Full wwPDB EM Validation Report (i)

Apr 16, 2024 – 03:25 am BST

PDB ID	:	7OII
EMDB ID	:	EMD-12930
Title	:	CspA-70 cotranslational folding intermediate 2
Authors	:	Agirrezabala, X.; Samatova, E.; Macher, M.; Liutkute, M.; Gil-Carton, D.; Novacek, J.; Valle, M.; Rodnina, M.V.
Deposited on	:	2021-05-11
Resolution	:	3.00 Å(reported)
Based on initial model	:	6ORE

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

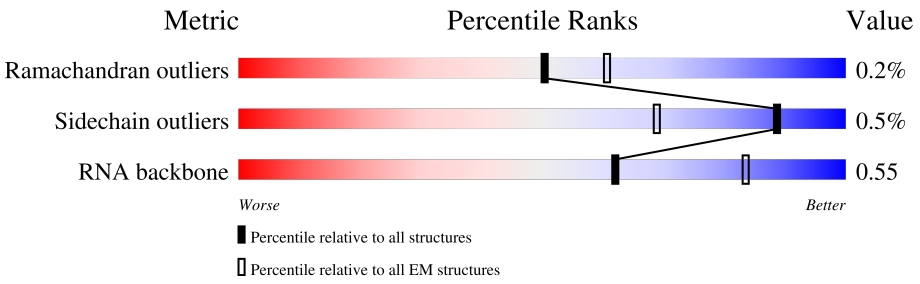
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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%

Mol	Chain	Length	Quality of chain
1	1	2903	71% 27% .
2	2	1534	77% 22% .
3	3	120	82% 17% .
4	C	271	100%
5	D	209	98% .
6	E	201	100%
7	F	177	99% .
8	G	175	99% .
9	H	149	98% .

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Mol	Chain	Length	Quality of chain
10	I	142	99%
11	J	123	99%
12	K	144	99%
13	L	136	99%
14	M	119	99%
15	N	116	100%
16	O	114	100%
17	P	117	99%
18	Q	103	98%
19	R	110	99%
20	S	94	100%
21	T	103	99%
22	U	94	99%
23	V	84	98%
24	W	77	100%
25	X	62	98%
26	Y	58	98%
27	Z	66	98%
28	a	56	98%
29	b	52	100%
30	c	46	100%
31	d	64	97%
32	e	38	97%
33	f	225	100%
34	g	208	99%

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Mol	Chain	Length	Quality of chain
35	h	205	100%
36	i	156	97%
37	j	104	100%
38	k	151	100%
39	l	129	100%
40	m	127	98%
41	n	99	98%
42	o	117	99%
43	p	123	99%
44	q	116	100%
45	r	100	100%
46	s	88	100%
47	t	82	100%
48	u	80	100%
49	v	66	100%
50	w	83	99%
51	x	86	100%
52	y	70	97%
53	4	6	67% 33%
54	z	85	52% 34% 14%
55	B	39	100%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 145171 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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 rRNA.

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 protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	V	84	634	391	129	113	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L31.

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

- Molecule 28 is a protein called 50S ribosomal protein L32.

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

- Molecule 29 is a protein called 50S ribosomal protein L33.

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

- Molecule 30 is a protein called 50S ribosomal protein L34.

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

- Molecule 31 is a protein called 50S ribosomal protein L35.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 30S ribosomal protein S2.

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

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

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

- Molecule 37 is a protein called 30S ribosomal protein S6.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

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

- Molecule 42 is a protein called 30S ribosomal protein S11.

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

- Molecule 43 is a protein called 30S ribosomal protein S12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called 30S ribosomal protein S14.

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

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

- Molecule 48 is a protein called 30S ribosomal protein S17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

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

- Molecule 50 is a protein called 30S ribosomal protein S19.

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

- Molecule 51 is a protein called 30S ribosomal protein S20.

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

- Molecule 52 is a protein called 30S ribosomal protein S21.

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	4	6	122	55	17	44	6	0	0

- Molecule 54 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	z	85	1830	822	328	595	85	0	0

- Molecule 55 is a protein called Cold-shock DNA-binding protein family.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	B	39	250	159	43	48	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ILE	VAL	conflict	UNP A0A1H2D2H5

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	1	282	282	282	0
56	2	119	119	119	0
56	3	8	8	8	0
56	C	1	1	1	0
56	D	1	1	1	0
56	M	1	1	1	0
56	P	1	1	1	0
56	a	2	2	2	0
56	h	1	1	1	0
56	q	1	1	1	0
56	4	1	1	1	0
56	z	4	4	4	0

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

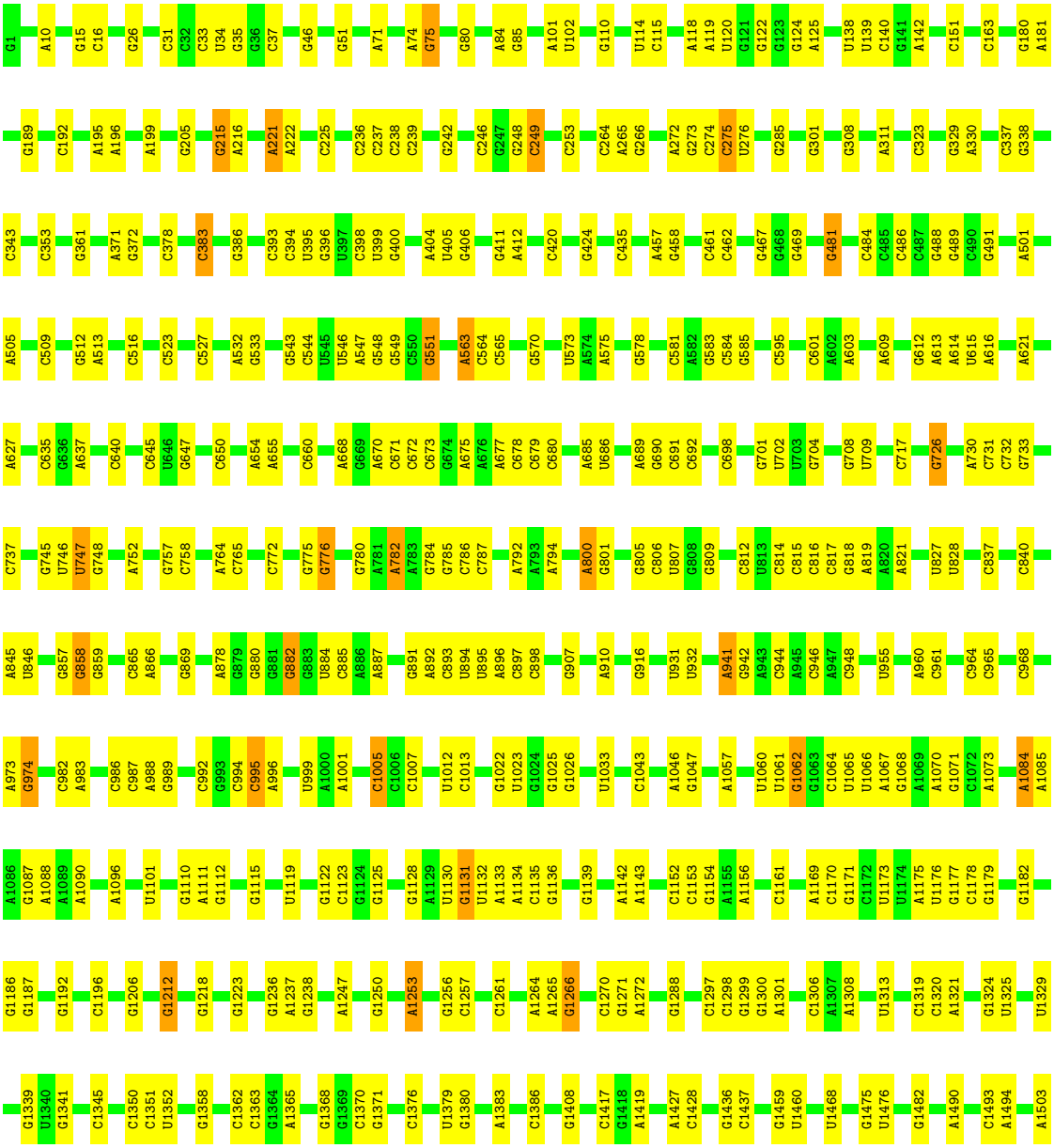
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	Z	1	1	1	0
57	e	1	1	1	0

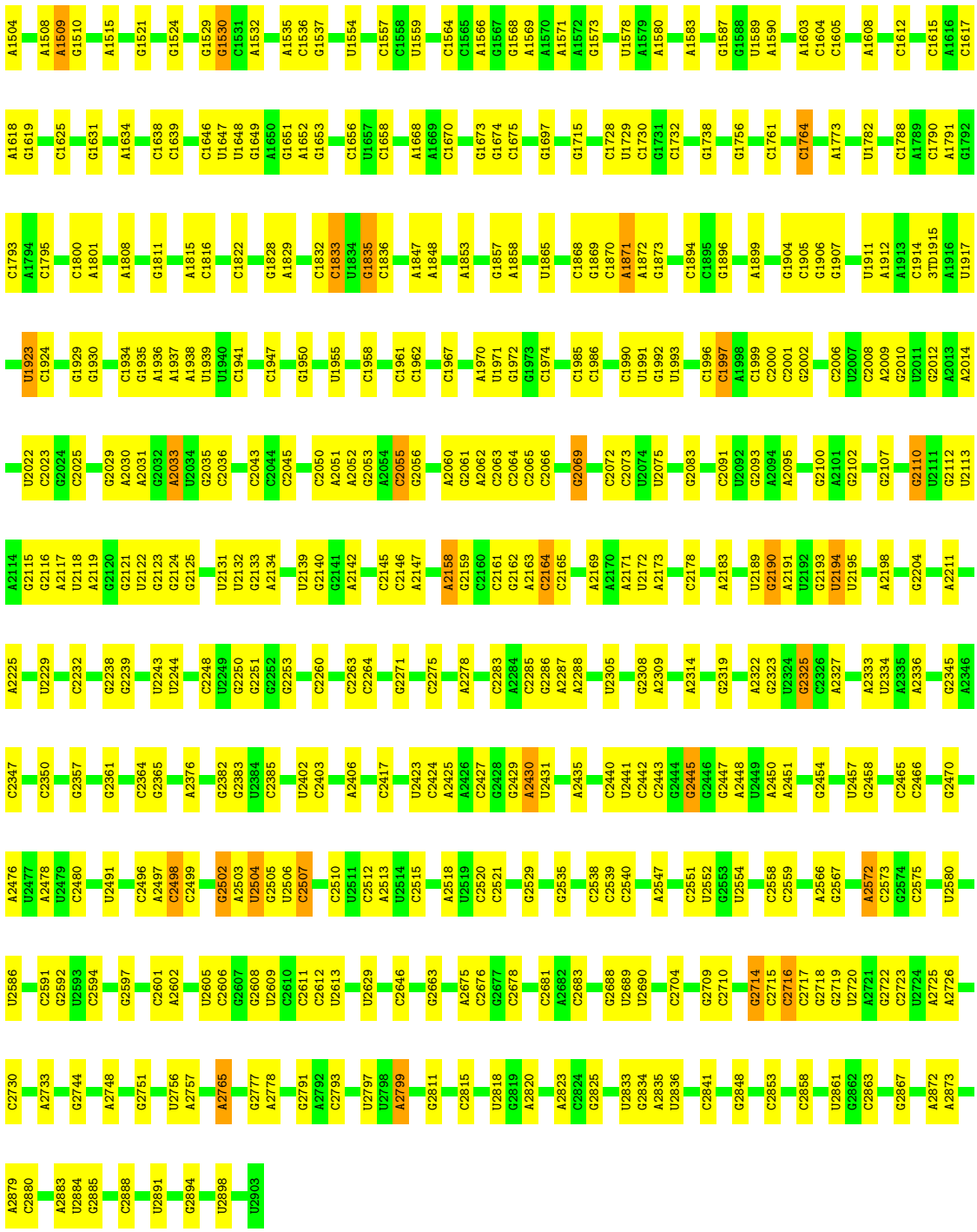
3 Residue-property plots (i)

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 rRNA

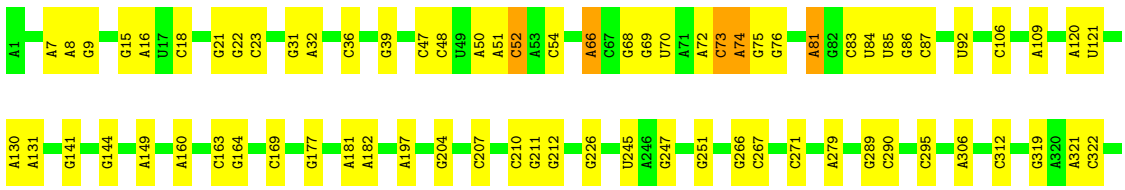
Chain 1: 71% 27%





- Molecule 2: 16S rRNA

Chain 2:



C328 A329 C330 G331 G332 U333 C334 C335 G347 C352 A353 G354 G362 U367 C372 G384 C392 U398 G399 C400 G406 A412 G413 A414 U421 C422 G423 G424 U429 C436 U439 G457 U458 U463 U464 U467 A468 U476 C477 A478 U479 U480

G481 G484 U485 U486 A496 A499 C504 A510 C511 U516 G517 C518 G521 G527 U531 A532 A533 A547 G548 C549 C556 G557 G558 A559 C564 G568 A572 A573 A574 G575 C576 G577 C578 A579 C580 G581 A596 C599 U605 A622 C623 C624

G633 G650 U653 C658 U659 C660 A665 G682 U686 G700 U701 A702 G703 C708 A718 C719 C720 G721 G722 U723 G724 G725 C726 G731 C732 G733 G734 C738 A747 G748 A753 C754 G755 C756 U757 C758 G765 C770 A777 A787 G791

A792 U793 A794 C795 C796 C797 C806 C810 C811 C812 A815 A816 C817 G821 U822 C823 U828 G829 G832 C841 U842 U843 G844 A845 G846 C856 C857 C858 C868 G869 C879 C882 C883 U884 G885 G886 G887 C897 G898 C899 A914 A919 C924 C931

G934 A935 U960 U965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 U982 G993 A994 C995 A996 A1004 U1009 A1019 G1020 A1021 A1022 U1025 G1026 C1027 C1028 U1029 U1030 C1031 G1032 G1033 G1034 G1043 A1046 U1065 C1069 G1079 U1085 G1089

G1094 U1095 A1101 G1104 C1107 G1108 C1109 G1124 U1125 C1132 C1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 A1145 A1146 A1151 A1152 C1158 U1159 G1160 A1167 U1168 A1169 G1175 A1176 G1184 A1196 A1197 C1200 G1207 U1212 A1213 C1214 G1215 G1221 G1222 C1223

A1227 C1228 A1238 A1239 A1257 G1258 C1259 G1260 A1261 G1266 A1275 G1279 A1280 U1286 A1287 G1297 U1298 A1299 C1302 C1303 C1304 G1305 G1312 C1317 A1318 A1319 C1320 G1331 U1335 C1336 A1340 A1346 G1353 A1363 U1364 G1365 C1366 G1370 G1373 G1379

U1380 U1381 C1389 A1396 C1402 C1403 C1407 G1419 A1446 G1482 G1494 G1497 U1498 A1499 A1500 C1501 A1502 A1503 U1506 C1509 A1513 G1516 G1517 A1518 A1519 C1520 C1521 C1524 G1529 G1530 A1534

- Molecule 3: 5S rRNA

Chain 3: 82% 17% •

U1 G2 G9 G13 U14 A15 G24 C31 C35 C36 A45 G51 G56 A66 G76 C88 U89 C90 C91 C92 C93 A99 G102 A109 G117 U120

- Molecule 4: 50S ribosomal protein L2

Chain C: 100%

A2 V162 S272

- Molecule 5: 50S ribosomal protein L3

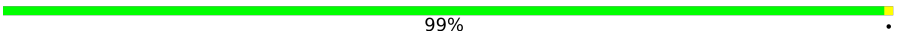
Chain D: 98% •

M1 T151 P152 G153 K154 V155 A209

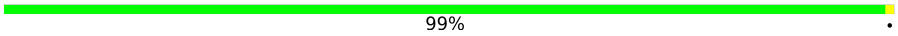
- Molecule 6: 50S ribosomal protein L4

Chain E: 100%

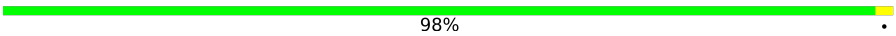
• Molecule 7: 50S ribosomal protein L5

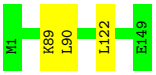
Chain F: 

• Molecule 8: 50S ribosomal protein L6

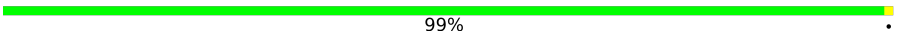
Chain G: 

• Molecule 9: 50S ribosomal protein L9

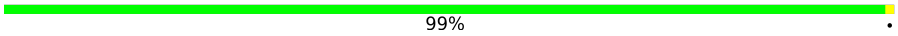
Chain H: 



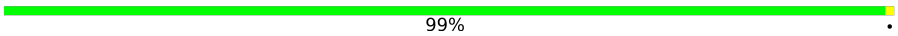
• Molecule 10: 50S ribosomal protein L13

Chain I: 

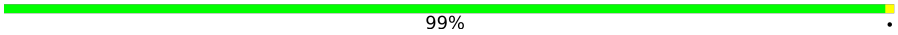
• Molecule 11: 50S ribosomal protein L14

Chain J: 

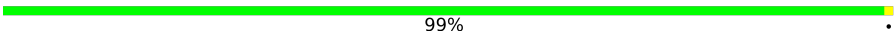
• Molecule 12: 50S ribosomal protein L15

Chain K: 

• Molecule 13: 50S ribosomal protein L16

Chain L: 

• Molecule 14: 50S ribosomal protein L17

Chain M: 

• Molecule 15: 50S ribosomal protein L18

Chain N:

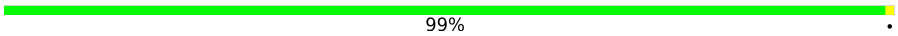
There are no outlier residues recorded for this chain.

