44	VAL
37	e	3	LYS
37	e	30	ARG
37	e	31	HIS
37	e	55	LEU
38	f	3	VAL
38	f	7	VAL

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Mol	Chain	Res	Type
38	f	11	CYS
38	f	26	ILE
38	f	27	CYS
39	g	4	VAL
39	g	5	SER
39	g	23	TRP
39	g	105	LYS
39	g	128	LYS
39	g	129	LEU
39	g	132	LYS
39	g	135	LEU
39	g	212	LEU
39	g	227	GLN
40	h	14	ILE
40	h	16	LYS
40	h	89	LYS
40	h	119	SER
40	h	154	SER
40	h	164	ARG
40	h	165	THR
40	h	172	ARG
40	h	175	LEU
40	h	176	HIS
40	h	178	LEU
40	h	179	ARG
40	h	200	VAL
41	i	5	LEU
41	i	47	ARG
41	i	95	GLU
41	i	104	ARG
41	i	116	GLN
41	i	138	SER
41	i	143	VAL
42	j	15	LEU
42	j	22	SER
42	j	34	THR
42	j	60	ILE
42	j	65	GLU
42	j	70	ASN
42	j	82	GLN
42	j	94	VAL
42	j	114	VAL

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Mol	Chain	Res	Type
42	j	115	LEU
42	j	123	VAL
42	j	138	ARG
42	j	149	SER
42	j	165	LEU
43	k	7	VAL
43	k	16	GLU
43	k	24	ARG
43	k	38	ARG
43	k	44	ARG
43	k	54	LEU
43	k	79	ARG
43	k	86	ARG
44	l	7	ILE
44	l	9	GLN
44	l	11	LYS
44	l	17	LYS
44	l	21	GLU
44	l	23	LEU
44	l	27	VAL
44	l	50	LEU
44	l	68	ASN
44	l	79	ARG
44	l	91	VAL
44	l	109	ARG
44	l	123	GLU
44	l	126	ASP
44	l	142	HIS
44	l	146	GLU
45	m	9	ASP
45	m	12	THR
45	m	80	ARG
45	m	96	MET
45	m	104	VAL
45	m	107	SER
46	n	12	ARG
46	n	25	ASN
46	n	27	LYS
46	n	56	ASP
46	n	60	LYS
46	n	61	LEU
46	n	63	LEU

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Mol	Chain	Res	Type
46	n	85	ARG
46	n	98	LEU
46	n	118	LEU
46	n	123	ARG
46	n	130	ARG
47	o	5	ARG
47	o	17	LEU
47	o	24	GLU
47	o	25	ILE
47	o	27	GLU
47	o	37	ARG
47	o	57	VAL
47	o	58	ASN
47	o	63	ASP
48	p	13	ARG
48	p	15	GLN
48	p	18	ASP
48	p	56	ARG
48	p	100	LEU
48	p	107	ILE
48	p	109	ASN
49	q	12	ARG
49	q	21	VAL
49	q	24	LEU
49	q	30	LYS
49	q	62	GLU
49	q	64	THR
49	q	74	LEU
49	q	86	ARG
49	q	102	LEU
50	r	11	ASP
50	r	16	VAL
50	r	25	VAL
50	r	29	ARG
50	r	59	GLU
50	r	68	ASP
50	r	93	ARG
51	s	45	VAL
51	s	46	LEU
51	s	89	MET
51	s	92	GLU
52	t	17	ARG

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Mol	Chain	Res	Type
52	t	39	LEU
52	t	40	GLN
52	t	64	ARG
52	t	66	LEU
52	t	67	LEU
52	t	80	GLN
52	t	84	ARG
52	t	85	LEU
53	u	2	VAL
53	u	3	THR
53	u	18	GLN
53	u	19	VAL
53	u	20	VAL
53	u	35	ARG
54	v	14	SER
54	v	22	VAL
54	v	75	LEU
54	v	81	LYS
55	w	14	THR
55	w	66	SER
55	w	71	THR
55	w	74	HIS
56	x	21	LYS
56	x	33	THR
56	x	49	ILE
56	x	69	HIS
56	x	81	ARG
57	y	43	ASP
57	y	48	GLN
57	y	54	MET
58	z	4	ILE
58	z	31	GLU
58	z	55	ARG
58	z	62	ARG
58	z	67	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
12	F	22	GLN
30	X	36	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2897/2904 (99%)	619 (21%)	91 (3%)
2	2	1528/1534 (99%)	332 (21%)	39 (2%)
3	3	119/120 (99%)	20 (16%)	1 (0%)
4	4	4/18 (22%)	1 (25%)	0
5	5	73/78 (93%)	24 (32%)	7 (9%)
All	All	4621/4654 (99%)	996 (21%)	138 (2%)

All (996) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	23	G
1	1	34	U
1	1	35	G
1	1	45	G
1	1	46	G
1	1	58	G
1	1	60	G
1	1	62	U
1	1	63	A
1	1	71	A
1	1	72	U
1	1	74	A
1	1	75	G
1	1	80	G
1	1	83	A
1	1	84	A
1	1	85	G
1	1	101	A
1	1	102	U
1	1	103	A
1	1	118	A
1	1	119	A
1	1	120	U
1	1	131	A
1	1	137	U
1	1	138	U
1	1	139	U
1	1	140	C
1	1	141	G

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Mol	Chain	Res	Type
1	1	142	A
1	1	143	C
1	1	144	A
1	1	149	A
1	1	163	C
1	1	165	A
1	1	181	A
1	1	186	G
1	1	196	A
1	1	199	A
1	1	200	U
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	241	A
1	1	248	G
1	1	249	C
1	1	264	C
1	1	265	A
1	1	266	G
1	1	271	G
1	1	272	A
1	1	275	C
1	1	276	U
1	1	278	A
1	1	279	A
1	1	285	G
1	1	291	G
1	1	303	G
1	1	311	A
1	1	312	G
1	1	324	A
1	1	327	G
1	1	329	G
1	1	330	A
1	1	353	C
1	1	361	G
1	1	362	A
1	1	366	C
1	1	371	A
1	1	372	G

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Mol	Chain	Res	Type
1	1	386	G
1	1	396	G
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	416	U
1	1	417	C
1	1	420	C
1	1	424	G
1	1	450	G
1	1	451	U
1	1	455	C
1	1	457	A
1	1	459	U
1	1	467	G
1	1	477	A
1	1	480	A
1	1	481	G
1	1	490	C
1	1	491	G
1	1	501	A
1	1	503	A
1	1	504	A
1	1	505	A
1	1	509	C
1	1	519	U
1	1	522	A
1	1	530	G
1	1	531	C
1	1	532	A
1	1	533	G
1	1	543	G
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	572	A
1	1	573	U
1	1	575	A

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Mol	Chain	Res	Type
1	1	586	A
1	1	603	A
1	1	609	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	618	G
1	1	620	G
1	1	621	A
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G
1	1	654	A
1	1	659	G
1	1	664	G
1	1	668	A
1	1	670	A
1	1	685	A
1	1	686	U
1	1	701	G
1	1	709	U
1	1	710	U
1	1	716	A
1	1	717	C
1	1	724	U
1	1	730	A
1	1	735	A
1	1	738	G
1	1	745	1MG
1	1	746	PSU
1	1	747	5MU
1	1	757	G
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	786	C

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Mol	Chain	Res	Type
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	831	G
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	878	A
1	1	881	G
1	1	883	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U
1	1	896	A
1	1	897	C
1	1	899	A
1	1	907	G
1	1	910	A
1	1	914	G
1	1	931	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G
1	1	961	C
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C

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Mol	Chain	Res	Type
1	1	1022	G
1	1	1023	U
1	1	1026	G
1	1	1033	U
1	1	1041	G
1	1	1043	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1060	U
1	1	1061	U
1	1	1063	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1073	A
1	1	1074	G
1	1	1076	C
1	1	1079	C
1	1	1080	A
1	1	1081	U
1	1	1082	U
1	1	1083	U
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1094	U
1	1	1095	A
1	1	1096	A
1	1	1097	U
1	1	1109	C
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1130	U
1	1	1132	U
1	1	1133	A

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Mol	Chain	Res	Type
1	1	1134	A
1	1	1135	C
1	1	1137	G
1	1	1142	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1178	C
1	1	1179	G
1	1	1180	U
1	1	1186	G
1	1	1206	G
1	1	1210	G
1	1	1227	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1248	G
1	1	1253	A
1	1	1256	G
1	1	1265	A
1	1	1266	G
1	1	1268	A
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1275	A
1	1	1287	A
1	1	1300	G
1	1	1301	A
1	1	1302	A
1	1	1321	A
1	1	1330	C
1	1	1345	C
1	1	1352	U
1	1	1363	C
1	1	1365	A
1	1	1368	G

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Mol	Chain	Res	Type
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1387	A
1	1	1395	A
1	1	1406	U
1	1	1408	G
1	1	1409	U
1	1	1414	C
1	1	1415	U
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1420	A
1	1	1428	C
1	1	1434	A
1	1	1452	G
1	1	1453	A
1	1	1455	G
1	1	1459	G
1	1	1460	U
1	1	1478	G
1	1	1482	G
1	1	1490	A
1	1	1491	G
1	1	1493	C
1	1	1496	A
1	1	1497	U
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1520	U
1	1	1529	G
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U

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Mol	Chain	Res	Type
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1570	A
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1583	A
1	1	1584	U
1	1	1589	U
1	1	1590	A
1	1	1593	A
1	1	1608	A
1	1	1609	A
1	1	1610	A
1	1	1613	G
1	1	1616	A
1	1	1619	G
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1654	A
1	1	1663	G
1	1	1664	A
1	1	1674	G
1	1	1677	A
1	1	1695	G
1	1	1703	G
1	1	1713	A
1	1	1714	U
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1733	G
1	1	1738	G
1	1	1742	U
1	1	1746	A
1	1	1750	G
1	1	1757	A
1	1	1758	U

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Mol	Chain	Res	Type
1	1	1764	C
1	1	1773	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1842	G
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1859	U
1	1	1869	G
1	1	1870	C
1	1	1872	A
1	1	1873	G
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1913	A
1	1	1914	C
1	1	1918	A
1	1	1919	A
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1938	A
1	1	1955	U
1	1	1960	A
1	1	1963	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1982	U
1	1	1991	U
1	1	1992	G
1	1	1993	U

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Mol	Chain	Res	Type
1	1	1997	C
1	1	2002	G
1	1	2020	A
1	1	2022	U
1	1	2023	C
1	1	2027	G
1	1	2033	A
1	1	2043	C
1	1	2049	G
1	1	2051	A
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2077	A
1	1	2093	G
1	1	2097	A
1	1	2099	U
1	1	2100	G
1	1	2103	C
1	1	2107	G
1	1	2108	A
1	1	2110	G
1	1	2111	U
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2121	G
1	1	2122	U
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2131	U
1	1	2132	U
1	1	2133	G

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Mol	Chain	Res	Type
1	1	2134	A
1	1	2139	U
1	1	2141	G
1	1	2146	C
1	1	2147	A
1	1	2154	A
1	1	2157	G
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2178	C
1	1	2182	U
1	1	2183	A
1	1	2185	U
1	1	2186	G
1	1	2187	U
1	1	2188	U
1	1	2189	U
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2203	U
1	1	2204	G
1	1	2209	G
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2213	U
1	1	2220	U
1	1	2225	A
1	1	2226	C
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2244	U