• Molecule 16: 50S ribosomal protein L19

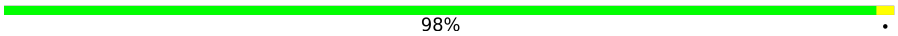
Chain O:

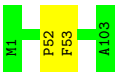
There are no outlier residues recorded for this chain.

• Molecule 17: 50S ribosomal protein L20

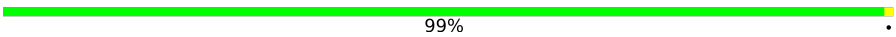
Chain P: 

• Molecule 18: 50S ribosomal protein L21

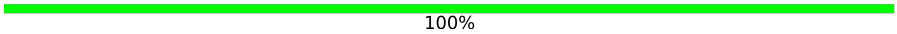
Chain Q: 



• Molecule 19: 50S ribosomal protein L22

Chain R: 

• Molecule 20: 50S ribosomal protein L23

Chain S: 

There are no outlier residues recorded for this chain.

• Molecule 21: 50S ribosomal protein L24

Chain T: 99%

• Molecule 22: 50S ribosomal protein L25

Chain U: 99%

• Molecule 23: 50S ribosomal protein L27

Chain V: 98%

• Molecule 24: 50S ribosomal protein L28

Chain W: 100%

There are no outlier residues recorded for this chain.

• Molecule 25: 50S ribosomal protein L29

Chain X: 98%

• Molecule 26: 50S ribosomal protein L30

Chain Y: 98%

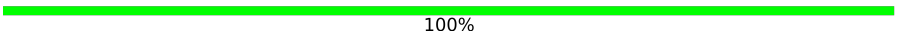
• Molecule 27: 50S ribosomal protein L31

Chain Z: 98%

• Molecule 28: 50S ribosomal protein L32

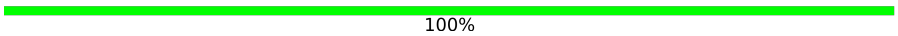
Chain a: 98%

• Molecule 29: 50S ribosomal protein L33

Chain b: 

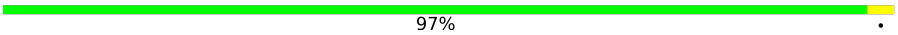
There are no outlier residues recorded for this chain.

• Molecule 30: 50S ribosomal protein L34

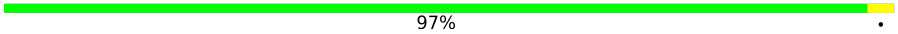
Chain c: 

There are no outlier residues recorded for this chain.

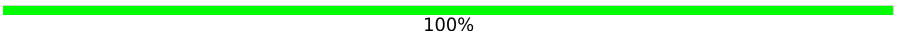
• Molecule 31: 50S ribosomal protein L35

Chain d: 

• Molecule 32: 50S ribosomal protein L36

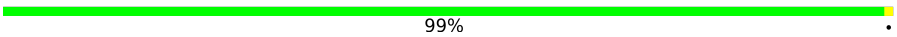
Chain e: 

• Molecule 33: 30S ribosomal protein S2

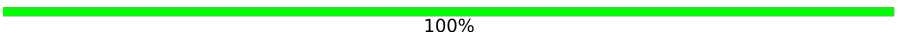
Chain f: 

There are no outlier residues recorded for this chain.

• Molecule 34: 30S ribosomal protein S3

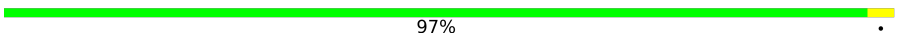
Chain g: 

• Molecule 35: 30S ribosomal protein S4

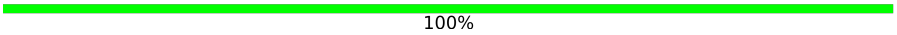
Chain h: 

There are no outlier residues recorded for this chain.

• Molecule 36: 30S ribosomal protein S5

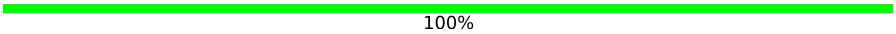
Chain i: 

• Molecule 37: 30S ribosomal protein S6

Chain j: 

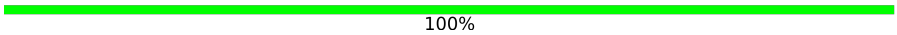
There are no outlier residues recorded for this chain.

• Molecule 38: 30S ribosomal protein S7

Chain k: 

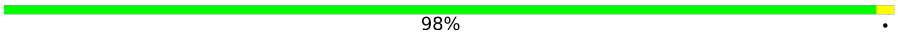
There are no outlier residues recorded for this chain.

• Molecule 39: 30S ribosomal protein S8

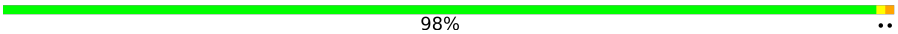
Chain l: 

There are no outlier residues recorded for this chain.

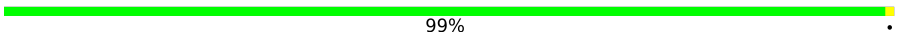
• Molecule 40: 30S ribosomal protein S9

Chain m: 

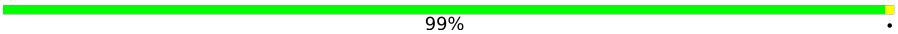
• Molecule 41: 30S ribosomal protein S10

Chain n: 

• Molecule 42: 30S ribosomal protein S11

Chain o: 

• Molecule 43: 30S ribosomal protein S12

Chain p: 

• Molecule 44: 30S ribosomal protein S13

Chain q: 100%

There are no outlier residues recorded for this chain.

• Molecule 45: 30S ribosomal protein S14

Chain r: 100%

There are no outlier residues recorded for this chain.

• Molecule 46: 30S ribosomal protein S15

Chain s: 100%

There are no outlier residues recorded for this chain.

• Molecule 47: 30S ribosomal protein S16

Chain t: 100%

There are no outlier residues recorded for this chain.

• Molecule 48: 30S ribosomal protein S17

Chain u: 100%

There are no outlier residues recorded for this chain.

• Molecule 49: 30S ribosomal protein S18

Chain v: 100%

There are no outlier residues recorded for this chain.

• Molecule 50: 30S ribosomal protein S19

Chain w: 99%

P2 R78 A84

• Molecule 51: 30S ribosomal protein S20

Chain x: 100%

There are no outlier residues recorded for this chain.

• Molecule 52: 30S ribosomal protein S21

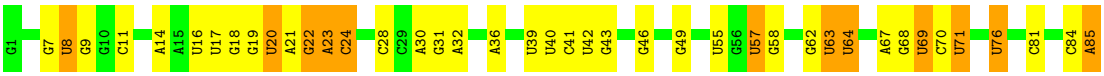
Chain y: 97%

• Molecule 53: mRNA

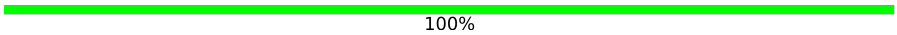
Chain 4:

• Molecule 54: tRNA-Leu

Chain z:



• Molecule 55: Cold-shock DNA-binding protein family

Chain B: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23782	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	2.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (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: OMG, MA6, ZN, 5MC, UR3, 0TD, G7M, OMU, PSU, 4OC, 6MZ, 5MU, OMC, 2MA, 3TD, 2MG, MG, 1MG

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	1.63	238/69286 (0.3%)	1.27	240/108087 (0.2%)
2	2	1.45	60/36590 (0.2%)	1.19	59/57074 (0.1%)
3	3	1.39	3/2872 (0.1%)	1.16	8/4478 (0.2%)
4	C	1.06	1/2121 (0.0%)	0.71	0/2852
5	D	1.07	1/1586 (0.1%)	0.72	1/2134 (0.0%)
6	E	0.96	0/1571	0.69	1/2113 (0.0%)
7	F	0.75	0/1434	0.68	0/1926
8	G	0.71	0/1333	0.64	0/1805
9	H	0.51	0/1122	0.79	0/1515
10	I	1.03	1/1152 (0.1%)	0.67	0/1551
11	J	0.98	0/955	0.74	0/1279
12	K	0.98	0/1062	0.76	0/1413
13	L	1.01	0/1093	0.69	0/1460
14	M	1.00	0/964	0.73	0/1289
15	N	0.89	0/902	0.68	0/1209
16	O	1.03	0/929	0.68	0/1242
17	P	1.19	0/960	0.75	0/1278
18	Q	1.02	0/829	0.70	0/1107
19	R	1.02	1/864 (0.1%)	0.73	0/1156
20	S	0.98	0/752	0.65	0/1005
21	T	0.89	0/796	0.66	0/1062
22	U	0.88	0/766	0.66	0/1025
23	V	1.04	0/642	0.70	0/848
24	W	0.99	0/635	0.71	0/848
25	X	0.76	0/502	0.74	1/667 (0.1%)
26	Y	0.93	0/452	0.73	1/605 (0.2%)
27	Z	0.64	1/531 (0.2%)	0.67	0/709
28	a	1.02	1/450 (0.2%)	0.74	0/599
29	b	0.83	0/433	0.62	0/576
30	c	1.03	0/380	0.78	0/498
31	d	1.05	0/513	0.74	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	1.05	1/303 (0.3%)	0.75	0/397
33	f	0.65	0/1791	0.66	0/2413
34	g	0.82	0/1663	0.66	0/2241
35	h	0.80	0/1665	0.64	0/2227
36	i	0.95	2/1165 (0.2%)	0.73	0/1568
37	j	0.76	0/867	0.67	0/1171
38	k	0.73	0/1195	0.68	0/1602
39	l	0.93	0/989	0.70	0/1326
40	m	0.82	0/1034	0.71	0/1375
41	n	0.74	0/800	0.79	1/1082 (0.1%)
42	o	0.80	0/893	0.68	0/1205
43	p	0.94	0/960	0.72	0/1286
44	q	0.71	0/909	0.69	0/1215
45	r	0.80	0/817	0.66	0/1088
46	s	0.80	0/722	0.68	0/964
47	t	0.90	0/659	0.67	0/884
48	u	0.81	0/657	0.71	0/881
49	v	0.84	0/553	0.69	0/743
50	w	0.69	0/680	0.62	0/915
51	x	0.78	0/675	0.69	0/895
52	y	0.71	0/597	0.66	0/792
53	4	1.64	1/134 (0.7%)	1.42	0/205
54	z	1.47	9/1768 (0.5%)	1.33	14/2759 (0.5%)
55	B	0.55	0/255	0.62	0/347
All	All	1.40	320/156228 (0.2%)	1.13	326/233667 (0.1%)

All (320) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	32	A	N9-C4	-8.67	1.32	1.37
1	1	2442	C	N1-C6	-7.47	1.32	1.37
54	z	84	C	N1-C6	-7.46	1.32	1.37
1	1	1999	C	N1-C6	-7.20	1.32	1.37
1	1	673	C	N1-C6	-7.17	1.32	1.37
1	1	786	C	N1-C6	-7.13	1.32	1.37
1	1	565	C	N1-C6	-7.02	1.32	1.37
1	1	964	C	N1-C6	-6.92	1.32	1.37
1	1	787	C	N1-C6	-6.91	1.33	1.37
1	1	691	C	N1-C6	-6.87	1.33	1.37
1	1	581	C	N1-C6	-6.87	1.33	1.37
1	1	2512	C	N1-C6	-6.81	1.33	1.37
53	4	4	C	N1-C6	-6.70	1.33	1.37