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Mol	Chain	Res	Type
1	1	2250	G
1	1	2251	OMG
1	1	2267	A
1	1	2268	A
1	1	2273	A
1	1	2275	C
1	1	2278	A
1	1	2282	G
1	1	2283	C
1	1	2287	A
1	1	2288	A
1	1	2294	G
1	1	2297	A
1	1	2305	U
1	1	2308	G
1	1	2309	A
1	1	2311	A
1	1	2314	A
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2339	C
1	1	2345	G
1	1	2347	C
1	1	2352	A
1	1	2361	G
1	1	2372	U
1	1	2376	A
1	1	2379	G
1	1	2382	G
1	1	2383	G
1	1	2385	C
1	1	2396	G
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2410	G
1	1	2423	U
1	1	2424	C
1	1	2425	A

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Mol	Chain	Res	Type
1	1	2426	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2434	A
1	1	2435	A
1	1	2436	G
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G
1	1	2473	U
1	1	2474	U
1	1	2476	A
1	1	2478	A
1	1	2491	U
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2512	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2525	G
1	1	2529	G
1	1	2534	A
1	1	2535	G
1	1	2547	A
1	1	2552	OMU
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2585	U
1	1	2586	U
1	1	2602	A
1	1	2603	G
1	1	2609	U

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Mol	Chain	Res	Type
1	1	2610	C
1	1	2613	U
1	1	2623	G
1	1	2629	U
1	1	2663	G
1	1	2671	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2722	G
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2757	A
1	1	2758	A
1	1	2762	C
1	1	2765	A
1	1	2777	G
1	1	2791	G
1	1	2796	U
1	1	2797	U
1	1	2798	U
1	1	2799	A
1	1	2801	G
1	1	2818	U
1	1	2820	A
1	1	2821	A
1	1	2824	C
1	1	2825	G
1	1	2849	U
1	1	2854	G
1	1	2859	G
1	1	2861	U
1	1	2867	G
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2891	U
1	1	2902	C

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Mol	Chain	Res	Type
2	2	4	U
2	2	5	U
2	2	8	A
2	2	9	G
2	2	22	G
2	2	29	U
2	2	32	A
2	2	38	G
2	2	39	G
2	2	41	G
2	2	47	C
2	2	48	C
2	2	51	A
2	2	52	C
2	2	54	C
2	2	58	C
2	2	68	G
2	2	69	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	74	A
2	2	76	G
2	2	82	G
2	2	83	C
2	2	84	U
2	2	87	C
2	2	90	C
2	2	94	G
2	2	95	C
2	2	96	U
2	2	108	G
2	2	116	A
2	2	120	A
2	2	121	U
2	2	122	G
2	2	128	G
2	2	131	A
2	2	141	G
2	2	144	G
2	2	147	G
2	2	149	A

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Mol	Chain	Res	Type
2	2	160	A
2	2	161	A
2	2	164	G
2	2	173	U
2	2	174	A
2	2	181	A
2	2	182	A
2	2	196	A
2	2	197	A
2	2	198	G
2	2	204	G
2	2	208	U
2	2	209	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	214	C
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	262	A
2	2	266	G
2	2	267	C
2	2	271	C
2	2	279	A
2	2	280	C
2	2	289	G
2	2	299	G
2	2	306	A
2	2	316	C
2	2	319	G
2	2	321	A
2	2	328	C
2	2	329	A
2	2	332	G
2	2	341	C
2	2	347	G
2	2	352	C
2	2	354	G
2	2	355	C
2	2	367	U

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Mol	Chain	Res	Type
2	2	372	C
2	2	373	A
2	2	376	G
2	2	382	A
2	2	384	G
2	2	388	G
2	2	389	A
2	2	392	C
2	2	393	A
2	2	397	A
2	2	406	G
2	2	411	A
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	436	C
2	2	439	U
2	2	446	G
2	2	451	A
2	2	457	G
2	2	458	U
2	2	460	A
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	469	C
2	2	478	A
2	2	479	U
2	2	480	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	495	A
2	2	496	A
2	2	497	G
2	2	511	C

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Mol	Chain	Res	Type
2	2	514	C
2	2	517	G
2	2	518	C
2	2	519	C
2	2	523	A
2	2	526	C
2	2	527	7MG
2	2	528	C
2	2	531	U
2	2	532	A
2	2	533	A
2	2	536	C
2	2	537	G
2	2	539	A
2	2	547	A
2	2	559	A
2	2	567	G
2	2	568	G
2	2	570	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	579	A
2	2	596	A
2	2	607	A
2	2	628	G
2	2	633	G
2	2	642	A
2	2	649	A
2	2	650	G
2	2	653	U
2	2	654	G
2	2	665	A
2	2	700	G
2	2	702	A
2	2	705	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	742	G

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Mol	Chain	Res	Type
2	2	747	A
2	2	748	G
2	2	755	G
2	2	760	G
2	2	777	A
2	2	793	U
2	2	794	A
2	2	799	G
2	2	802	A
2	2	813	U
2	2	814	A
2	2	815	A
2	2	817	C
2	2	828	U
2	2	832	G
2	2	841	C
2	2	844	G
2	2	845	A
2	2	846	G
2	2	849	G
2	2	872	A
2	2	874	G
2	2	876	C
2	2	885	G
2	2	887	G
2	2	902	G
2	2	914	A
2	2	916	U
2	2	928	G
2	2	934	C
2	2	935	A
2	2	936	C
2	2	945	G
2	2	958	A
2	2	960	U
2	2	966	2MG
2	2	967	5MC
2	2	968	A
2	2	969	A
2	2	972	C
2	2	975	A
2	2	976	G

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Mol	Chain	Res	Type
2	2	978	A
2	2	984	C
2	2	987	G
2	2	989	U
2	2	991	U
2	2	992	U
2	2	993	G
2	2	996	A
2	2	1004	A
2	2	1005	A
2	2	1008	U
2	2	1009	U
2	2	1017	U
2	2	1018	G
2	2	1021	A
2	2	1024	G
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1037	C
2	2	1042	A
2	2	1043	G
2	2	1044	A
2	2	1046	A
2	2	1065	U
2	2	1074	G
2	2	1085	U
2	2	1094	G
2	2	1095	U
2	2	1099	G
2	2	1101	A
2	2	1124	G
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1142	G
2	2	1143	G