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	672	C	N1-C6	-6.68	1.33	1.37
1	1	584	C	N1-C6	-6.64	1.33	1.37
1	1	2066	C	N1-C6	-6.63	1.33	1.37
1	1	671	C	N1-C6	-6.60	1.33	1.37
1	1	2515	C	N1-C6	-6.60	1.33	1.37
1	1	944	C	N1-C6	-6.59	1.33	1.37
1	1	987	C	N1-C6	-6.54	1.33	1.37
1	1	1376	C	N1-C6	-6.53	1.33	1.37
1	1	1985	C	N1-C6	-6.51	1.33	1.37
54	z	85	A	N9-C4	-6.42	1.33	1.37
1	1	679	C	N1-C6	-6.42	1.33	1.37
1	1	772	C	N1-C6	-6.40	1.33	1.37
1	1	2065	C	N1-C6	-6.36	1.33	1.37
1	1	2264	C	N1-C6	-6.35	1.33	1.37
2	2	18	C	N1-C6	-6.34	1.33	1.37
1	1	2841	C	N1-C6	-6.34	1.33	1.37
1	1	523	C	N1-C6	-6.29	1.33	1.37
1	1	2443	C	N1-C6	-6.29	1.33	1.37
1	1	2540	C	N1-C6	-6.26	1.33	1.37
1	1	2681	C	N1-C6	-6.26	1.33	1.37
1	1	2064	C	N1-C6	-6.26	1.33	1.37
1	1	1370	C	N1-C6	-6.23	1.33	1.37
1	1	1656	C	N1-C6	-6.23	1.33	1.37
1	1	1084	A	O3'-P	-6.21	1.53	1.61
1	1	1363	C	N1-C6	-6.21	1.33	1.37
1	1	782	A	N9-C4	-6.19	1.34	1.37
1	1	1270	C	N1-C6	-6.19	1.33	1.37
1	1	2601	C	N1-C6	-6.19	1.33	1.37
1	1	968	C	N1-C6	-6.18	1.33	1.37
1	1	678	C	N1-C6	-6.18	1.33	1.37
1	1	31	C	N1-C6	-6.17	1.33	1.37
1	1	1604	C	N1-C6	-6.16	1.33	1.37
1	1	1298	C	N1-C6	-6.15	1.33	1.37
1	1	800	A	N9-C4	-6.12	1.34	1.37
2	2	758	C	N1-C6	-6.11	1.33	1.37
1	1	1638	C	N1-C6	-6.10	1.33	1.37
1	1	1257	C	N1-C6	-6.08	1.33	1.37
2	2	1520	C	N1-C6	-6.07	1.33	1.37
2	2	879	C	N1-C6	-6.07	1.33	1.37
1	1	2683	C	N1-C6	-6.06	1.33	1.37
1	1	817	C	N1-C6	-6.04	1.33	1.37
2	2	719	C	N1-C6	-6.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2050	C	N1-C6	-6.03	1.33	1.37
1	1	2499	C	N1-C6	-6.03	1.33	1.37
1	1	806	C	N3-C4	-6.03	1.29	1.33
1	1	239	C	N1-C6	-6.00	1.33	1.37
1	1	2260	C	N1-C6	-5.98	1.33	1.37
1	1	2073	C	N1-C6	-5.96	1.33	1.37
1	1	635	C	N1-C6	-5.96	1.33	1.37
2	2	756	C	N1-C6	-5.96	1.33	1.37
1	1	1790	C	N1-C6	-5.95	1.33	1.37
36	i	137	VAL	CB-CG1	-5.93	1.40	1.52
1	1	2521	C	N1-C6	-5.92	1.33	1.37
1	1	2417	C	N1-C6	-5.90	1.33	1.37
1	1	2591	C	N1-C6	-5.90	1.33	1.37
1	1	1007	C	N1-C6	-5.88	1.33	1.37
1	1	815	C	N1-C6	-5.88	1.33	1.37
1	1	398	C	N1-C6	-5.87	1.33	1.37
1	1	816	C	N1-C6	-5.87	1.33	1.37
1	1	692	C	N1-C6	-5.87	1.33	1.37
1	1	680	C	N1-C6	-5.86	1.33	1.37
1	1	2676	C	N1-C6	-5.86	1.33	1.37
1	1	660	C	N1-C6	-5.85	1.33	1.37
1	1	1958	C	N1-C6	-5.85	1.33	1.37
1	1	2466	C	N1-C6	-5.83	1.33	1.37
2	2	919	A	N9-C4	-5.83	1.34	1.37
1	1	1005	C	N1-C6	-5.82	1.33	1.37
1	1	698	C	N1-C6	-5.81	1.33	1.37
1	1	585	G	N9-C8	-5.81	1.33	1.37
1	1	1557	C	N1-C6	-5.80	1.33	1.37
1	1	1905	C	N1-C6	-5.80	1.33	1.37
1	1	337	C	N1-C6	-5.79	1.33	1.37
1	1	806	C	N1-C6	-5.78	1.33	1.37
1	1	1795	C	N1-C6	-5.78	1.33	1.37
2	2	549	C	N1-C6	-5.77	1.33	1.37
1	1	2036	C	C4-C5	-5.77	1.38	1.43
54	z	36	A	N9-C4	-5.77	1.34	1.37
1	1	516	C	N1-C6	-5.76	1.33	1.37
1	1	988	A	N9-C4	-5.76	1.34	1.37
2	2	23	C	N1-C6	-5.75	1.33	1.37
1	1	840	C	N1-C6	-5.74	1.33	1.37
1	1	965	C	N1-C6	-5.74	1.33	1.37
1	1	1658	C	N1-C6	-5.72	1.33	1.37
1	1	737	C	N1-C6	-5.71	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1639	C	N1-C6	-5.71	1.33	1.37
36	i	136	VAL	CB-CG1	-5.69	1.40	1.52
1	1	2051	A	N9-C4	-5.69	1.34	1.37
1	1	564	C	N1-C6	-5.69	1.33	1.37
1	1	2091	C	N1-C6	-5.68	1.33	1.37
1	1	948	C	N1-C6	-5.66	1.33	1.37
1	1	2263	C	N1-C6	-5.66	1.33	1.37
1	1	1261	C	N1-C6	-5.66	1.33	1.37
1	1	2008	C	N1-C6	-5.66	1.33	1.37
1	1	2559	C	N1-C6	-5.66	1.33	1.37
2	2	924	C	N1-C6	-5.64	1.33	1.37
54	z	41	C	N1-C6	-5.63	1.33	1.37
1	1	2009	A	N9-C4	-5.62	1.34	1.37
2	2	1223	C	N1-C6	-5.62	1.33	1.37
1	1	2710	C	N1-C6	-5.62	1.33	1.37
1	1	2538	C	N1-C6	-5.62	1.33	1.37
1	1	2248	C	N1-C6	-5.61	1.33	1.37
1	1	994	C	N1-C6	-5.61	1.33	1.37
54	z	84	C	C4-C5	-5.60	1.38	1.43
1	1	2539	C	N1-C6	-5.60	1.33	1.37
1	1	2716	C	N1-C6	-5.58	1.33	1.37
1	1	1153	C	N1-C6	-5.58	1.33	1.37
2	2	295	C	N1-C6	-5.57	1.33	1.37
1	1	814	C	N1-C6	-5.57	1.33	1.37
2	2	109	A	N9-C4	-5.56	1.34	1.37
3	3	93	C	N1-C6	-5.55	1.33	1.37
1	1	809	G	N9-C8	-5.55	1.33	1.37
1	1	1612	C	N1-C6	-5.55	1.33	1.37
1	1	758	C	N1-C6	-5.54	1.33	1.37
1	1	1319	C	N1-C6	-5.54	1.33	1.37
1	1	1833	C	N1-C6	-5.54	1.33	1.37
1	1	1605	C	N1-C6	-5.53	1.33	1.37
1	1	668	A	N9-C4	-5.53	1.34	1.37
1	1	2055	C	N1-C6	-5.53	1.33	1.37
2	2	52	C	N1-C6	-5.53	1.33	1.37
1	1	1668	A	N9-C4	-5.52	1.34	1.37
1	1	237	C	N1-C6	-5.52	1.33	1.37
2	2	1389	C	N1-C6	-5.51	1.33	1.37
1	1	1001	A	N9-C4	-5.51	1.34	1.37
2	2	726	C	N1-C6	-5.51	1.33	1.37
1	1	2717	C	N1-C6	-5.50	1.33	1.37
1	1	2063	C	N1-C6	-5.50	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1221	G	N9-C4	-5.49	1.33	1.38
1	1	2427	C	N1-C6	-5.49	1.33	1.37
1	1	2730	C	N1-C6	-5.48	1.33	1.37
2	2	36	C	N1-C6	-5.48	1.33	1.37
2	2	16	A	N9-C4	-5.47	1.34	1.37
1	1	2551	C	N1-C6	-5.47	1.33	1.37
2	2	578	C	N1-C6	-5.47	1.33	1.37
2	2	1509	C	N1-C6	-5.47	1.33	1.37
2	2	811	C	N1-C6	-5.47	1.33	1.37
1	1	2507	C	N1-C6	-5.46	1.33	1.37
1	1	2364	C	N1-C6	-5.46	1.33	1.37
1	1	1832	C	N1-C6	-5.45	1.33	1.37
1	1	2606	C	N1-C6	-5.45	1.33	1.37
2	2	622	A	N9-C4	-5.45	1.34	1.37
1	1	992	C	N1-C6	-5.45	1.33	1.37
1	1	1670	C	C4-C5	-5.45	1.38	1.43
19	R	50	VAL	CB-CG1	-5.44	1.41	1.52
1	1	527	C	N1-C6	-5.44	1.33	1.37
1	1	2006	C	N1-C6	-5.44	1.33	1.37
32	e	3	VAL	CB-CG1	-5.44	1.41	1.52
1	1	2014	A	N9-C4	-5.43	1.34	1.37
1	1	486	C	N1-C6	-5.43	1.33	1.37
1	1	601	C	N1-C6	-5.43	1.33	1.37
1	1	1815	A	N9-C4	-5.43	1.34	1.37
1	1	1997	C	N1-C6	-5.43	1.33	1.37
2	2	599	C	N1-C6	-5.43	1.33	1.37
1	1	757	G	N9-C4	-5.42	1.33	1.38
2	2	1513	A	N9-C4	-5.42	1.34	1.37
2	2	1109	C	N1-C6	-5.42	1.33	1.37
2	2	897	C	N1-C6	-5.41	1.33	1.37
1	1	393	C	N1-C6	-5.41	1.33	1.37
1	1	195	A	N9-C4	-5.41	1.34	1.37
1	1	2072	C	N1-C6	-5.39	1.33	1.37
1	1	1571	A	N9-C4	-5.39	1.34	1.37
1	1	1986	C	N1-C6	-5.39	1.33	1.37
1	1	1990	C	N1-C6	-5.39	1.33	1.37
1	1	2450	A	N9-C4	-5.39	1.34	1.37
54	z	32	A	N3-C4	-5.39	1.31	1.34
1	1	2612	C	N1-C6	-5.38	1.33	1.37
1	1	1822	C	N1-C6	-5.38	1.33	1.37
1	1	672	C	C4-C5	-5.38	1.38	1.43
2	2	792	A	N9-C4	-5.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2010	G	N9-C4	-5.38	1.33	1.38
1	1	1670	C	N1-C6	-5.36	1.33	1.37
1	1	1947	C	N1-C6	-5.36	1.33	1.37
2	2	931	C	N1-C6	-5.36	1.33	1.37
2	2	504	C	N1-C6	-5.36	1.33	1.37
1	1	640	C	N1-C6	-5.36	1.33	1.37
1	1	1899	A	N9-C4	-5.36	1.34	1.37
1	1	2719	G	C2-N2	-5.36	1.29	1.34
1	1	115	C	N1-C6	-5.35	1.33	1.37
1	1	1625	C	N1-C6	-5.34	1.33	1.37
3	3	76	G	N9-C4	-5.34	1.33	1.38
1	1	2497	A	N9-C4	-5.34	1.34	1.37
1	1	2010	G	N9-C8	-5.34	1.34	1.37
1	1	794	A	N9-C4	-5.34	1.34	1.37
1	1	246	C	N1-C6	-5.34	1.33	1.37
1	1	1297	C	N1-C6	-5.33	1.33	1.37
2	2	1524	C	N1-C6	-5.33	1.33	1.37
2	2	708	C	N1-C6	-5.33	1.33	1.37
1	1	2001	C	N1-C6	-5.33	1.33	1.37
1	1	2499	C	C5-C6	-5.33	1.30	1.34
1	1	151	C	N1-C6	-5.33	1.33	1.37
2	2	556	C	N1-C6	-5.32	1.33	1.37
2	2	810	C	N1-C6	-5.32	1.33	1.37
1	1	2688	G	N9-C4	-5.32	1.33	1.38
1	1	2815	C	N1-C6	-5.32	1.33	1.37
2	2	882	C	N1-C6	-5.31	1.33	1.37
1	1	1615	C	N1-C6	-5.31	1.33	1.37
1	1	1934	C	N1-C6	-5.31	1.33	1.37
1	1	1123	C	N1-C6	-5.30	1.33	1.37
1	1	378	C	N1-C6	-5.30	1.33	1.37
1	1	1362	C	N1-C6	-5.29	1.33	1.37
1	1	704	G	N9-C4	-5.29	1.33	1.38
54	z	30	A	N9-C4	-5.29	1.34	1.37
1	1	394	C	N1-C6	-5.29	1.33	1.37
1	1	2594	C	N1-C6	-5.29	1.33	1.37
2	2	795	C	N1-C6	-5.29	1.33	1.37
1	1	1152	C	N1-C6	-5.28	1.33	1.37
2	2	335	C	N1-C6	-5.28	1.33	1.37
1	1	192	C	N1-C6	-5.28	1.33	1.37
1	1	1196	C	N1-C6	-5.28	1.33	1.37
1	1	238	C	C4-C5	-5.27	1.38	1.43
1	1	1264	A	N9-C4	-5.27	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1996	C	N1-C6	-5.26	1.33	1.37
1	1	732	C	N1-C6	-5.26	1.33	1.37
1	1	1670	C	C4-N4	-5.26	1.29	1.33
2	2	400	C	N1-C6	-5.26	1.33	1.37
1	1	2496	C	N1-C6	-5.25	1.33	1.37
2	2	868	C	N1-C6	-5.25	1.33	1.37
1	1	383	C	N1-C6	-5.25	1.34	1.37
1	1	2502	G	N9-C4	-5.25	1.33	1.38
1	1	2440	C	N1-C6	-5.25	1.34	1.37
2	2	1501	C	N1-C6	-5.24	1.34	1.37
1	1	986	C	N1-C6	-5.24	1.34	1.37
1	1	2000	C	N1-C6	-5.24	1.34	1.37
1	1	2719	G	N9-C4	-5.24	1.33	1.38
1	1	2232	C	N1-C6	-5.23	1.34	1.37
1	1	2510	C	N1-C6	-5.23	1.34	1.37
2	2	797	C	N1-C6	-5.23	1.34	1.37
4	C	162	VAL	CB-CG1	-5.22	1.41	1.52
1	1	2036	C	N1-C6	-5.22	1.34	1.37
1	1	2465	C	N1-C6	-5.22	1.34	1.37
1	1	1265	A	N9-C4	-5.22	1.34	1.37
1	1	1974	C	N1-C6	-5.21	1.34	1.37
1	1	731	C	N1-C6	-5.21	1.34	1.37
1	1	1564	C	N1-C6	-5.20	1.34	1.37
1	1	780	G	N9-C4	-5.20	1.33	1.38
1	1	2678	C	N1-C6	-5.20	1.34	1.37
1	1	1192	G	N9-C4	-5.20	1.33	1.38
1	1	1161	C	N1-C6	-5.19	1.34	1.37
1	1	236	C	N1-C6	-5.19	1.34	1.37
1	1	690	G	N9-C8	-5.18	1.34	1.37
2	2	312	C	N1-C6	-5.18	1.34	1.37
2	2	624	C	N1-C6	-5.18	1.34	1.37
1	1	1257	C	C4-C5	-5.17	1.38	1.43
5	D	155	VAL	CB-CG2	-5.16	1.42	1.52
1	1	1237	A	N9-C4	-5.16	1.34	1.37
2	2	658	C	N1-C6	-5.16	1.34	1.37
2	2	334	C	N1-C6	-5.16	1.34	1.37
1	1	2033	A	N9-C4	-5.15	1.34	1.37
1	1	37	C	N1-C6	-5.15	1.34	1.37
1	1	1603	A	N9-C4	-5.15	1.34	1.37
1	1	1617	C	N1-C6	-5.15	1.34	1.37
54	z	85	A	C6-N6	-5.15	1.29	1.33
1	1	1961	C	N1-C6	-5.14	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1253	A	N9-C4	-5.14	1.34	1.37
1	1	253	C	N1-C6	-5.14	1.34	1.37
1	1	1646	C	N1-C6	-5.14	1.34	1.37
1	1	2451	A	N9-C4	-5.14	1.34	1.37
10	I	73	VAL	CB-CG1	-5.13	1.42	1.52
2	2	290	C	N1-C6	-5.13	1.34	1.37
1	1	2675	A	N9-C4	-5.13	1.34	1.37
1	1	2715	C	N1-C6	-5.13	1.34	1.37
2	2	1318	A	N9-C4	-5.13	1.34	1.37
1	1	461	C	N1-C6	-5.13	1.34	1.37
1	1	249	C	N1-C6	-5.12	1.34	1.37
1	1	2053	G	N9-C8	-5.12	1.34	1.37
1	1	2045	C	N1-C6	-5.12	1.34	1.37
2	2	580	C	N1-C6	-5.11	1.34	1.37
28	a	3	VAL	CB-CG1	-5.11	1.42	1.52
1	1	462	C	N1-C6	-5.11	1.34	1.37
1	1	2558	C	N1-C6	-5.11	1.34	1.37
1	1	1351	C	N1-C6	-5.10	1.34	1.37
1	1	1764	C	N1-C6	-5.10	1.34	1.37
2	2	823	C	N1-C6	-5.10	1.34	1.37
1	1	995	C	N1-C6	-5.09	1.34	1.37
1	1	865	C	N1-C6	-5.08	1.34	1.37
2	2	106	C	N1-C6	-5.08	1.34	1.37
1	1	2863	C	N1-C6	-5.08	1.34	1.37
1	1	578	G	C6-N1	-5.08	1.35	1.39
1	1	677	A	N9-C4	-5.08	1.34	1.37
1	1	16	C	N1-C6	-5.07	1.34	1.37
1	1	501	A	N9-C4	-5.07	1.34	1.37
2	2	856	C	N1-C6	-5.07	1.34	1.37
2	2	1521	C	N1-C6	-5.06	1.34	1.37
1	1	2575	C	N1-C6	-5.06	1.34	1.37
1	1	595	C	N1-C6	-5.05	1.34	1.37
1	1	2499	C	C4-C5	-5.05	1.39	1.43
2	2	330	C	N1-C6	-5.05	1.34	1.37
1	1	2704	C	N1-C6	-5.05	1.34	1.37
2	2	899	C	N1-C6	-5.05	1.34	1.37
1	1	1652	A	N9-C4	-5.04	1.34	1.37
27	Z	5	ILE	C-N	-5.04	1.22	1.34
1	1	420	C	N1-C6	-5.04	1.34	1.37
1	1	1152	C	N3-C4	-5.04	1.30	1.33
1	1	1793	C	N1-C6	-5.04	1.34	1.37
2	2	806	C	N1-C6	-5.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2611	C	N1-C6	-5.03	1.34	1.37
2	2	578	C	C4-C5	-5.03	1.39	1.43
1	1	2025	C	N1-C6	-5.03	1.34	1.37
2	2	1069	C	N1-C6	-5.03	1.34	1.37
1	1	1853	A	N9-C4	-5.02	1.34	1.37
1	1	821	A	N9-C4	-5.02	1.34	1.37
1	1	2853	C	N1-C6	-5.02	1.34	1.37
3	3	92	C	N1-C6	-5.02	1.34	1.37
1	1	1308	A	C6-N6	-5.02	1.29	1.33
2	2	765	G	N9-C4	-5.01	1.33	1.38
1	1	2285	C	N1-C6	-5.01	1.34	1.37
2	2	738	C	N1-C6	-5.01	1.34	1.37
2	2	718	A	N9-C4	-5.01	1.34	1.37