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Mol	Chain	Res	Type
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1171	A
2	2	1174	G
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1200	C
2	2	1206	G
2	2	1211	U
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1225	A
2	2	1226	C
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1248	A
2	2	1256	A
2	2	1257	A
2	2	1275	A
2	2	1278	G
2	2	1279	G
2	2	1280	A
2	2	1285	A
2	2	1286	U
2	2	1287	A
2	2	1299	A
2	2	1300	G
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C

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Mol	Chain	Res	Type
2	2	1320	C
2	2	1332	A
2	2	1338	G
2	2	1340	A
2	2	1346	A
2	2	1347	G
2	2	1348	U
2	2	1353	G
2	2	1363	A
2	2	1370	G
2	2	1378	C
2	2	1379	G
2	2	1381	U
2	2	1383	C
2	2	1396	A
2	2	1397	C
2	2	1403	C
2	2	1414	U
2	2	1419	G
2	2	1429	A
2	2	1441	A
2	2	1446	A
2	2	1447	A
2	2	1448	C
2	2	1452	C
2	2	1453	G
2	2	1475	G
2	2	1480	A
2	2	1492	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	15	A
3	3	16	G
3	3	17	C

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Mol	Chain	Res	Type
3	3	21	G
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	64	G
3	3	66	A
3	3	67	G
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	105	G
3	3	109	A
3	3	120	U
4	4	15	A
5	5	3	G
5	5	5	G
5	5	8	4SU
5	5	9	G
5	5	13	A
5	5	15	C
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	20	H2U
5	5	21	A
5	5	22	G
5	5	25	C
5	5	31	G
5	5	47	U
5	5	48	C
5	5	49	G
5	5	55	PSU
5	5	56	C
5	5	57	A
5	5	59	A
5	5	69	C
5	5	74	C

All (138) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	62	U
1	1	101	A
1	1	138	U
1	1	140	C
1	1	196	A
1	1	199	A
1	1	271	G
1	1	369	U
1	1	404	A
1	1	446	G
1	1	503	A
1	1	546	U
1	1	548	G
1	1	571	U
1	1	573	U
1	1	603	A
1	1	614	A
1	1	620	G
1	1	682	G
1	1	752	A
1	1	764	A
1	1	784	G
1	1	805	G
1	1	883	G
1	1	892	A
1	1	894	U
1	1	895	U
1	1	896	A
1	1	984	A
1	1	995	C
1	1	1061	U
1	1	1063	G
1	1	1064	C
1	1	1070	A
1	1	1082	U
1	1	1094	U
1	1	1109	C
1	1	1110	G
1	1	1128	G
1	1	1133	A
1	1	1142	A
1	1	1173	U
1	1	1253	A

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Mol	Chain	Res	Type
1	1	1272	A
1	1	1275	A
1	1	1320	C
1	1	1344	U
1	1	1379	U
1	1	1395	A
1	1	1396	U
1	1	1415	U
1	1	1490	A
1	1	1497	U
1	1	1509	A
1	1	1583	A
1	1	1584	U
1	1	1608	A
1	1	1647	U
1	1	1913	A
1	1	1918	A
1	1	1923	U
1	1	1962	5MC
1	1	2062	A
1	1	2146	C
1	1	2162	G
1	1	2193	G
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2225	A
1	1	2244	U
1	1	2250	G
1	1	2275	C
1	1	2282	G
1	1	2296	U
1	1	2324	U
1	1	2326	C
1	1	2382	G
1	1	2425	A
1	1	2447	G
1	1	2473	U
1	1	2506	U
1	1	2572	A
1	1	2602	A
1	1	2610	C

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Mol	Chain	Res	Type
1	1	2756	U
1	1	2796	U
1	1	2797	U
1	1	2798	U
1	1	2820	A
1	1	2873	A
2	2	70	U
2	2	121	U
2	2	181	A
2	2	183	C
2	2	197	A
2	2	209	U
2	2	305	G
2	2	421	U
2	2	428	G
2	2	429	U
2	2	481	G
2	2	496	A
2	2	517	G
2	2	531	U
2	2	559	A
2	2	575	G
2	2	641	U
2	2	653	U
2	2	702	A
2	2	733	G
2	2	793	U
2	2	966	2MG
2	2	967	5MC
2	2	991	U
2	2	992	U
2	2	1145	A
2	2	1196	A
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1225	A
2	2	1299	A
2	2	1346	A
2	2	1363	A
2	2	1396	A
2	2	1403	C

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Mol	Chain	Res	Type
2	2	1407	5MC
2	2	1447	A
2	2	1516	2MG
3	3	48	U
5	5	8	4SU
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	47	U
5	5	60	U