All (326) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1670	C	C5-C4-N4	-9.67	113.43	120.20
1	1	1670	C	N3-C4-C5	9.66	125.76	121.90
1	1	2719	G	C2-N3-C4	-9.16	107.32	111.90
1	1	2193	G	C4-N9-C1'	9.01	138.21	126.50
1	1	1509	A	O4'-C1'-N9	8.55	115.04	108.20
1	1	2193	G	C8-N9-C1'	-8.22	116.31	127.00
1	1	1871	A	O4'-C1'-N9	8.00	114.60	108.20
1	1	512	G	O4'-C1'-N9	7.92	114.53	108.20
1	1	2499	C	C5-C4-N4	-7.91	114.66	120.20
1	1	1923	U	O4'-C1'-N1	7.88	114.50	108.20
1	1	221	A	O4'-C1'-N9	7.58	114.26	108.20
1	1	481	G	O4'-C1'-N9	7.50	114.20	108.20
41	n	87	LEU	CA-CB-CG	7.47	132.48	115.30
54	z	32	A	C2-N3-C4	-7.42	106.89	110.60
1	1	275	C	C2-N1-C1'	-7.35	110.72	118.80
1	1	2799	A	N9-C4-C5	-7.30	102.88	105.80
1	1	2193	G	C6-C5-N7	-7.29	126.02	130.40
1	1	75	G	N3-C4-N9	-7.12	121.73	126.00
1	1	1857	G	O4'-C1'-N9	6.98	113.79	108.20
1	1	274	C	N1-C2-O2	6.97	123.08	118.90
1	1	801	G	C2-N3-C4	-6.97	108.42	111.90
1	1	1670	C	C6-N1-C2	6.94	123.07	120.30
1	1	982	C	N3-C4-C5	6.80	124.62	121.90
1	1	1905	C	N3-C4-C5	6.76	124.61	121.90
1	1	1187	G	C2-N3-C4	-6.75	108.53	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	z	84	C	N3-C4-C5	6.75	124.60	121.90
1	1	308	G	C2-N3-C4	-6.74	108.53	111.90
1	1	752	A	N1-C6-N6	6.74	122.64	118.60
1	1	2688	G	C2-N3-C4	-6.73	108.53	111.90
1	1	323	C	C2-N1-C1'	6.72	126.19	118.80
1	1	1615	C	C5-C4-N4	-6.71	115.51	120.20
1	1	1697	G	C2-N3-C4	-6.71	108.55	111.90
2	2	1221	G	N3-C4-C5	6.70	131.95	128.60
1	1	1728	C	N1-C2-O2	-6.70	114.88	118.90
2	2	581	G	C2-N3-C4	-6.67	108.57	111.90
1	1	2365	G	C2-N3-C4	-6.66	108.57	111.90
1	1	2430	A	N1-C6-N6	6.64	122.58	118.60
2	2	74	A	O4'-C1'-N9	6.63	113.51	108.20
2	2	1200	C	C5-C4-N4	-6.62	115.57	120.20
1	1	2719	G	N1-C2-N3	6.60	127.86	123.90
1	1	806	C	N1-C2-O2	6.59	122.85	118.90
2	2	686	U	O4'-C1'-N1	6.58	113.47	108.20
1	1	675	A	N1-C6-N6	6.57	122.54	118.60
1	1	2799	A	C4-C5-N7	6.55	113.97	110.70
1	1	818	G	C2-N3-C4	-6.46	108.67	111.90
1	1	2161	C	N3-C2-O2	-6.46	117.38	121.90
6	E	153	LEU	CA-CB-CG	6.44	130.12	115.30
1	1	2314	A	O4'-C1'-N9	6.43	113.35	108.20
2	2	976	G	N3-C2-N2	-6.42	115.40	119.90
1	1	469	G	C2-N3-C4	-6.41	108.70	111.90
1	1	1358	G	C2-N3-C4	-6.40	108.70	111.90
1	1	1313	U	C2-N1-C1'	6.35	125.32	117.70
1	1	2848	G	O4'-C1'-N9	6.32	113.26	108.20
1	1	2765	A	O4'-C1'-N9	6.32	113.26	108.20
1	1	733	G	C2-N3-C4	-6.29	108.75	111.90
1	1	916	G	C2-N3-C4	-6.29	108.75	111.90
1	1	757	G	N3-C4-C5	6.26	131.73	128.60
2	2	1403	C	C5-C4-N4	-6.26	115.81	120.20
2	2	575	G	N3-C4-N9	-6.26	122.24	126.00
2	2	792	A	O4'-C1'-N9	6.26	113.20	108.20
1	1	2158	A	O4'-C1'-N9	6.24	113.19	108.20
1	1	1670	C	C2-N3-C4	-6.23	116.78	119.90
2	2	1221	G	N3-C4-N9	-6.22	122.27	126.00
2	2	354	G	C2-N3-C4	-6.21	108.79	111.90
1	1	2454	G	C2-N3-C4	-6.20	108.80	111.90
2	2	1033	G	N3-C4-C5	6.20	131.70	128.60
1	1	1143	A	C5-C6-N6	-6.17	118.76	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	76	G	C2-N3-C4	-6.17	108.82	111.90
2	2	31	G	N3-C4-N9	-6.16	122.30	126.00
1	1	974	G	O4'-C1'-N9	6.14	113.11	108.20
1	1	275	C	C6-N1-C1'	6.13	128.15	120.80
54	z	84	C	C5-C4-N4	-6.13	115.91	120.20
1	1	308	G	N1-C2-N2	-6.10	110.71	116.20
1	1	323	C	C6-N1-C1'	-6.10	113.48	120.80
54	z	81	C	C6-N1-C2	6.07	122.73	120.30
2	2	1482	G	C2-N3-C4	-6.07	108.86	111.90
1	1	786	C	C6-N1-C2	6.06	122.72	120.30
2	2	765	G	C2-N3-C4	-6.04	108.88	111.90
1	1	1530	G	N9-C4-C5	-6.02	102.99	105.40
1	1	2799	A	N1-C6-N6	6.01	122.21	118.60
2	2	976	G	N3-C4-N9	-6.00	122.40	126.00
2	2	1160	G	N3-C4-N9	-6.00	122.40	126.00
1	1	1625	C	N1-C2-O2	6.00	122.50	118.90
2	2	791	G	C2-N3-C4	-6.00	108.90	111.90
2	2	993	G	O4'-C1'-N9	6.00	113.00	108.20
1	1	1459	G	N3-C4-C5	5.99	131.59	128.60
1	1	807	U	O4'-C1'-N1	5.97	112.98	108.20
3	3	76	G	N3-C4-C5	5.97	131.58	128.60
1	1	585	G	C2-N3-C4	-5.94	108.93	111.90
1	1	1062	G	C4-N9-C1'	5.93	134.21	126.50
1	1	2799	A	C6-C5-N7	-5.92	128.16	132.30
1	1	982	C	C5-C4-N4	-5.92	116.06	120.20
1	1	2714	G	C2-N3-C4	-5.92	108.94	111.90
1	1	1941	C	C5-C4-N4	-5.91	116.06	120.20
1	1	2036	C	N1-C2-O2	5.89	122.44	118.90
1	1	400	G	C2-N3-C4	-5.89	108.95	111.90
1	1	2164	C	P-O3'-C3'	-5.89	112.63	119.70
1	1	1788	C	N1-C2-O2	5.88	122.43	118.90
2	2	1502	A	N1-C6-N6	5.88	122.13	118.60
2	2	1033	G	N3-C4-N9	-5.87	122.48	126.00
1	1	942	G	C5-C6-O6	5.86	132.12	128.60
2	2	1396	A	C5-C6-N6	-5.86	119.01	123.70
1	1	1261	C	N3-C4-C5	5.86	124.24	121.90
1	1	2572	A	O4'-C1'-N9	5.86	112.88	108.20
1	1	1154	G	C2-N3-C4	-5.85	108.98	111.90
2	2	1109	C	O4'-C1'-N1	5.85	112.88	108.20
1	1	180	G	N3-C4-N9	-5.84	122.49	126.00
1	1	2382	G	C2-N3-C4	-5.84	108.98	111.90
1	1	780	G	C2-N3-C4	-5.83	108.99	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1339	G	C2-N3-C4	-5.82	108.99	111.90
1	1	26	G	C2-N3-C4	-5.80	109.00	111.90
1	1	2715	C	C2-N1-C1'	5.79	125.17	118.80
1	1	551	G	C8-N9-C1'	-5.79	119.47	127.00
1	1	189	G	C2-N3-C4	-5.78	109.01	111.90
1	1	708	G	O3'-P-O5'	-5.78	93.01	104.00
1	1	1062	G	C8-N9-C1'	-5.78	119.48	127.00
1	1	565	C	C6-N1-C2	5.76	122.61	120.30
1	1	704	G	O4'-C1'-N9	5.76	112.81	108.20
1	1	1062	G	C6-C5-N7	-5.76	126.95	130.40
1	1	882	G	C8-N9-C1'	-5.75	119.53	127.00
1	1	2722	G	C2-N3-C4	-5.74	109.03	111.90
1	1	395	U	O4'-C1'-N1	5.74	112.79	108.20
1	1	458	G	O4'-C1'-N9	5.73	112.78	108.20
1	1	2688	G	N3-C4-C5	5.71	131.46	128.60
1	1	2244	U	N3-C4-O4	5.71	123.40	119.40
54	z	43	G	N3-C4-N9	-5.71	122.58	126.00
1	1	180	G	N3-C4-C5	5.70	131.45	128.60
2	2	81	A	C8-N9-C4	-5.70	103.52	105.80
1	1	837	C	N3-C2-O2	-5.70	117.91	121.90
1	1	1131	G	C2-N3-C4	-5.69	109.06	111.90
1	1	2012	G	C2-N3-C4	-5.69	109.06	111.90
1	1	1115	G	O4'-C1'-N9	5.69	112.75	108.20
1	1	1790	C	C6-N1-C2	5.68	122.57	120.30
3	3	31	C	C2-N1-C1'	5.68	125.05	118.80
1	1	1143	A	N1-C6-N6	5.68	122.01	118.60
1	1	1261	C	C6-N1-C2	5.67	122.57	120.30
2	2	1028	C	C2-N1-C1'	-5.67	112.57	118.80
1	1	124	G	C2-N3-C4	-5.66	109.07	111.90
1	1	2715	C	C6-N1-C1'	-5.66	114.00	120.80
1	1	114	U	C2-N1-C1'	5.66	124.48	117.70
1	1	2248	C	C6-N1-C1'	-5.66	114.01	120.80
2	2	31	G	N3-C4-C5	5.65	131.43	128.60
1	1	726	G	N3-C4-C5	5.65	131.42	128.60
54	z	23	A	O4'-C1'-N9	5.65	112.72	108.20
1	1	2365	G	N1-C2-N2	-5.64	111.12	116.20
1	1	2075	U	N3-C4-O4	5.63	123.34	119.40
1	1	1950	G	N3-C4-N9	-5.63	122.62	126.00
1	1	672	C	N1-C2-O2	5.63	122.28	118.90
1	1	858	G	C2-N3-C4	-5.62	109.09	111.90
1	1	672	C	C2-N1-C1'	5.62	124.98	118.80
1	1	801	G	N3-C4-C5	5.61	131.40	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1905	C	C6-N1-C2	5.60	122.54	120.30
1	1	987	C	C6-N1-C2	5.58	122.53	120.30
1	1	2608	G	C2-N3-C4	-5.58	109.11	111.90
1	1	551	G	C4-N9-C1'	5.56	133.72	126.50
1	1	1828	G	C2-N3-C4	-5.55	109.12	111.90
3	3	31	C	C6-N1-C1'	-5.55	114.13	120.80
54	z	22	G	C2-N3-C4	-5.55	109.12	111.90
1	1	565	C	N3-C4-C5	5.55	124.12	121.90
1	1	2194	U	C2-N1-C1'	-5.54	111.05	117.70
1	1	2275	C	N1-C2-O2	5.53	122.22	118.90
1	1	1306	C	N3-C4-C5	5.52	124.11	121.90
1	1	2888	C	N1-C2-O2	5.51	122.21	118.90
1	1	675	A	C5-C6-N6	-5.51	119.29	123.70
1	1	2502	G	N3-C4-N9	-5.51	122.70	126.00
2	2	558	G	C2-N3-C4	-5.50	109.15	111.90
2	2	770	C	N3-C4-C5	5.50	124.10	121.90
1	1	2723	C	C6-N1-C1'	-5.50	114.20	120.80
2	2	271	C	C6-N1-C2	5.49	122.50	120.30
1	1	1564	C	N1-C2-O2	5.49	122.19	118.90
1	1	2253	G	C2-N3-C4	-5.49	109.16	111.90
1	1	2195	U	O4'-C1'-N1	5.47	112.58	108.20
2	2	1275	A	N1-C6-N6	5.47	121.88	118.60
2	2	73	C	C6-N1-C2	-5.47	118.11	120.30
25	X	48	ARG	CA-CB-CG	5.46	125.42	113.40
1	1	274	C	N3-C2-O2	-5.45	118.08	121.90
1	1	2308	G	C8-N9-C1'	5.45	134.08	127.00
1	1	1568	G	N3-C4-C5	5.45	131.32	128.60
2	2	1396	A	C4-C5-N7	5.45	113.42	110.70
1	1	748	G	O4'-C1'-N9	5.45	112.56	108.20
5	D	152	PRO	CA-N-CD	-5.44	103.89	111.50
2	2	1107	C	N3-C4-C5	5.43	124.07	121.90
1	1	780	G	N3-C4-C5	5.43	131.31	128.60
3	3	102	G	N3-C4-N9	-5.43	122.75	126.00
1	1	1371	G	C2-N3-C4	-5.42	109.19	111.90
1	1	33	C	O4'-C1'-N1	5.42	112.54	108.20
1	1	2308	G	C4-N9-C1'	-5.42	119.45	126.50
1	1	2193	G	N3-C4-N9	5.42	129.25	126.00
1	1	570	G	C2-N3-C4	-5.42	109.19	111.90
1	1	960	A	C5-C6-N1	5.42	120.41	117.70
1	1	1192	G	N3-C4-C5	5.41	131.31	128.60
1	1	2430	A	C5-C6-N6	-5.41	119.37	123.70
2	2	869	G	C2-N3-C4	-5.41	109.20	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2248	C	C2-N1-C1'	5.40	124.74	118.80
1	1	205	G	O4'-C1'-N9	5.40	112.52	108.20
54	z	32	A	N3-C4-C5	5.40	130.58	126.80
2	2	1222	G	N3-C4-N9	-5.40	122.76	126.00
1	1	2597	G	C2-N3-C4	-5.40	109.20	111.90
2	2	1304	G	C2-N3-C4	-5.39	109.20	111.90
1	1	2719	G	C5-C6-N1	-5.39	108.81	111.50
1	1	689	A	C5-C6-N6	-5.38	119.39	123.70
1	1	2035	G	O4'-C1'-N9	5.38	112.51	108.20
2	2	1079	G	C2-N3-C4	-5.38	109.21	111.90
2	2	322	C	N3-C4-C5	5.37	124.05	121.90
1	1	2499	C	C6-N1-C1'	-5.37	114.36	120.80
2	2	207	C	N1-C2-O2	-5.36	115.68	118.90
1	1	2271	G	C2-N3-C4	-5.36	109.22	111.90
2	2	1373	G	C2-N3-C4	-5.35	109.22	111.90
1	1	2894	G	N3-C4-N9	-5.35	122.79	126.00
1	1	2440	C	C5-C4-N4	-5.35	116.46	120.20
1	1	563	A	N1-C6-N6	-5.34	115.40	118.60
1	1	2190	G	C6-C5-N7	-5.34	127.20	130.40
1	1	484	C	C5-C4-N4	-5.34	116.46	120.20
1	1	1905	C	C2-N3-C4	-5.33	117.23	119.90
2	2	682	G	N3-C4-C5	5.33	131.26	128.60
1	1	726	G	N3-C4-N9	-5.33	122.80	126.00
54	z	24	C	C2-N1-C1'	5.33	124.66	118.80
1	1	338	G	C2-N3-C4	-5.33	109.24	111.90
1	1	1761	C	N3-C4-C5	5.31	124.03	121.90
1	1	2715	C	N1-C2-O2	5.31	122.08	118.90
1	1	2124	G	N3-C4-N9	-5.30	122.82	126.00
2	2	1366	C	N1-C2-O2	5.30	122.08	118.90
2	2	1034	G	O4'-C1'-N9	5.29	112.44	108.20
1	1	680	C	N1-C2-O2	5.29	122.07	118.90
1	1	882	G	C4-N9-C1'	5.29	133.38	126.50
1	1	2193	G	C4-C5-N7	5.29	112.92	110.80
1	1	1996	C	C5-C4-N4	-5.29	116.50	120.20
2	2	66	A	C4-C5-N7	5.29	113.34	110.70
2	2	770	C	C6-N1-C2	5.29	122.41	120.30
54	z	9	G	OP1-P-OP2	5.29	127.53	119.60
1	1	1212	G	N3-C4-C5	5.28	131.24	128.60
1	1	2720	U	N3-C4-O4	5.27	123.09	119.40
1	1	2323	G	C2-N3-C4	-5.27	109.26	111.90
1	1	1788	C	C2-N1-C1'	5.27	124.60	118.80
1	1	2592	G	C2-N3-C4	-5.27	109.27	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1299	G	C2-N3-C4	-5.26	109.27	111.90
2	2	1502	A	C5-C6-N6	-5.26	119.49	123.70
1	1	2083	G	C2-N3-C4	-5.26	109.27	111.90
1	1	215	G	C2-N3-C4	-5.25	109.28	111.90
1	1	1894	C	N1-C2-O2	5.23	122.04	118.90
1	1	488	G	C2-N3-C4	-5.23	109.28	111.90
1	1	2709	G	C2-N3-C4	-5.23	109.29	111.90
54	z	28	C	N1-C2-O2	5.23	122.04	118.90
1	1	581	C	C6-N1-C1'	-5.22	114.54	120.80
1	1	1266	G	N3-C4-N9	-5.22	122.87	126.00
1	1	1673	G	C2-N3-C4	-5.21	109.30	111.90
1	1	1350	C	C6-N1-C2	5.20	122.38	120.30
1	1	1143	A	C4-C5-N7	5.20	113.30	110.70
1	1	726	G	C2-N3-C4	-5.20	109.30	111.90
3	3	117	G	N3-C4-C5	5.20	131.20	128.60
1	1	2858	C	C5-C4-N4	-5.19	116.57	120.20
54	z	31	G	N1-C6-O6	5.19	123.01	119.90
1	1	2123	G	O4'-C1'-N9	5.19	112.35	108.20
2	2	15	G	C2-N3-C4	-5.19	109.31	111.90
1	1	2325	G	C2-N3-C4	-5.18	109.31	111.90
2	2	879	C	C6-N1-C2	5.18	122.37	120.30
2	2	858	G	C2-N3-C4	-5.18	109.31	111.90
1	1	37	C	N3-C4-C5	5.18	123.97	121.90
1	1	1339	G	N3-C4-N9	-5.17	122.90	126.00
1	1	1631	G	C2-N3-C4	-5.17	109.32	111.90
1	1	1223	G	C2-N3-C4	-5.16	109.32	111.90
1	1	1761	C	C5-C4-N4	-5.16	116.59	120.20
1	1	1904	G	C2-N3-C4	-5.16	109.32	111.90
3	3	66	A	N1-C6-N6	5.16	121.69	118.60
3	3	15	A	N1-C6-N6	5.15	121.69	118.60
1	1	583	G	C2-N3-C4	-5.15	109.33	111.90
1	1	1257	C	C6-N1-C2	5.15	122.36	120.30
1	1	801	G	N3-C4-N9	-5.15	122.91	126.00
1	1	2502	G	C2-N3-C4	-5.15	109.33	111.90
1	1	585	G	N1-C2-N3	5.14	126.99	123.90
1	1	383	C	C5-C4-N4	-5.14	116.60	120.20
1	1	794	A	C5-N7-C8	-5.13	101.33	103.90
1	1	2458	G	C2-N3-C4	-5.13	109.33	111.90
1	1	2723	C	C2-N1-C1'	5.13	124.44	118.80
1	1	1521	G	C2-N3-C4	-5.12	109.34	111.90
1	1	704	G	N3-C4-C5	5.12	131.16	128.60
1	1	242	G	N3-C4-N9	-5.12	122.93	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1459	G	N3-C4-N9	-5.11	122.93	126.00
1	1	1675	C	C5-C4-N4	-5.11	116.62	120.20
1	1	2029	G	C2-N3-C4	-5.11	109.34	111.90
2	2	21	G	C2-N3-C4	-5.11	109.34	111.90
26	Y	16	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	1	1935	G	C2-N3-C4	-5.11	109.34	111.90
1	1	2447	G	C2-N3-C4	-5.10	109.35	111.90
2	2	580	C	N1-C2-O2	5.10	121.96	118.90
1	1	748	G	N3-C4-N9	-5.09	122.94	126.00
1	1	1653	G	C2-N3-C4	-5.09	109.36	111.90
1	1	2443	C	N1-C2-O2	5.09	121.95	118.90
1	1	941	A	C5-C6-N6	-5.09	119.63	123.70
1	1	757	G	N3-C4-N9	-5.08	122.95	126.00
1	1	1436	G	C2-N3-C4	-5.08	109.36	111.90
1	1	581	C	N3-C4-C5	5.08	123.93	121.90
1	1	704	G	N3-C4-N9	-5.07	122.96	126.00
1	1	1530	G	C8-N9-C1'	-5.07	120.42	127.00
1	1	2502	G	N3-C4-C5	5.07	131.13	128.60
1	1	1836	C	N3-C4-C5	5.06	123.93	121.90
54	z	11	C	C6-N1-C2	5.06	122.33	120.30
1	1	601	C	O4'-C1'-N1	5.06	112.25	108.20
1	1	2440	C	N3-C4-C5	5.06	123.92	121.90
1	1	2194	U	O4'-C1'-N1	5.06	112.25	108.20
54	z	31	G	C2-N3-C4	-5.06	109.37	111.90
1	1	709	U	C6-N1-C2	-5.06	117.97	121.00
1	1	1313	U	C6-N1-C1'	-5.06	114.12	121.20
1	1	1573	G	C2-N3-C4	-5.06	109.37	111.90
1	1	2417	C	N1-C2-O2	5.05	121.93	118.90
1	1	1288	G	C2-N3-C4	-5.05	109.38	111.90
1	1	701	G	C2-N3-C4	-5.05	109.38	111.90
1	1	857	G	C2-N3-C4	-5.05	109.38	111.90
2	2	1331	G	O4'-C1'-N9	5.04	112.23	108.20
1	1	2834	G	C2-N3-C4	-5.04	109.38	111.90
2	2	1266	G	N3-C4-N9	-5.04	122.98	126.00
1	1	1320	C	O4'-C1'-N1	5.03	112.23	108.20
1	1	2110	G	N9-C1'-C2'	5.03	120.54	114.00
2	2	812	G	C2-N3-C4	-5.03	109.39	111.90
2	2	765	G	N3-C4-N9	-5.03	122.98	126.00
1	1	2676	C	N1-C2-O2	5.02	121.91	118.90
2	2	733	G	O4'-C1'-N9	5.02	112.22	108.20
1	1	776	G	C2-N3-C4	-5.01	109.39	111.90
1	1	1568	G	N3-C4-N9	-5.01	122.99	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	650	C	N1-C2-O2	5.01	121.91	118.90
2	2	169	C	O4'-C1'-N1	5.01	112.21	108.20
2	2	580	C	C2-N1-C1'	5.01	124.31	118.80
1	1	1125	G	C2-N3-C4	-5.00	109.40	111.90
1	1	2723	C	N1-C2-O2	5.00	121.90	118.90
2	2	335	C	N3-C4-C5	5.00	123.90	121.90
1	1	1728	C	C2-N1-C1'	-5.00	113.30	118.80

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	
4	C	269/271 (99%)	256 (95%)	13 (5%)	0	100	100
5	D	207/209 (99%)	201 (97%)	3 (1%)	3 (1%)	11	43
6	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
7	F	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	25	64
8	G	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
9	H	147/149 (99%)	135 (92%)	10 (7%)	2 (1%)	11	43
10	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	J	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
12	K	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
13	L	134/136 (98%)	130 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	M	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
15	N	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
16	O	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
17	P	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
18	Q	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	7	34
19	R	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
20	S	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
21	T	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
22	U	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
23	V	82/84 (98%)	73 (89%)	7 (8%)	2 (2%)	6	29
24	W	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
25	X	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	Z	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
28	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	b	50/52 (96%)	50 (100%)	0	0	100	100
30	c	44/46 (96%)	44 (100%)	0	0	100	100
31	d	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
32	e	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
33	f	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
34	g	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
35	h	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
36	i	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
37	j	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
38	k	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
39	l	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
40	m	125/127 (98%)	117 (94%)	8 (6%)	0	100	100
41	n	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
42	o	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
43	p	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
44	q	114/116 (98%)	109 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	r	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
46	s	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
47	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
48	u	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
49	v	64/66 (97%)	64 (100%)	0	0	100	100
50	w	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
51	x	84/86 (98%)	84 (100%)	0	0	100	100
52	y	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
55	B	37/39 (95%)	29 (78%)	8 (22%)	0	100	100
All	All	5653/5754 (98%)	5440 (96%)	203 (4%)	10 (0%)	50	82

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	152	PRO
5	D	153	GLY
5	D	154	LYS
9	H	90	LEU
23	V	5	LYS
23	V	11	ARG
18	Q	52	PRO
18	Q	53	PHE
9	H	89	LYS
7	F	124	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	216/216 (100%)	216 (100%)	0	100	100
5	D	164/164 (100%)	163 (99%)	1 (1%)	86	95
6	E	165/165 (100%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	148/148 (100%)	148 (100%)	0	100	100
8	G	136/136 (100%)	135 (99%)	1 (1%)	84	94
9	H	114/114 (100%)	113 (99%)	1 (1%)	78	92
10	I	116/116 (100%)	116 (100%)	0	100	100
11	J	104/104 (100%)	103 (99%)	1 (1%)	76	91
12	K	103/103 (100%)	102 (99%)	1 (1%)	76	91
13	L	109/109 (100%)	108 (99%)	1 (1%)	78	92
14	M	99/99 (100%)	98 (99%)	1 (1%)	76	91
15	N	86/86 (100%)	86 (100%)	0	100	100
16	O	99/99 (100%)	99 (100%)	0	100	100
17	P	89/89 (100%)	88 (99%)	1 (1%)	73	90
18	Q	84/84 (100%)	84 (100%)	0	100	100
19	R	93/93 (100%)	93 (100%)	0	100	100
20	S	81/81 (100%)	81 (100%)	0	100	100
21	T	84/84 (100%)	83 (99%)	1 (1%)	71	90
22	U	78/78 (100%)	77 (99%)	1 (1%)	69	89
23	V	62/62 (100%)	62 (100%)	0	100	100
24	W	67/67 (100%)	67 (100%)	0	100	100
25	X	54/54 (100%)	54 (100%)	0	100	100
26	Y	48/48 (100%)	48 (100%)	0	100	100
27	Z	59/59 (100%)	59 (100%)	0	100	100
28	a	47/47 (100%)	47 (100%)	0	100	100
29	b	47/47 (100%)	47 (100%)	0	100	100
30	c	38/38 (100%)	38 (100%)	0	100	100
31	d	51/51 (100%)	49 (96%)	2 (4%)	32	69
32	e	34/34 (100%)	34 (100%)	0	100	100
33	f	187/187 (100%)	187 (100%)	0	100	100
34	g	171/171 (100%)	169 (99%)	2 (1%)	71	90
35	h	172/172 (100%)	172 (100%)	0	100	100
36	i	119/119 (100%)	117 (98%)	2 (2%)	60	85
37	j	91/91 (100%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	k	124/124 (100%)	124 (100%)	0	100	100
39	l	104/104 (100%)	104 (100%)	0	100	100
40	m	105/105 (100%)	103 (98%)	2 (2%)	57	84
41	n	86/86 (100%)	84 (98%)	2 (2%)	50	80
42	o	90/90 (100%)	89 (99%)	1 (1%)	73	90
43	p	102/102 (100%)	102 (100%)	0	100	100
44	q	94/94 (100%)	94 (100%)	0	100	100
45	r	83/83 (100%)	83 (100%)	0	100	100
46	s	76/76 (100%)	76 (100%)	0	100	100
47	t	65/65 (100%)	65 (100%)	0	100	100
48	u	74/74 (100%)	74 (100%)	0	100	100
49	v	57/57 (100%)	57 (100%)	0	100	100
50	w	72/72 (100%)	71 (99%)	1 (1%)	67	88
51	x	65/65 (100%)	65 (100%)	0	100	100
52	y	60/60 (100%)	58 (97%)	2 (3%)	38	73
55	B	16/28 (57%)	16 (100%)	0	100	100
All	All	4688/4700 (100%)	4664 (100%)	24 (0%)	89	96

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	151	THR
8	G	47	ASP
9	H	122	LEU
11	J	17	ARG
12	K	48	ARG
13	L	59	ARG
14	M	80	PHE
17	P	78	LYS
21	T	68	SER
22	U	10	LYS
31	d	31	HIS
31	d	51	SER
34	g	118	ASP
34	g	164	ARG
36	i	29	ARG

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Mol	Chain	Res	Type
36	i	93	ARG
40	m	25	ASN
40	m	106	ARG
41	n	5	ARG
41	n	87	LEU
42	o	56	ARG
50	w	78	ARG
52	y	5	LYS
52	y	13	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
8	G	38	ASN
9	H	128	HIS
31	d	31	HIS
33	f	36	ASN
50	w	69	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2903 (99%)	494 (17%)	10 (0%)
2	2	1529/1534 (99%)	255 (16%)	5 (0%)
3	3	119/120 (99%)	16 (13%)	0
53	4	5/6 (83%)	1 (20%)	0
54	z	84/85 (98%)	26 (30%)	0
All	All	4635/4648 (99%)	792 (17%)	15 (0%)

All (792) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	51	G
1	1	71	A
1	1	74	A

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Mol	Chain	Res	Type
1	1	75	G
1	1	80	G
1	1	84	A
1	1	85	G
1	1	101	A
1	1	102	U
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U
1	1	122	G
1	1	125	A
1	1	138	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A
1	1	221	A
1	1	222	A
1	1	225	C
1	1	248	G
1	1	249	C
1	1	264	C
1	1	265	A
1	1	266	G
1	1	272	A
1	1	273	G
1	1	275	C
1	1	276	U
1	1	285	G
1	1	301	G
1	1	311	A
1	1	329	G
1	1	330	A
1	1	343	C
1	1	353	C
1	1	361	G

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Mol	Chain	Res	Type
1	1	371	A
1	1	372	G
1	1	383	C
1	1	386	G
1	1	396	G
1	1	399	U
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	435	C
1	1	457	A
1	1	467	G
1	1	481	G
1	1	489	G
1	1	491	G
1	1	505	A
1	1	509	C
1	1	513	A
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C
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	573	U
1	1	575	A
1	1	603	A
1	1	609	A
1	1	612	G
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	621	A
1	1	627	A
1	1	637	A

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Mol	Chain	Res	Type
1	1	645	C
1	1	647	G
1	1	654	A
1	1	655	A
1	1	670	A
1	1	685	A
1	1	686	U
1	1	702	U
1	1	717	C
1	1	726	G
1	1	730	A
1	1	747	5MU
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	792	A
1	1	800	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	866	A
1	1	869	G
1	1	878	A
1	1	880	G
1	1	882	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U

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Mol	Chain	Res	Type
1	1	896	A
1	1	897	C
1	1	898	C
1	1	907	G
1	1	910	A
1	1	931	U
1	1	932	U
1	1	941	A
1	1	946	C
1	1	961	C
1	1	973	A
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
1	1	1022	G
1	1	1023	U
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1060	U
1	1	1061	U
1	1	1062	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	1071	G
1	1	1073	A
1	1	1084	A
1	1	1085	A

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Mol	Chain	Res	Type
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1096	A
1	1	1101	U
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1122	G
1	1	1128	G
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1136	G
1	1	1139	G
1	1	1142	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1171	G
1	1	1173	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1182	G
1	1	1186	G
1	1	1206	G
1	1	1212	G
1	1	1218	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1250	G
1	1	1253	A
1	1	1256	G
1	1	1266	G