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

40 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	$\#\|Z\| > 2$
2	4OC	2	1402	2	20,23,24	0.68	0	26,32,35	1.59	3 (11%)
2	7MG	2	527	2	22,26,27	1.46	4 (18%)	29,39,42	2.99	10 (34%)
2	2MG	2	966	2	18,26,27	1.17	3 (16%)	16,38,41	2.07	3 (18%)
1	PSU	1	746	59,1	18,21,22	2.01	1 (5%)	22,30,33	2.10	3 (13%)
2	MA6	2	1519	2	18,26,27	0.65	0	19,38,41	0.85	1 (5%)
1	5MU	1	747	1	19,22,23	0.75	1 (5%)	28,32,35	1.08	4 (14%)
1	PSU	1	1911	1	18,21,22	0.83	1 (5%)	22,30,33	1.11	2 (9%)
1	2MG	1	2445	1	18,26,27	1.31	3 (16%)	16,38,41	1.50	3 (18%)
1	PSU	1	1917	1	18,21,22	1.23	2 (11%)	22,30,33	1.34	4 (18%)
1	OMC	1	2498	59,1	19,22,23	1.17	2 (10%)	26,31,34	1.61	3 (11%)
1	2MA	1	2503	59,1	17,25,26	1.14	3 (17%)	17,37,40	3.15	6 (35%)
1	PSU	1	2605	1	18,21,22	1.90	1 (5%)	22,30,33	1.69	3 (13%)
5	5MU	5	54	5	19,22,23	0.67	0	28,32,35	0.97	2 (7%)
1	OMG	1	2251	1,5	18,26,27	1.29	4 (22%)	19,38,41	3.06	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	PSU	2	516	59,2	18,21,22	1.55	1 (5%)	22,30,33	1.62	2 (9%)
1	PSU	1	2457	1	18,21,22	2.22	1 (5%)	22,30,33	1.42	4 (18%)
1	6MZ	1	1618	1	18,25,26	0.83	1 (5%)	16,36,39	1.72	2 (12%)
1	PSU	1	2504	1	18,21,22	1.86	1 (5%)	22,30,33	1.64	3 (13%)
2	MA6	2	1518	2	18,26,27	0.59	0	19,38,41	0.83	1 (5%)
5	H2U	5	20	5	18,21,22	0.65	0	21,30,33	1.92	4 (19%)
1	2MG	1	1835	1	18,26,27	1.20	3 (16%)	16,38,41	1.74	3 (18%)
2	UR3	2	1498	2	19,22,23	0.81	0	26,32,35	1.02	1 (3%)
2	2MG	2	1516	2	18,26,27	1.20	3 (16%)	16,38,41	1.73	2 (12%)
1	3TD	1	1915	1	18,22,23	2.41	6 (33%)	22,32,35	1.85	4 (18%)
1	6MZ	1	2030	1	18,25,26	0.87	0	16,36,39	2.24	4 (25%)
5	4SU	5	8	5	18,21,22	1.55	3 (16%)	26,30,33	2.78	12 (46%)
2	5MC	2	1407	2	18,22,23	0.84	1 (5%)	26,32,35	1.29	3 (11%)
5	PSU	5	55	5	18,21,22	1.79	1 (5%)	22,30,33	1.60	3 (13%)
1	1MG	1	745	1	18,26,27	1.83	3 (16%)	19,39,42	2.19	4 (21%)
49	0TD	q	89	49	7,9,10	6.74	5 (71%)	6,11,13	4.11	2 (33%)
1	OMU	1	2552	1	19,22,23	0.53	0	26,31,34	0.81	1 (3%)
5	8AN	5	76	59,60,1,5	19,24,25	0.67	0	13,35,38	0.88	1 (7%)
2	2MG	2	1207	2	18,26,27	1.64	4 (22%)	16,38,41	1.11	1 (6%)
1	G7M	1	2069	1	20,26,27	1.82	2 (10%)	17,39,42	2.08	4 (23%)
1	PSU	1	955	1	18,21,22	1.87	1 (5%)	22,30,33	1.66	3 (13%)
1	5MC	1	1962	1	18,22,23	0.85	1 (5%)	26,32,35	1.52	3 (11%)
5	4OC	5	32	5	20,23,24	0.58	0	26,32,35	1.23	2 (7%)
1	PSU	1	2580	1	18,21,22	1.88	1 (5%)	22,30,33	1.37	3 (13%)
1	5MU	1	1939	1	19,22,23	0.79	1 (5%)	28,32,35	1.05	3 (10%)
2	5MC	2	967	2	18,22,23	0.76	1 (5%)	26,32,35	1.30	3 (11%)

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
2	4OC	2	1402	2	-	1/9/29/30	0/2/2/2
2	7MG	2	527	2	-	3/7/37/38	0/3/3/3
2	2MG	2	966	2	-	4/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	746	59,1	-	2/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	6/7/29/30	0/3/3/3
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	59,1	-	2/9/27/28	0/2/2/2
1	2MA	1	2503	59,1	-	1/3/25/26	0/3/3/3
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
5	5MU	5	54	5	-	0/7/25/26	0/2/2/2
1	OMG	1	2251	1,5	-	4/5/27/28	0/3/3/3
2	PSU	2	516	59,2	-	2/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	1/7/25/26	0/2/2/2
1	6MZ	1	1618	1	-	4/5/27/28	0/3/3/3
1	PSU	1	2504	1	-	1/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
5	H2U	5	20	5	-	4/7/38/39	0/2/2/2
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	3TD	1	1915	1	-	2/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	1/5/27/28	0/3/3/3
5	4SU	5	8	5	-	3/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
5	PSU	5	55	5	-	3/7/25/26	0/2/2/2
1	1MG	1	745	1	-	2/3/25/26	0/3/3/3
49	0TD	q	89	49	-	2/7/12/14	-
1	OMU	1	2552	1	-	2/9/27/28	0/2/2/2
5	8AN	5	76	59,60,1,5	-	1/3/25/26	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
1	G7M	1	2069	1	-	2/3/25/26	0/3/3/3
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	1/7/25/26	0/2/2/2
5	4OC	5	32	5	-	0/9/29/30	0/2/2/2
1	PSU	1	2580	1	-	2/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	5/7/25/26	0/2/2/2