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Mol	Chain	Res	Type
1	1	1271	G
1	1	1272	A
1	1	1300	G
1	1	1301	A
1	1	1321	A
1	1	1324	G
1	1	1325	U
1	1	1329	U
1	1	1341	G
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1408	G
1	1	1417	C
1	1	1419	A
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1460	U
1	1	1468	U
1	1	1476	U
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1494	A
1	1	1503	A
1	1	1504	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1532	A
1	1	1535	A
1	1	1536	C

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Mol	Chain	Res	Type
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1583	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1608	A
1	1	1619	G
1	1	1634	A
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1756	G
1	1	1764	C
1	1	1773	A
1	1	1782	U
1	1	1791	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	1835	2MG
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1865	U
1	1	1868	C

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Mol	Chain	Res	Type
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1896	G
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1914	C
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A
1	1	1938	A
1	1	1955	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2033	A
1	1	2043	C
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	2093	G
1	1	2095	A
1	1	2100	G

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Mol	Chain	Res	Type
1	1	2102	G
1	1	2107	G
1	1	2110	G
1	1	2112	G
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2121	G
1	1	2122	U
1	1	2125	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2140	G
1	1	2142	A
1	1	2145	C
1	1	2146	C
1	1	2147	A
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	2173	A
1	1	2178	C
1	1	2183	A
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2211	A

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Mol	Chain	Res	Type
1	1	2225	A
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2278	A
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2305	U
1	1	2309	A
1	1	2319	G
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G

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Mol	Chain	Res	Type
1	1	2476	A
1	1	2478	A
1	1	2480	C
1	1	2491	U
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2586	U
1	1	2602	A
1	1	2609	U
1	1	2613	U
1	1	2629	U
1	1	2646	C
1	1	2663	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2725	A
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	2765	A
1	1	2777	G

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Mol	Chain	Res	Type
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2797	U
1	1	2799	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2825	G
1	1	2833	U
1	1	2835	A
1	1	2836	U
1	1	2861	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2898	U
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	66	A
2	2	68	G
2	2	69	G
2	2	70	U
2	2	72	A
2	2	73	C

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Mol	Chain	Res	Type
2	2	74	A
2	2	75	G
2	2	76	G
2	2	81	A
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	92	U
2	2	120	A
2	2	121	U
2	2	130	A
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A
2	2	160	A
2	2	163	C
2	2	164	G
2	2	177	G
2	2	181	A
2	2	182	A
2	2	197	A
2	2	204	G
2	2	210	C
2	2	211	G
2	2	212	G
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	266	G
2	2	267	C
2	2	279	A
2	2	289	G
2	2	306	A
2	2	319	G
2	2	321	A
2	2	328	C
2	2	332	G
2	2	347	G

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Mol	Chain	Res	Type
2	2	352	C
2	2	354	G
2	2	362	G
2	2	367	U
2	2	372	C
2	2	384	G
2	2	392	C
2	2	398	U
2	2	406	G
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	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	476	U
2	2	478	A
2	2	479	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	496	A
2	2	499	A
2	2	510	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	521	G
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	533	A

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Mol	Chain	Res	Type
2	2	547	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	605	U
2	2	633	G
2	2	650	G
2	2	653	U
2	2	660	C
2	2	665	A
2	2	700	G
2	2	701	U
2	2	702	A
2	2	703	G
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	753	A
2	2	755	G
2	2	777	A
2	2	787	A
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
2	2	821	G
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	843	U
2	2	844	G

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Mol	Chain	Res	Type
2	2	845	A
2	2	846	G
2	2	884	U
2	2	885	G
2	2	887	G
2	2	914	A
2	2	934	C
2	2	935	A
2	2	960	U
2	2	965	U
2	2	966	2MG
2	2	967	5MC
2	2	969	A
2	2	971	G
2	2	972	C
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	982	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1004	A
2	2	1009	U
2	2	1019	A
2	2	1020	G
2	2	1022	A
2	2	1025	U
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1034	G
2	2	1043	G
2	2	1046	A
2	2	1065	U
2	2	1085	U
2	2	1089	G
2	2	1094	G
2	2	1095	U

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Mol	Chain	Res	Type
2	2	1101	A
2	2	1104	G
2	2	1108	G
2	2	1124	G
2	2	1125	U
2	2	1132	C
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1169	A
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1212	U
2	2	1213	A
2	2	1215	G
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G

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Mol	Chain	Res	Type
2	2	1299	A
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1335	U
2	2	1336	C
2	2	1340	A
2	2	1346	A
2	2	1353	G
2	2	1363	A
2	2	1364	U
2	2	1370	G
2	2	1379	G
2	2	1381	U
2	2	1419	G
2	2	1446	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	9	G
3	3	13	G
3	3	24	G
3	3	31	C
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A

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Mol	Chain	Res	Type
3	3	109	A
53	4	6	A
54	z	7	G
54	z	8	5MU
54	z	14	A
54	z	16	U
54	z	17	U
54	z	18	G
54	z	19	G
54	z	20	5MU
54	z	21	A
54	z	22	G
54	z	23	A
54	z	24	C
54	z	46	G
54	z	49	G
54	z	57	5MU
54	z	58	G
54	z	62	G
54	z	63	5MU
54	z	64	5MU
54	z	67	A
54	z	68	G
54	z	69	5MU
54	z	70	C
54	z	71	5MU
54	z	76	5MU
54	z	85	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	372	G
1	1	404	A
1	1	613	A
1	1	784	G
1	1	891	G
1	1	894	U
1	1	1379	U
1	1	1475	G
1	1	2189	U
1	1	2756	U

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Mol	Chain	Res	Type
2	2	85	U
2	2	86	G
2	2	516	PSU
2	2	1109	C
2	2	1145	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	3TD	1	1915	1	18,22,23	4.04	7 (38%)	22,32,35	1.54	3 (13%)
1	PSU	1	2457	1	18,21,22	1.18	2 (11%)	22,30,33	2.20	5 (22%)
1	5MU	1	1939	56,1	19,22,23	4.39	7 (36%)	28,32,35	3.71	10 (35%)
1	2MA	1	2503	56,1	17,25,26	2.14	3 (17%)	17,37,40	1.30	3 (17%)
54	5MU	z	39	54	19,22,23	1.44	5 (26%)	28,32,35	2.17	9 (32%)
54	5MU	z	42	54,2	19,22,23	4.34	7 (36%)	28,32,35	3.84	11 (39%)
1	2MG	1	1835	1	18,26,27	2.04	7 (38%)	16,38,41	1.45	3 (18%)
2	5MC	2	1407	2	18,22,23	3.12	7 (38%)	26,32,35	0.90	1 (3%)
1	2MG	1	2445	1	18,26,27	2.15	7 (38%)	16,38,41	1.25	4 (25%)
1	PSU	1	2605	1	18,21,22	1.05	1 (5%)	22,30,33	1.92	4 (18%)
1	PSU	1	2580	56,1	18,21,22	1.14	1 (5%)	22,30,33	2.23	6 (27%)
2	MA6	2	1519	2	18,26,27	1.37	1 (5%)	19,38,41	3.65	2 (10%)
1	OMC	1	2498	56,1	19,22,23	2.51	6 (31%)	26,31,34	0.96	0
2	PSU	2	516	56,2	18,21,22	0.97	1 (5%)	22,30,33	1.88	3 (13%)
54	5MU	z	71	54	19,22,23	1.34	5 (26%)	28,32,35	2.21	9 (32%)
54	5MU	z	57	54	19,22,23	4.54	7 (36%)	28,32,35	3.71	9 (32%)
1	OMG	1	2251	54,1	18,26,27	2.01	7 (38%)	19,38,41	1.44	4 (21%)
54	5MU	z	55	54	19,22,23	4.68	7 (36%)	28,32,35	3.48	9 (32%)
2	2MG	2	1207	2	18,26,27	2.22	7 (38%)	16,38,41	1.35	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	0TD	p	89	43	7,9,10	1.49	1 (14%)	6,11,13	1.92	2 (33%)
2	4OC	2	1402	2	20,23,24	2.69	8 (40%)	26,32,35	1.08	1 (3%)
54	5MU	z	64	54	19,22,23	1.44	6 (31%)	28,32,35	2.32	7 (25%)
2	2MG	2	1516	2	18,26,27	2.21	7 (38%)	16,38,41	1.47	4 (25%)
1	PSU	1	1911	1	18,21,22	0.90	0	22,30,33	1.87	3 (13%)
2	5MC	2	967	2	18,22,23	3.27	7 (38%)	26,32,35	1.12	2 (7%)
54	5MU	z	40	54	19,22,23	1.38	5 (26%)	28,32,35	2.27	11 (39%)
1	PSU	1	746	56,1	18,21,22	1.04	2 (11%)	22,30,33	1.74	3 (13%)
1	G7M	1	2069	1	20,26,27	2.17	8 (40%)	17,39,42	1.29	2 (11%)
2	MA6	2	1518	2	18,26,27	1.31	1 (5%)	19,38,41	3.44	2 (10%)
1	PSU	1	2504	1	18,21,22	0.98	1 (5%)	22,30,33	1.85	4 (18%)
54	5MU	z	20	56,54	19,22,23	4.78	7 (36%)	28,32,35	3.73	9 (32%)
1	PSU	1	1917	1	18,21,22	1.01	1 (5%)	22,30,33	2.13	5 (22%)
2	G7M	2	527	2	20,26,27	2.23	9 (45%)	17,39,42	1.11	1 (5%)
1	5MU	1	747	1	19,22,23	4.50	7 (36%)	28,32,35	3.78	9 (32%)
54	5MU	z	69	54	19,22,23	6.60	6 (31%)	28,32,35	28.78	14 (50%)
1	PSU	1	955	1	18,21,22	1.08	1 (5%)	22,30,33	1.99	5 (22%)
1	6MZ	1	1618	1	18,25,26	1.89	5 (27%)	16,36,39	3.26	3 (18%)
1	OMU	1	2552	1	19,22,23	2.74	6 (31%)	26,31,34	1.67	6 (23%)
1	6MZ	1	2030	1	18,25,26	1.89	4 (22%)	16,36,39	3.27	3 (18%)
54	5MU	z	8	54	19,22,23	4.51	7 (36%)	28,32,35	3.93	9 (32%)
2	2MG	2	966	2	18,26,27	2.27	7 (38%)	16,38,41	1.32	3 (18%)
2	UR3	2	1498	2	19,22,23	2.41	6 (31%)	26,32,35	1.04	2 (7%)
1	5MC	1	1962	1	18,22,23	3.04	7 (38%)	26,32,35	1.26	5 (19%)
54	5MU	z	63	54	19,22,23	1.45	6 (31%)	28,32,35	2.45	13 (46%)
1	1MG	1	745	1	18,26,27	2.61	5 (27%)	19,39,42	1.62	4 (21%)
54	5MU	z	76	54	19,22,23	1.43	6 (31%)	28,32,35	2.14	9 (32%)

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
1	3TD	1	1915	1	-	3/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1	1939	56,1	-	0/7/25/26	0/2/2/2
1	2MA	1	2503	56,1	-	2/3/25/26	0/3/3/3
54	5MU	z	39	54	-	4/7/25/26	0/2/2/2
54	5MU	z	42	54,2	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2580	56,1	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	5/7/29/30	0/3/3/3
1	OMC	1	2498	56,1	-	0/9/27/28	0/2/2/2
2	PSU	2	516	56,2	-	2/7/25/26	0/2/2/2
54	5MU	z	71	54	-	3/7/25/26	0/2/2/2
54	5MU	z	57	54	-	2/7/25/26	0/2/2/2
1	OMG	1	2251	54,1	-	0/5/27/28	0/3/3/3
54	5MU	z	55	54	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
43	0TD	p	89	43	-	3/7/12/14	-
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
54	5MU	z	64	54	-	2/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	2/7/25/26	0/2/2/2
54	5MU	z	40	54	-	2/7/25/26	0/2/2/2
1	PSU	1	746	56,1	-	1/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	1/3/25/26	0/3/3/3
2	MA6	2	1518	2	-	3/7/29/30	0/3/3/3
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
54	5MU	z	20	56,54	-	4/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
2	G7M	2	527	2	-	3/3/25/26	0/3/3/3
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
54	5MU	z	69	54	-	2/7/25/26	1/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	1618	1	-	3/5/27/28	0/3/3/3
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MU	z	8	54	-	2/7/25/26	0/2/2/2
2	2MG	2	966	2	-	0/5/27/28	0/3/3/3
2	UR3	2	1498	2	-	1/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
54	5MU	z	63	54	-	2/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
54	5MU	z	76	54	-	2/7/25/26	0/2/2/2