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	q	89	0TD	CB-SB	-16.93	1.65	1.82
1	1	2457	PSU	C2'-C1'	-9.03	1.42	1.53
1	1	746	PSU	C2'-C1'	-8.32	1.42	1.53
1	1	2605	PSU	C2'-C1'	-7.74	1.43	1.53
1	1	2504	PSU	C2'-C1'	-7.60	1.43	1.53
1	1	2580	PSU	C2'-C1'	-7.58	1.43	1.53
5	5	55	PSU	C2'-C1'	-7.36	1.44	1.53
1	1	955	PSU	C2'-C1'	-7.21	1.44	1.53
1	1	2069	G7M	C2'-C1'	-6.64	1.43	1.53
2	2	516	PSU	C2'-C1'	-6.32	1.45	1.53
1	1	1915	3TD	C1'-C5	-6.19	1.36	1.50
1	1	1915	3TD	C6-C5	-5.83	1.28	1.35
1	1	745	1MG	C2'-C1'	-5.76	1.45	1.53
5	5	8	4SU	C4-S4	-4.52	1.59	1.68
1	1	2498	OMC	C3'-C2'	-3.75	1.44	1.52
2	2	1207	2MG	C2'-C1'	-3.61	1.48	1.53
2	2	527	7MG	C4-N9	-3.41	1.33	1.37
49	q	89	0TD	CA-N	-3.17	1.37	1.47
1	1	745	1MG	C5-C6	-3.08	1.38	1.47
1	1	2445	2MG	C5-C6	-3.02	1.41	1.47
1	1	1835	2MG	C5-C6	-3.02	1.41	1.47
2	2	1207	2MG	C6-N1	2.89	1.42	1.37
1	1	1915	3TD	O5'-C5'	2.87	1.51	1.44
1	1	1915	3TD	O2-C2	-2.83	1.17	1.23
1	1	1915	3TD	C4-N3	-2.73	1.34	1.40
5	5	8	4SU	C5-C4	-2.71	1.39	1.42
1	1	1962	5MC	C2'-C1'	-2.71	1.44	1.53
2	2	1516	2MG	C5-C6	-2.71	1.41	1.47
49	q	89	0TD	OD2-CG	-2.70	1.21	1.30
2	2	1207	2MG	C5-C6	-2.69	1.41	1.47
49	q	89	0TD	CB-CG	-2.68	1.47	1.52
2	2	966	2MG	C5-C6	-2.64	1.42	1.47
2	2	527	7MG	C6-N1	-2.63	1.34	1.38
1	1	2251	OMG	C5-C6	-2.62	1.42	1.47
1	1	1911	PSU	C2'-C1'	-2.57	1.50	1.53
1	1	2445	2MG	C5-C4	-2.55	1.36	1.43
2	2	527	7MG	C5-C4	2.54	1.46	1.38
2	2	966	2MG	C6-N1	2.53	1.41	1.37
49	q	89	0TD	CSB-SB	-2.53	1.74	1.79
1	1	1939	5MU	C2'-C1'	-2.52	1.45	1.53
2	2	1516	2MG	C6-N1	2.52	1.41	1.37
1	1	2069	G7M	O2'-C2'	-2.52	1.37	1.43
1	1	2498	OMC	C2'-C1'	-2.49	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	8	4SU	C2-N1	2.46	1.42	1.38
2	2	527	7MG	C5-N7	-2.39	1.32	1.35
1	1	2503	2MA	C2'-C3'	-2.38	1.46	1.53
1	1	2251	OMG	C5-C4	-2.33	1.37	1.43
1	1	1835	2MG	C5-C4	-2.32	1.37	1.43
1	1	2251	OMG	C6-N1	2.30	1.41	1.37
1	1	747	5MU	C2'-C1'	-2.29	1.46	1.53
2	2	1516	2MG	C5-C4	-2.28	1.37	1.43
1	1	2251	OMG	C3'-C2'	-2.27	1.47	1.52
2	2	966	2MG	C5-C4	-2.25	1.37	1.43
2	2	1207	2MG	C5-C4	-2.22	1.37	1.43
1	1	1917	PSU	C2'-C1'	-2.19	1.50	1.53
1	1	2445	2MG	C6-N1	2.18	1.41	1.37
2	2	967	5MC	C2'-C1'	-2.10	1.46	1.53
1	1	1835	2MG	C6-N1	2.10	1.41	1.37
1	1	1618	6MZ	C2'-C1'	-2.09	1.50	1.53
1	1	1917	PSU	C6-N1	-2.06	1.32	1.36
2	2	1407	5MC	C2'-C1'	-2.05	1.46	1.53
1	1	2503	2MA	C5-C4	-2.05	1.37	1.43
1	1	2503	2MA	C8-N7	-2.04	1.31	1.35
1	1	745	1MG	C5-C4	-2.03	1.37	1.43
1	1	1915	3TD	C2-N1	2.01	1.39	1.37

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2251	OMG	O2'-C2'-C1'	10.15	129.21	109.09
2	2	527	7MG	N9-C4-N3	9.24	139.29	125.47
1	1	2503	2MA	C3'-C2'-C1'	-8.61	88.01	100.98
1	1	746	PSU	C3'-C2'-C1'	7.62	110.52	101.64
49	q	89	0TD	CB-CA-N	-7.52	93.08	109.10
1	1	1915	3TD	C6-C5-C4	6.86	122.96	118.22
5	5	8	4SU	C5-C4-S4	-6.64	115.91	124.47
2	2	1402	4OC	O3'-C3'-C2'	6.64	130.03	111.17
5	5	8	4SU	C5-C4-N3	6.64	120.84	114.69
5	5	8	4SU	C4-N3-C2	-6.42	121.11	127.34
1	1	2498	OMC	O3'-C3'-C2'	6.40	129.33	111.17
2	2	966	2MG	O3'-C3'-C4'	6.30	129.27	111.05
49	q	89	0TD	CSB-SB-CB	6.19	113.63	102.44
1	1	745	1MG	C3'-C2'-C1'	6.13	110.21	100.98
1	1	2030	6MZ	C3'-C2'-C1'	-5.99	91.96	100.98
2	2	527	7MG	O4'-C1'-N9	5.92	117.36	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1962	5MC	O3'-C3'-C4'	5.75	127.66	111.05
2	2	527	7MG	N9-C8-N7	-5.72	95.19	103.38
2	2	527	7MG	C5-C4-N3	-5.56	117.53	128.13
2	2	516	PSU	O2'-C2'-C3'	5.48	129.56	111.82
1	1	745	1MG	O3'-C3'-C4'	5.44	126.77	111.05
1	1	1618	6MZ	O3'-C3'-C4'	5.37	126.56	111.05
1	1	2503	2MA	O3'-C3'-C2'	5.28	128.91	111.82
1	1	2251	OMG	O3'-C3'-C2'	5.27	126.12	111.17
2	2	1516	2MG	O3'-C3'-C2'	5.19	128.59	111.82
5	5	55	PSU	O2'-C2'-C3'	5.05	128.14	111.82
1	1	2251	OMG	O3'-C3'-C4'	4.99	125.47	111.05
1	1	2030	6MZ	O3'-C3'-C4'	4.92	125.28	111.05
1	1	2504	PSU	O2'-C2'-C3'	4.77	127.27	111.82
1	1	2605	PSU	O2'-C2'-C3'	4.69	127.00	111.82
1	1	955	PSU	O2'-C2'-C3'	4.65	126.86	111.82
5	5	20	H2U	O2'-C2'-C3'	4.63	126.79	111.82
1	1	2605	PSU	O2'-C2'-C1'	4.59	122.17	111.23
2	2	527	7MG	C2-N3-C4	4.58	120.46	112.30
1	1	2503	2MA	O2'-C2'-C1'	4.51	127.50	110.85
2	2	1407	5MC	O3'-C3'-C2'	4.46	126.24	111.82
1	1	955	PSU	O2'-C2'-C1'	4.40	121.71	111.23
5	5	20	H2U	O3'-C3'-C4'	4.39	123.73	111.05
1	1	2069	G7M	C3'-C2'-C1'	-4.34	94.44	100.98
1	1	746	PSU	O2'-C2'-C3'	4.21	125.46	111.82
1	1	2069	G7M	O2'-C2'-C3'	4.18	125.33	111.82
5	5	20	H2U	O3'-C3'-C2'	4.15	125.24	111.82
1	1	2498	OMC	O2'-C2'-C1'	4.09	117.07	109.08
1	1	2503	2MA	O4'-C1'-C2'	4.09	112.90	106.93
1	1	1835	2MG	O3'-C3'-C4'	4.06	122.79	111.05
1	1	2069	G7M	O2'-C2'-C1'	4.06	125.83	110.85
1	1	2504	PSU	O2'-C2'-C1'	4.05	120.89	111.23
1	1	2457	PSU	O2'-C2'-C3'	3.92	124.52	111.82
5	5	55	PSU	O2'-C2'-C1'	3.91	120.55	111.23
5	5	32	4OC	O3'-C3'-C2'	3.85	122.10	111.17
1	1	2580	PSU	O2'-C2'-C3'	3.85	124.27	111.82
1	1	2503	2MA	O3'-C3'-C4'	3.84	122.17	111.05
5	5	8	4SU	C1'-N1-C2	3.83	124.50	117.57
2	2	967	5MC	O3'-C3'-C2'	3.69	123.77	111.82
5	5	20	H2U	O2'-C2'-C1'	3.62	122.14	110.02
1	1	2251	OMG	C3'-C2'-C1'	3.62	109.69	102.89
2	2	516	PSU	O2'-C2'-C1'	3.53	119.66	111.23
1	1	1939	5MU	C2'-C1'-N1	3.46	123.03	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2580	PSU	O2'-C2'-C1'	3.40	119.33	111.23
1	1	1835	2MG	C3'-C2'-C1'	3.38	106.06	100.98
1	1	2445	2MG	O3'-C3'-C2'	3.34	122.61	111.82
2	2	966	2MG	C2'-C3'-C4'	-3.29	96.26	102.64
1	1	745	1MG	O3'-C3'-C2'	3.28	122.44	111.82
5	5	8	4SU	N3-C2-N1	3.24	119.19	114.89
1	1	746	PSU	O2'-C2'-C1'	3.24	118.95	111.23
2	2	1516	2MG	O3'-C3'-C4'	3.19	120.28	111.05
1	1	2503	2MA	O2'-C2'-C3'	3.18	122.09	111.82
1	1	1917	PSU	C3'-C2'-C1'	3.16	105.32	101.64
1	1	2504	PSU	C2'-C3'-C4'	-3.16	96.51	102.64
5	5	8	4SU	S4-C4-N3	3.09	123.25	120.21
1	1	2457	PSU	O2'-C2'-C1'	3.07	118.55	111.23
1	1	1835	2MG	O3'-C3'-C2'	3.05	121.70	111.82
2	2	967	5MC	O3'-C3'-C4'	3.02	119.79	111.05
2	2	527	7MG	C5-C6-N1	3.01	116.30	110.99
2	2	1498	UR3	O4'-C1'-C2'	-2.99	100.13	106.64
1	1	955	PSU	C2'-C3'-C4'	-2.98	96.84	102.64
1	1	1618	6MZ	C2-N1-C6	2.97	119.14	116.59
5	5	55	PSU	C3'-C2'-C1'	2.97	105.09	101.64
1	1	2445	2MG	O3'-C3'-C4'	2.92	119.48	111.05
5	5	32	4OC	O3'-C3'-C4'	2.91	119.46	111.05
2	2	527	7MG	O4'-C4'-C3'	-2.89	99.39	105.11
1	1	1915	3TD	O4'-C4'-C5'	-2.89	99.86	109.37
1	1	1911	PSU	C3'-C2'-C1'	2.81	104.91	101.64
1	1	2030	6MZ	C2-N1-C6	2.79	118.98	116.59
1	1	747	5MU	C2'-C1'-N1	2.77	121.06	113.22
1	1	2445	2MG	C3'-C2'-C1'	2.74	105.11	100.98
5	5	8	4SU	C2'-C1'-N1	2.70	120.87	113.22
2	2	1402	4OC	O3'-C3'-C4'	2.67	118.78	111.05
1	1	1917	PSU	O2-C2-N1	-2.67	119.85	122.79
1	1	2069	G7M	C2'-C3'-C4'	-2.64	97.51	102.64
1	1	2457	PSU	C3'-C2'-C1'	2.63	104.69	101.64
1	1	2605	PSU	C2'-C3'-C4'	-2.62	97.56	102.64
2	2	1402	4OC	O4'-C4'-C3'	-2.58	100.00	105.11
5	5	54	5MU	C2'-C1'-N1	2.57	120.50	113.22
2	2	1518	MA6	C2'-C3'-C4'	-2.56	97.66	102.64
1	1	2030	6MZ	O3'-C3'-C2'	2.56	120.10	111.82
2	2	966	2MG	O3'-C3'-C2'	2.53	119.99	111.82
1	1	1962	5MC	O3'-C3'-C2'	2.51	119.95	111.82
2	2	527	7MG	C5-C4-N9	-2.46	103.16	106.35
2	2	967	5MC	C2'-C1'-N1	2.40	120.02	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2580	PSU	C3'-C2'-C1'	2.39	104.42	101.64
1	1	2457	PSU	C2'-C3'-C4'	-2.36	98.05	102.64
2	2	527	7MG	O6-C6-C5	-2.35	121.76	127.54
1	1	1917	PSU	N1-C2-N3	2.34	117.78	115.13
1	1	1911	PSU	O3'-C3'-C4'	2.31	117.72	111.05
2	2	1207	2MG	O2'-C2'-C1'	-2.26	102.52	110.85
2	2	1407	5MC	C2'-C1'-N1	2.24	119.58	113.22
1	1	747	5MU	C3'-C2'-C1'	2.24	105.68	101.43
2	2	1407	5MC	O3'-C3'-C4'	2.20	117.42	111.05
1	1	1939	5MU	N3-C2-N1	2.20	117.81	114.89
2	2	1519	MA6	C2'-C3'-C4'	-2.20	98.36	102.64
1	1	1939	5MU	C4-N3-C2	-2.20	124.51	127.35
1	1	2552	OMU	N3-C2-N1	2.15	117.75	114.89
1	1	747	5MU	N3-C2-N1	2.15	117.74	114.89
1	1	1917	PSU	C6-C5-C4	2.14	119.69	118.20
5	5	54	5MU	N3-C2-N1	2.13	117.72	114.89
1	1	747	5MU	C4-N3-C2	-2.12	124.61	127.35
5	5	8	4SU	C4'-O4'-C1'	-2.11	104.81	109.47
1	1	1915	3TD	C3'-C2'-C1'	2.11	104.09	101.64
1	1	1962	5MC	C3'-C2'-C1'	2.11	105.43	101.43
5	5	8	4SU	O4'-C1'-C2'	-2.10	102.07	106.64
1	1	745	1MG	O2'-C2'-C3'	2.09	118.59	111.82
5	5	8	4SU	C1'-N1-C6	-2.09	116.29	120.84
5	5	8	4SU	O2-C2-N1	-2.07	120.04	122.79
1	1	2498	OMC	C3'-C2'-C1'	2.03	106.71	102.89
5	5	76	8AN	C5-C6-N6	2.03	123.43	120.35
1	1	1915	3TD	C4-N3-C2	-2.01	122.43	124.61
2	2	527	7MG	O2'-C2'-C1'	-2.01	103.32	110.02
5	5	8	4SU	C6-C5-C4	-2.00	118.22	119.95