All (231) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	69	5MU	C6-C5	23.78	1.73	1.34
1	1	1915	3TD	C6-C5	11.71	1.49	1.35
54	z	57	5MU	C2-N1	11.02	1.56	1.38
54	z	20	5MU	C2-N1	10.76	1.55	1.38
54	z	20	5MU	C6-N1	10.47	1.55	1.38
54	z	42	5MU	C2-N1	10.46	1.55	1.38
54	z	55	5MU	C2-N1	10.34	1.55	1.38
54	z	20	5MU	C4-C5	10.30	1.61	1.44
54	z	55	5MU	C6-N1	10.22	1.55	1.38
1	1	747	5MU	C2-N1	10.12	1.54	1.38
1	1	1939	5MU	C2-N1	9.97	1.54	1.38
54	z	69	5MU	C4-C5	-9.95	1.28	1.44
54	z	8	5MU	C2-N1	9.91	1.54	1.38
1	1	747	5MU	C6-N1	9.67	1.54	1.38
54	z	55	5MU	C4-C5	9.54	1.60	1.44
54	z	8	5MU	C6-N1	9.25	1.53	1.38
54	z	57	5MU	C6-N1	9.21	1.53	1.38
54	z	8	5MU	C4-C5	9.20	1.60	1.44
54	z	69	5MU	C6-N1	9.20	1.53	1.38
1	1	1939	5MU	C6-N1	9.01	1.53	1.38
1	1	1915	3TD	C2-N1	8.95	1.48	1.37
1	1	1939	5MU	C4-C5	8.85	1.59	1.44
1	1	747	5MU	C4-C5	8.50	1.58	1.44
54	z	42	5MU	C6-N1	8.50	1.52	1.38
54	z	42	5MU	C4-N3	-8.42	1.23	1.38
54	z	57	5MU	C4-C5	8.37	1.58	1.44
2	2	1407	5MC	C6-C5	8.23	1.48	1.34
54	z	57	5MU	C4-N3	-8.16	1.23	1.38
54	z	42	5MU	C4-C5	8.05	1.58	1.44
1	1	747	5MU	C4-N3	-7.99	1.24	1.38
2	2	967	5MC	C6-C5	7.97	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1939	5MU	C4-N3	-7.86	1.24	1.38
54	z	8	5MU	C4-N3	-7.86	1.24	1.38
54	z	55	5MU	C4-N3	-7.64	1.24	1.38
1	1	745	1MG	C2-N2	7.49	1.47	1.34
1	1	1962	5MC	C6-C5	7.07	1.46	1.34
54	z	69	5MU	C4-N3	6.96	1.51	1.38
54	z	20	5MU	C4-N3	-6.96	1.25	1.38
2	2	1402	4OC	C4-N3	6.27	1.43	1.32
1	1	1962	5MC	C4-N3	6.24	1.44	1.34
2	2	967	5MC	C4-N3	6.19	1.44	1.34
1	1	2552	OMU	C2-N3	6.10	1.48	1.38
54	z	55	5MU	C6-C5	6.04	1.44	1.34
1	1	2503	2MA	C2-N3	6.04	1.44	1.31
54	z	20	5MU	C6-C5	5.96	1.44	1.34
2	2	1498	UR3	C6-C5	5.95	1.48	1.35
2	2	967	5MC	C2-N3	5.85	1.48	1.36
1	1	2552	OMU	C2-N1	5.76	1.47	1.38
1	1	1915	3TD	C6-N1	5.70	1.45	1.36
1	1	1618	6MZ	C6-N6	5.70	1.44	1.35
1	1	2498	OMC	C2-N3	5.50	1.47	1.36
1	1	2030	6MZ	C6-N6	5.38	1.43	1.35
1	1	1962	5MC	C2-N3	5.32	1.47	1.36
1	1	747	5MU	C6-C5	5.30	1.43	1.34
54	z	8	5MU	C6-C5	5.22	1.43	1.34
2	2	1402	4OC	C2-N3	5.22	1.46	1.36
1	1	2552	OMU	C6-C5	5.20	1.47	1.35
2	2	1407	5MC	C4-N3	5.17	1.42	1.34
2	2	1407	5MC	C2-N3	5.08	1.46	1.36
54	z	57	5MU	C6-C5	5.08	1.42	1.34
2	2	1402	4OC	C6-C5	5.07	1.46	1.35
2	2	966	2MG	C2-N2	5.04	1.44	1.33
2	2	527	G7M	C2-N3	4.98	1.45	1.33
2	2	966	2MG	C4-N3	4.93	1.49	1.37
2	2	1498	UR3	C2-N1	4.92	1.45	1.38
1	1	2498	OMC	C6-C5	4.74	1.46	1.35
2	2	1207	2MG	C2-N2	4.66	1.43	1.33
1	1	1915	3TD	C2-N3	4.60	1.48	1.38
1	1	1939	5MU	C6-C5	4.57	1.42	1.34
2	2	527	G7M	C2-N2	4.46	1.44	1.34
1	1	2251	OMG	C2-N3	4.40	1.43	1.33
2	2	1207	2MG	C4-N3	4.35	1.47	1.37
2	2	527	G7M	C4-N3	4.34	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2445	2MG	C2-N2	4.32	1.43	1.33
1	1	2069	G7M	C2-N3	4.30	1.43	1.33
1	1	2498	OMC	C4-N3	4.27	1.43	1.34
1	1	2503	2MA	C4-N3	4.26	1.47	1.37
1	1	1835	2MG	C4-N3	4.22	1.47	1.37
2	2	967	5MC	C4-N4	4.17	1.44	1.34
1	1	745	1MG	C2-N3	4.12	1.41	1.34
2	2	1516	2MG	C2-N2	4.08	1.42	1.33
1	1	1835	2MG	C2-N2	4.07	1.42	1.33
54	z	42	5MU	C6-C5	4.05	1.41	1.34
2	2	1498	UR3	C2-N3	4.05	1.46	1.39
2	2	1516	2MG	C2-N1	4.02	1.43	1.36
1	1	745	1MG	C4-N3	4.00	1.47	1.37
1	1	2498	OMC	C4-N4	4.00	1.43	1.33
2	2	1516	2MG	C4-N3	4.00	1.47	1.37
54	z	69	5MU	C2-N1	3.99	1.44	1.38
1	1	2445	2MG	C4-N3	3.98	1.47	1.37
2	2	1407	5MC	C6-N1	3.97	1.44	1.38
1	1	745	1MG	O6-C6	-3.95	1.14	1.22
1	1	2069	G7M	C4-N3	3.94	1.46	1.37
1	1	2069	G7M	C2-N2	3.90	1.43	1.34
1	1	2552	OMU	C4-N3	3.85	1.45	1.38
2	2	1402	4OC	C4-N4	3.76	1.43	1.35
2	2	1207	2MG	C2-N1	3.75	1.42	1.36
1	1	1962	5MC	C4-N4	3.74	1.43	1.34
2	2	1407	5MC	C4-N4	3.70	1.43	1.34
1	1	1962	5MC	C2-N1	3.66	1.47	1.40
2	2	1519	MA6	C5-C4	-3.63	1.31	1.40
2	2	966	2MG	C2-N1	3.60	1.42	1.36
54	z	42	5MU	O4-C4	-3.55	1.16	1.23
1	1	2251	OMG	C4-N3	3.55	1.46	1.37
1	1	747	5MU	O4-C4	-3.53	1.16	1.23
2	2	967	5MC	C2-N1	3.50	1.47	1.40
54	z	8	5MU	O4-C4	-3.48	1.17	1.23
1	1	2498	OMC	C2-N1	3.41	1.47	1.40
2	2	967	5MC	C6-N1	3.39	1.43	1.38
54	z	8	5MU	O2-C2	-3.39	1.16	1.23
1	1	2030	6MZ	C5-C4	-3.36	1.32	1.40
1	1	2445	2MG	C2-N1	3.34	1.42	1.36
2	2	1402	4OC	C2-N1	3.31	1.47	1.40
1	1	2503	2MA	C5-C4	-3.30	1.34	1.43
2	2	1407	5MC	O2-C2	-3.29	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1518	MA6	C5-C4	-3.29	1.32	1.40
2	2	1407	5MC	C2-N1	3.27	1.47	1.40
1	1	2251	OMG	C5-C4	-3.25	1.34	1.43
54	z	57	5MU	O4-C4	-3.23	1.17	1.23
1	1	1835	2MG	C2-N1	3.23	1.41	1.36
1	1	2445	2MG	C5-C4	-3.22	1.34	1.43
2	2	1498	UR3	C3U-N3	-3.18	1.41	1.47
2	2	967	5MC	O2-C2	-3.18	1.17	1.23
1	1	1962	5MC	O2-C2	-3.18	1.17	1.23
1	1	1618	6MZ	C5-C4	-3.16	1.32	1.40
1	1	2069	G7M	C6-N1	3.16	1.42	1.37
1	1	1939	5MU	O4-C4	-3.16	1.17	1.23
1	1	2498	OMC	O2-C2	-3.12	1.17	1.23
2	2	1402	4OC	O2-C2	-3.11	1.17	1.23
54	z	55	5MU	O4-C4	-2.96	1.18	1.23
54	z	20	5MU	O4-C4	-2.96	1.18	1.23
2	2	1516	2MG	C5-C4	-2.95	1.35	1.43
1	1	1962	5MC	C6-N1	2.94	1.43	1.38
2	2	1207	2MG	C5-C4	-2.93	1.35	1.43
1	1	2552	OMU	O4-C4	-2.92	1.18	1.24
2	2	1516	2MG	C6-N1	2.88	1.42	1.37
1	1	1939	5MU	O2-C2	-2.87	1.17	1.23
1	1	2552	OMU	O2-C2	-2.82	1.17	1.23
1	1	1835	2MG	C5-C4	-2.82	1.35	1.43
2	2	1402	4OC	C5-C4	2.81	1.46	1.40
1	1	2251	OMG	O6-C6	-2.80	1.17	1.23
2	2	966	2MG	C5-C4	-2.78	1.36	1.43
1	1	747	5MU	O2-C2	-2.77	1.18	1.23
54	z	64	5MU	C4-N3	-2.76	1.33	1.38
2	2	1207	2MG	C5-C6	2.75	1.53	1.47
1	1	745	1MG	C5-C4	-2.75	1.36	1.43
54	z	57	5MU	O2-C2	-2.75	1.18	1.23
54	z	39	5MU	C4-N3	-2.72	1.33	1.38
54	z	39	5MU	C6-C5	2.70	1.39	1.34
2	2	1516	2MG	C5-C6	2.70	1.52	1.47
54	z	42	5MU	O2-C2	-2.68	1.18	1.23
54	z	76	5MU	C4-N3	-2.68	1.33	1.38
54	z	69	5MU	O2-C2	-2.66	1.18	1.23
54	z	63	5MU	C4-N3	-2.63	1.34	1.38
1	1	1915	3TD	O4-C4	-2.60	1.17	1.23
2	2	1207	2MG	C6-N1	2.60	1.41	1.37
54	z	55	5MU	O2-C2	-2.59	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	64	5MU	C6-C5	2.57	1.38	1.34
1	1	2445	2MG	O6-C6	-2.55	1.18	1.23
54	z	76	5MU	C6-C5	2.55	1.38	1.34
54	z	63	5MU	C6-C5	2.55	1.38	1.34
2	2	1498	UR3	O2-C2	-2.55	1.17	1.22
1	1	2580	PSU	C4-C5	-2.53	1.36	1.44
1	1	1835	2MG	O6-C6	-2.52	1.18	1.23
1	1	2069	G7M	O6-C6	-2.52	1.18	1.23
2	2	527	G7M	O6-C6	-2.51	1.18	1.23
54	z	63	5MU	C4-C5	2.51	1.48	1.44
2	2	966	2MG	O6-C6	-2.51	1.18	1.23
1	1	2069	G7M	CN7-N7	-2.50	1.41	1.47
1	1	1915	3TD	O2-C2	-2.48	1.18	1.23
54	z	76	5MU	C4-C5	2.48	1.48	1.44
54	z	64	5MU	C6-N1	-2.48	1.33	1.38
54	z	39	5MU	C2-N1	2.48	1.42	1.38
54	z	71	5MU	C4-N3	-2.47	1.34	1.38
1	1	2069	G7M	C5-C4	-2.46	1.34	1.39
2	2	527	G7M	C6-N1	2.46	1.41	1.37
54	z	40	5MU	C6-C5	2.45	1.38	1.34
1	1	1835	2MG	C5-C6	2.44	1.52	1.47
54	z	40	5MU	C4-N3	-2.43	1.34	1.38
2	2	516	PSU	C4-C5	-2.41	1.37	1.44
1	1	1618	6MZ	C6-N1	-2.40	1.30	1.34
54	z	40	5MU	C6-N1	-2.39	1.34	1.38
54	z	76	5MU	C6-N1	-2.39	1.34	1.38
54	z	40	5MU	C4-C5	2.38	1.48	1.44
1	1	2457	PSU	C4-C5	-2.37	1.37	1.44
2	2	966	2MG	C6-N1	2.36	1.41	1.37
2	2	1207	2MG	O6-C6	-2.34	1.18	1.23
54	z	20	5MU	O2-C2	-2.34	1.18	1.23
2	2	527	G7M	C5-C6	2.33	1.51	1.45
54	z	71	5MU	C6-C5	2.32	1.38	1.34
1	1	955	PSU	C4-C5	-2.32	1.37	1.44
2	2	1516	2MG	O6-C6	-2.30	1.18	1.23
54	z	64	5MU	C4-C5	2.30	1.48	1.44
2	2	1498	UR3	C6-N1	2.30	1.43	1.38
54	z	39	5MU	C4-C5	2.29	1.48	1.44
54	z	71	5MU	C2-N1	2.29	1.42	1.38
1	1	2251	OMG	C2-N2	2.28	1.39	1.34
1	1	2069	G7M	C5-C6	2.28	1.51	1.45
1	1	2445	2MG	C2'-C1'	-2.27	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	40	5MU	C2-N1	2.27	1.42	1.38
2	2	966	2MG	C5-C6	2.25	1.52	1.47
54	z	39	5MU	C6-N1	-2.25	1.34	1.38
1	1	2251	OMG	C6-N1	2.25	1.41	1.37
54	z	63	5MU	C6-N1	-2.24	1.34	1.38
1	1	1917	PSU	C4-C5	-2.24	1.37	1.44
1	1	2030	6MZ	C5-N7	-2.23	1.31	1.39
43	p	89	0TD	CSB-SB	-2.20	1.75	1.79
2	2	1402	4OC	C6-N1	2.20	1.43	1.38
54	z	64	5MU	C2-N1	2.20	1.42	1.38
1	1	2030	6MZ	C6-N1	-2.19	1.30	1.34
54	z	71	5MU	C6-N1	-2.19	1.34	1.38
1	1	2605	PSU	C4-C5	-2.14	1.38	1.44
54	z	76	5MU	C2-N3	-2.12	1.34	1.38
54	z	63	5MU	C2-N1	2.12	1.41	1.38
54	z	63	5MU	C2-N3	-2.12	1.34	1.38
2	2	527	G7M	C2-N1	2.11	1.42	1.37
1	1	746	PSU	C4-C5	-2.10	1.38	1.44
54	z	64	5MU	C2-N3	-2.10	1.34	1.38
2	2	527	G7M	C5-C4	-2.10	1.34	1.39
1	1	1618	6MZ	C4-N3	-2.09	1.32	1.35
54	z	76	5MU	C2-N1	2.09	1.41	1.38
1	1	746	PSU	C6-C5	2.08	1.37	1.35
1	1	2251	OMG	C5-C6	2.08	1.51	1.47
1	1	2504	PSU	C4-C5	-2.08	1.38	1.44
2	2	527	G7M	CN7-N7	-2.08	1.42	1.47
1	1	1618	6MZ	C5-N7	-2.07	1.32	1.39
1	1	1835	2MG	C6-N1	2.06	1.40	1.37
54	z	71	5MU	C4-C5	2.06	1.48	1.44
1	1	2457	PSU	C6-N1	-2.05	1.32	1.36
1	1	2445	2MG	CM2-N2	-2.05	1.41	1.45
1	1	1915	3TD	O4'-C1'	-2.02	1.41	1.43

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	z	69	5MU	C6-C5-C4	-115.15	21.76	118.03
54	z	69	5MU	C5-C4-N3	-87.09	40.98	115.31
54	z	69	5MU	C6-N1-C2	-29.10	91.84	121.30
54	z	69	5MU	O4-C4-C5	-25.79	95.01	124.90
54	z	69	5MU	N3-C2-N1	-18.31	90.58	114.89
2	2	1519	MA6	N1-C6-N6	-14.61	101.68	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1518	MA6	N1-C6-N6	-13.91	102.42	117.06
54	z	20	5MU	C5-C4-N3	12.87	126.29	115.31
1	1	747	5MU	C5-C4-N3	12.70	126.15	115.31
54	z	8	5MU	C5-C4-N3	12.60	126.06	115.31
54	z	42	5MU	C5-C4-N3	12.09	125.63	115.31
54	z	55	5MU	C5-C4-N3	11.91	125.48	115.31
1	1	1618	6MZ	C1'-N9-C4	-11.73	106.04	126.64
54	z	57	5MU	C5-C4-N3	11.68	125.28	115.31
1	1	2030	6MZ	C1'-N9-C4	-11.47	106.49	126.64
1	1	1939	5MU	C5-C4-N3	11.44	125.08	115.31
54	z	69	5MU	C1'-N1-C2	10.72	136.98	117.57
54	z	57	5MU	C5-C6-N1	-10.51	112.52	123.34
54	z	42	5MU	C5-C6-N1	-10.27	112.77	123.34
1	1	747	5MU	C5-C6-N1	-9.96	113.09	123.34
1	1	1939	5MU	C5-C6-N1	-9.82	113.24	123.34
54	z	8	5MU	C5-C6-N1	-9.67	113.39	123.34
54	z	69	5MU	O2-C2-N1	9.36	135.23	122.79
54	z	55	5MU	C5-C6-N1	-8.98	114.10	123.34
54	z	20	5MU	C5-C6-N1	-8.81	114.28	123.34
54	z	69	5MU	O4-C4-N3	8.28	135.99	120.12
54	z	69	5MU	C5M-C5-C6	7.90	133.40	122.85
54	z	69	5MU	O2-C2-N3	6.80	134.17	121.50
54	z	20	5MU	C5M-C5-C4	6.62	126.06	118.77
54	z	69	5MU	C5M-C5-C4	-6.47	111.65	118.77
1	1	747	5MU	O4-C4-C5	-6.13	117.79	124.90
54	z	69	5MU	C1'-N1-C6	6.03	131.16	121.12
54	z	8	5MU	C4-N3-C2	-6.02	119.56	127.35
54	z	42	5MU	O4-C4-C5	-6.02	117.93	124.90
1	1	2457	PSU	C4-N3-C2	-5.93	117.80	126.34
2	2	1519	MA6	N3-C2-N1	-5.70	119.77	128.68
54	z	57	5MU	O4-C4-C5	-5.69	118.31	124.90
1	1	2457	PSU	N1-C2-N3	5.65	121.53	115.13
1	1	747	5MU	C4-N3-C2	-5.58	120.13	127.35
54	z	57	5MU	C4-N3-C2	-5.56	120.15	127.35
1	1	1939	5MU	C5M-C5-C6	-5.50	115.50	122.85
54	z	42	5MU	C4-N3-C2	-5.47	120.28	127.35
54	z	8	5MU	O4-C4-C5	-5.44	118.60	124.90
54	z	64	5MU	C4-N3-C2	-5.39	120.37	127.35
1	1	2580	PSU	C4-N3-C2	-5.39	118.58	126.34
1	1	1917	PSU	C4-N3-C2	-5.39	118.58	126.34
54	z	69	5MU	C5-C6-N1	-5.36	117.83	123.34
2	2	516	PSU	C4-N3-C2	-5.35	118.63	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2580	PSU	N1-C2-N3	5.31	121.14	115.13
1	1	2605	PSU	C4-N3-C2	-5.25	118.77	126.34
54	z	63	5MU	C4-N3-C2	-5.25	120.56	127.35
1	1	1939	5MU	C4-N3-C2	-5.23	120.58	127.35
54	z	76	5MU	C4-N3-C2	-5.22	120.60	127.35
54	z	8	5MU	N3-C2-N1	5.19	121.78	114.89
1	1	1911	PSU	C4-N3-C2	-5.13	118.94	126.34
54	z	71	5MU	C4-N3-C2	-5.11	120.73	127.35
1	1	1917	PSU	N1-C2-N3	5.11	120.92	115.13
54	z	8	5MU	C5M-C5-C4	5.11	124.39	118.77
54	z	39	5MU	N3-C2-N1	5.09	121.64	114.89
1	1	1939	5MU	C5M-C5-C4	5.06	124.33	118.77
1	1	746	PSU	C4-N3-C2	-5.04	119.08	126.34
1	1	1939	5MU	O4-C4-C5	-5.04	119.06	124.90
54	z	8	5MU	C5M-C5-C6	-5.00	116.17	122.85
54	z	20	5MU	C5M-C5-C6	-4.99	116.18	122.85
1	1	2504	PSU	C4-N3-C2	-4.99	119.15	126.34
1	1	955	PSU	C4-N3-C2	-4.98	119.16	126.34
54	z	64	5MU	N3-C2-N1	4.97	121.49	114.89
1	1	955	PSU	N1-C2-N3	4.92	120.71	115.13
54	z	39	5MU	C4-N3-C2	-4.91	120.99	127.35
54	z	40	5MU	C4-N3-C2	-4.90	121.01	127.35
2	2	1518	MA6	N3-C2-N1	-4.89	121.03	128.68
1	1	2552	OMU	C4-N3-C2	-4.83	120.21	126.58
54	z	76	5MU	N3-C2-N1	4.81	121.27	114.89
54	z	20	5MU	O4-C4-C5	-4.79	119.35	124.90
54	z	57	5MU	N3-C2-N1	4.78	121.23	114.89
54	z	42	5MU	C5M-C5-C6	-4.77	116.48	122.85
54	z	63	5MU	N3-C2-N1	4.75	121.20	114.89
54	z	71	5MU	N3-C2-N1	4.71	121.14	114.89
54	z	71	5MU	C5-C4-N3	4.69	119.32	115.31
1	1	2605	PSU	N1-C2-N3	4.69	120.44	115.13
54	z	63	5MU	C5-C4-N3	4.65	119.28	115.31
1	1	747	5MU	N3-C2-N1	4.63	121.03	114.89
1	1	1911	PSU	N1-C2-N3	4.60	120.35	115.13
54	z	55	5MU	C5M-C5-C4	4.59	123.82	118.77
54	z	40	5MU	N3-C2-N1	4.59	120.98	114.89
54	z	20	5MU	C4-N3-C2	-4.58	121.42	127.35
1	1	2504	PSU	N1-C2-N3	4.56	120.30	115.13
1	1	1939	5MU	N3-C2-N1	4.56	120.94	114.89
1	1	2030	6MZ	N3-C2-N1	-4.55	121.56	128.68
54	z	71	5MU	O4-C4-C5	-4.50	119.69	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	z	76	5MU	C5-C4-N3	4.50	119.15	115.31
54	z	64	5MU	C5-C4-N3	4.46	119.12	115.31
54	z	55	5MU	C4-N3-C2	-4.45	121.59	127.35
1	1	1618	6MZ	N3-C2-N1	-4.45	121.72	128.68
54	z	55	5MU	O4-C4-C5	-4.42	119.78	124.90
1	1	1915	3TD	N1-C2-N3	4.38	119.59	116.14
1	1	746	PSU	N1-C2-N3	4.37	120.08	115.13
2	2	516	PSU	N1-C2-N3	4.34	120.05	115.13
54	z	64	5MU	C5-C6-N1	-4.22	118.99	123.34
54	z	55	5MU	N3-C2-N1	4.21	120.47	114.89
1	1	745	1MG	CM1-N1-C2	-4.16	116.40	120.72
1	1	2580	PSU	O2-C2-N1	-4.15	118.22	122.79
54	z	42	5MU	N3-C2-N1	4.14	120.39	114.89
54	z	8	5MU	O2-C2-N1	-4.07	117.38	122.79
54	z	40	5MU	C5-C4-N3	4.06	118.78	115.31
54	z	63	5MU	C5-C6-N1	-4.01	119.21	123.34
54	z	55	5MU	C5M-C5-C6	-4.00	117.51	122.85
54	z	39	5MU	C5-C4-N3	3.99	118.71	115.31
54	z	76	5MU	C5-C6-N1	-3.93	119.29	123.34
54	z	64	5MU	O4-C4-C5	-3.85	120.44	124.90
54	z	57	5MU	C6-C5-C4	3.82	121.22	118.03
54	z	63	5MU	O4-C4-C5	-3.81	120.48	124.90
54	z	69	5MU	C4-N3-C2	-3.77	122.47	127.35
54	z	63	5MU	C2'-C1'-N1	-3.77	102.54	113.22
54	z	40	5MU	O4-C4-C5	-3.73	120.58	124.90
54	z	42	5MU	C5M-C5-C4	3.71	122.85	118.77
1	1	2503	2MA	C5-C6-N1	3.71	120.42	114.02
1	1	1835	2MG	CM2-N2-C2	-3.68	115.72	123.86
43	p	89	0TD	OD2-CG-CB	3.66	121.06	113.15
54	z	39	5MU	O4-C4-C5	-3.57	120.76	124.90
54	z	76	5MU	O4-C4-C5	-3.55	120.78	124.90
1	1	2552	OMU	N3-C2-N1	3.55	119.60	114.89
1	1	2030	6MZ	C9-N6-C6	-3.53	119.83	122.87
1	1	1917	PSU	C6-C5-C4	3.50	120.65	118.20
1	1	2580	PSU	C6-C5-C4	3.48	120.63	118.20
1	1	2457	PSU	O2-C2-N1	-3.47	118.97	122.79
54	z	20	5MU	N3-C2-N1	3.44	119.45	114.89
1	1	747	5MU	C5M-C5-C6	-3.42	118.28	122.85
1	1	2251	OMG	C2-N1-C6	-3.39	118.85	125.10
1	1	1915	3TD	C4-N3-C2	-3.39	120.93	124.61
1	1	1917	PSU	O2-C2-N1	-3.32	119.13	122.79
1	1	747	5MU	O2-C2-N1	-3.32	118.38	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	966	2MG	C5-C6-N1	3.31	119.79	113.95
54	z	40	5MU	C5-C6-N1	-3.28	119.97	123.34
54	z	57	5MU	C5M-C5-C6	-3.25	118.50	122.85
2	2	1516	2MG	CM2-N2-C2	-3.21	116.76	123.86
2	2	1207	2MG	C5-C6-N1	3.20	119.61	113.95
1	1	745	1MG	CM1-N1-C6	3.16	121.88	117.55
54	z	42	5MU	C6-C5-C4	3.16	120.67	118.03
54	z	39	5MU	C5-C6-N1	-3.11	120.14	123.34
1	1	955	PSU	O2-C2-N1	-3.11	119.37	122.79
54	z	39	5MU	C1'-N1-C2	3.09	123.17	117.57
2	2	1407	5MC	C5-C6-N1	-3.09	120.16	123.34
1	1	1835	2MG	C5-C6-N1	3.08	119.38	113.95
2	2	1498	UR3	C4-N3-C2	-3.07	121.67	124.56
54	z	64	5MU	C2'-C1'-N1	-3.04	104.62	113.22
1	1	1911	PSU	O2-C2-N1	-3.04	119.45	122.79
1	1	745	1MG	C5-C6-N1	3.03	118.45	113.90
54	z	20	5MU	O4-C4-N3	-3.01	114.35	120.12
54	z	40	5MU	C1'-N1-C2	2.98	122.96	117.57
2	2	1402	4OC	CM4-N4-C4	-2.96	116.66	122.45
1	1	2552	OMU	O4-C4-C5	-2.96	119.95	125.16
54	z	63	5MU	O3'-C3'-C2'	2.96	121.39	111.82
1	1	747	5MU	C5M-C5-C4	2.94	122.01	118.77
2	2	1516	2MG	C5-C6-N1	2.94	119.14	113.95
54	z	40	5MU	O4'-C1'-N1	2.88	114.96	108.36
54	z	40	5MU	C1'-N1-C6	-2.87	116.34	121.12
54	z	71	5MU	C5-C6-N1	-2.87	120.39	123.34
54	z	63	5MU	O3'-C3'-C4'	2.86	119.31	111.05
2	2	527	G7M	C2-N1-C6	-2.83	119.89	125.10
54	z	55	5MU	O4-C4-N3	-2.80	114.74	120.12
1	1	2504	PSU	O2-C2-N1	-2.80	119.71	122.79
1	1	1939	5MU	O2-C2-N1	-2.78	119.09	122.79
1	1	2251	OMG	C5-C6-N1	2.76	118.83	113.95
1	1	2552	OMU	C5-C4-N3	2.76	118.97	114.84
1	1	2445	2MG	C5-C6-N1	2.76	118.82	113.95
54	z	55	5MU	O2-C2-N1	-2.74	119.14	122.79
1	1	2552	OMU	CM2-O2'-C2'	-2.72	107.39	114.52
54	z	40	5MU	C5M-C5-C4	2.70	121.74	118.77
1	1	746	PSU	O2-C2-N1	-2.69	119.83	122.79
2	2	1207	2MG	CM2-N2-C2	-2.64	118.02	123.86
54	z	42	5MU	C1'-N1-C2	2.64	122.34	117.57
54	z	63	5MU	O2-C2-N1	-2.62	119.31	122.79
1	1	2069	G7M	C2-N1-C6	-2.61	120.30	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1498	UR3	C3U-N3-C4	2.61	121.61	117.89
54	z	40	5MU	C2'-C1'-N1	-2.60	105.86	113.22
1	1	1962	5MC	CM5-C5-C6	-2.59	119.39	122.85
1	1	1618	6MZ	C9-N6-C6	-2.58	120.65	122.87
1	1	1939	5MU	C6-C5-C4	2.55	120.16	118.03
54	z	71	5MU	C5'-C4'-C3'	-2.53	105.72	115.18
1	1	955	PSU	C6-N1-C2	-2.52	120.11	122.68
2	2	516	PSU	O2-C2-N1	-2.52	120.02	122.79
1	1	2457	PSU	C6-N1-C2	-2.51	120.12	122.68
54	z	8	5MU	O4-C4-N3	-2.49	115.34	120.12
54	z	39	5MU	O4'-C1'-N1	2.49	114.06	108.36
54	z	63	5MU	O4'-C4'-C3'	-2.48	100.21	105.11
54	z	39	5MU	C1'-N1-C6	-2.47	117.02	121.12
1	1	1962	5MC	C5-C4-N4	-2.47	117.79	121.48
2	2	1207	2MG	C8-N7-C5	2.44	107.64	102.99
54	z	20	5MU	O2-C2-N1	-2.43	119.56	122.79
43	p	89	0TD	OD1-CG-CB	-2.42	117.37	122.44
1	1	2503	2MA	C8-N7-C5	2.40	107.56	102.99
1	1	1962	5MC	C1'-N1-C6	-2.39	117.14	121.12
54	z	57	5MU	C1'-N1-C2	2.39	121.90	117.57
1	1	2251	OMG	C8-N7-C5	2.39	107.54	102.99
1	1	1962	5MC	C5-C6-N1	-2.39	120.88	123.34
54	z	40	5MU	C5M-C5-C6	-2.38	119.68	122.85
1	1	2504	PSU	C6-C5-C4	2.36	119.85	118.20
1	1	955	PSU	C6-C5-C4	2.36	119.85	118.20
1	1	2580	PSU	O4'-C1'-C2'	2.33	108.43	105.14
2	2	966	2MG	C8-N7-C5	2.32	107.41	102.99
1	1	2069	G7M	N2-C2-N1	2.31	121.64	116.71
54	z	76	5MU	O2-C2-N1	-2.31	119.72	122.79
54	z	76	5MU	C2'-C1'-N1	-2.28	106.75	113.22
54	z	63	5MU	C5M-C5-C4	2.28	121.28	118.77
2	2	966	2MG	O6-C6-C5	-2.28	119.92	124.37
54	z	63	5MU	C3'-C2'-C1'	-2.27	97.11	101.43
1	1	2445	2MG	CM2-N2-C2	-2.27	118.85	123.86
54	z	71	5MU	C2'-C3'-C4'	2.27	107.05	102.64
1	1	2605	PSU	C6-C5-C4	2.26	119.78	118.20
1	1	2580	PSU	C6-N1-C2	-2.25	120.38	122.68
54	z	42	5MU	C1'-N1-C6	-2.25	117.38	121.12
1	1	745	1MG	C8-N7-C5	2.25	107.27	102.99
2	2	1516	2MG	C8-N7-C5	2.24	107.26	102.99
54	z	76	5MU	C5M-C5-C4	2.24	121.23	118.77
1	1	1939	5MU	O4-C4-N3	-2.22	115.86	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	z	39	5MU	O2-C2-N3	-2.22	117.37	121.50
1	1	2552	OMU	O2-C2-N1	-2.20	119.86	122.79
2	2	1516	2MG	O6-C6-C5	-2.20	120.08	124.37
1	1	2605	PSU	O2-C2-N1	-2.17	120.40	122.79
54	z	71	5MU	O2-C2-N1	-2.15	119.93	122.79
1	1	2457	PSU	O4'-C1'-C2'	2.14	108.16	105.14
1	1	1915	3TD	C6-C5-C4	2.14	119.70	118.22
54	z	57	5MU	O2-C2-N1	-2.13	119.95	122.79
1	1	2445	2MG	C8-N7-C5	2.13	107.05	102.99
1	1	747	5MU	O4-C4-N3	-2.12	116.05	120.12
1	1	1917	PSU	C6-N1-C2	-2.10	120.53	122.68
1	1	2251	OMG	CM2-O2'-C2'	-2.10	109.01	114.52
1	1	1835	2MG	C8-N7-C5	2.06	106.92	102.99
1	1	2445	2MG	O6-C6-C5	-2.06	120.35	124.37
2	2	967	5MC	CM5-C5-C6	-2.05	120.11	122.85
54	z	71	5MU	C5M-C5-C4	2.04	121.01	118.77
2	2	967	5MC	C5-C6-N1	-2.04	121.24	123.34
54	z	42	5MU	O2-C2-N1	-2.01	120.11	122.79
54	z	64	5MU	O4'-C1'-N1	2.01	112.95	108.36
1	1	1962	5MC	C1'-N1-C2	2.01	122.90	118.42
1	1	2503	2MA	CM2-C2-N1	2.00	120.69	116.23
54	z	76	5MU	C5M-C5-C6	-2.00	120.17	122.85
54	z	63	5MU	C5M-C5-C6	-2.00	120.17	122.85

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C9
2	2	1518	MA6	C5-C6-N6-C10
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C9
2	2	1519	MA6	C5-C6-N6-C10
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	1915	3TD	C2'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
54	z	8	5MU	O4'-C4'-C5'-O5'
54	z	39	5MU	O4'-C1'-N1-C2
54	z	39	5MU	O4'-C1'-N1-C6
54	z	40	5MU	O4'-C1'-N1-C2
54	z	40	5MU	O4'-C1'-N1-C6
54	z	64	5MU	O4'-C1'-N1-C2
54	z	64	5MU	O4'-C1'-N1-C6
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
54	z	8	5MU	C3'-C4'-C5'-O5'
54	z	57	5MU	C3'-C4'-C5'-O5'
54	z	57	5MU	O4'-C4'-C5'-O5'
54	z	63	5MU	C3'-C4'-C5'-O5'
54	z	69	5MU	C3'-C4'-C5'-O5'
54	z	69	5MU	O4'-C4'-C5'-O5'
54	z	71	5MU	C3'-C4'-C5'-O5'
54	z	71	5MU	O4'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
54	z	20	5MU	O4'-C4'-C5'-O5'
2	2	1518	MA6	N1-C6-N6-C10
2	2	1519	MA6	N1-C6-N6-C10
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
54	z	20	5MU	C3'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
54	z	39	5MU	O4'-C4'-C5'-O5'
54	z	63	5MU	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
43	p	89	0TD	CG-CB-SB-CSB
2	2	527	G7M	C4'-C5'-O5'-P
43	p	89	0TD	SB-CB-CG-OD1
54	z	71	5MU	C4'-C5'-O5'-P
54	z	76	5MU	O4'-C4'-C5'-O5'
54	z	39	5MU	C3'-C4'-C5'-O5'
1	1	2503	2MA	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	z	76	5MU	C3'-C4'-C5'-O5'
43	p	89	0TD	SB-CB-CG-OD2
54	z	20	5MU	C2'-C1'-N1-C2
2	2	1402	4OC	C3'-C4'-C5'-O5'
2	2	1498	UR3	O4'-C4'-C5'-O5'
1	1	746	PSU	O4'-C1'-C5-C6
1	1	2069	G7M	O4'-C4'-C5'-O5'
54	z	20	5MU	C4'-C5'-O5'-P

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	z	69	5MU	C2-C4-C5-C6-N1-N3

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 424 ligands modelled in this entry, 424 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12930. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

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

7 Map analysis (i)

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

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

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

8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

This section was not generated.