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	746	PSU	C2'-C1'-C5-C4
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1835	2MG	N1-C2-N2-CM2
1	1	1835	2MG	N3-C2-N2-CM2
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
1	1	2069	G7M	O4'-C4'-C5'-O5'
1	1	2251	OMG	C1'-C2'-O2'-CM2
1	1	2445	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	N1-C2-N2-CM2
2	2	966	2MG	N3-C2-N2-CM2
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
5	5	20	H2U	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C6
5	5	55	PSU	C3'-C4'-C5'-O5'
49	q	89	0TD	SB-CB-CG-OD2
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
5	5	20	H2U	C3'-C4'-C5'-O5'
1	1	2552	OMU	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
2	2	1519	MA6	N1-C6-N6-C10
5	5	20	H2U	O4'-C1'-N1-C2
1	1	745	1MG	O4'-C4'-C5'-O5'
1	1	745	1MG	C3'-C4'-C5'-O5'
2	2	527	7MG	C3'-C4'-C5'-O5'
1	1	2552	OMU	C3'-C4'-C5'-O5'
5	5	55	PSU	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2498	OMC	O4'-C4'-C5'-O5'
2	2	527	7MG	O4'-C4'-C5'-O5'
5	5	76	8AN	C4'-C5'-O5'-P
2	2	1519	MA6	C5-C6-N6-C9
1	1	2498	OMC	C3'-C4'-C5'-O5'
2	2	516	PSU	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C5-C6-N6-C9
49	q	89	0TD	CG-CB-SB-CSB
5	5	8	4SU	O4'-C1'-N1-C6
5	5	8	4SU	O4'-C1'-N1-C2
1	1	2069	G7M	C4'-C5'-O5'-P
2	2	967	5MC	C4'-C5'-O5'-P
1	1	2251	OMG	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	527	7MG	C4'-C5'-O5'-P
2	2	1519	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	1	2457	PSU	O4'-C1'-C5-C4
1	1	2580	PSU	O4'-C1'-C5-C4
1	1	2251	OMG	C3'-C2'-O2'-CM2
2	2	967	5MC	C2'-C1'-N1-C6
1	1	2251	OMG	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
2	2	516	PSU	C3'-C4'-C5'-O5'
2	2	967	5MC	C2'-C1'-N1-C2
1	1	1962	5MC	O4'-C1'-N1-C6
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	746	PSU	O4'-C1'-C5-C6
1	1	2580	PSU	O4'-C1'-C5-C6
5	5	8	4SU	C4'-C5'-O5'-P
5	5	55	PSU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 453 ligands modelled in this entry, 452 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	FME	5	103	5	8,9,10	0.55	0	7,9,11	1.31	1 (14%)

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	FME	5	103	5	-	2/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	5	103	FME	O-C-CA	-3.24	116.30	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	5	103	FME	O1-CN-N-CA
60	5	103	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	2196:C	O3'	2197:U	P	2.71

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-3492. 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 ⓘ

This section was not generated.

6.2 Central slices ⓘ

This section was not generated.

6.3 Largest variance slices ⓘ

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

This section was not generated.

6.5 Orthogonal surface views ⓘ

This section was not generated.

6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section was not generated.