Full wwPDB EM Validation Report ⓘ

Sep 21, 2021 – 08:49 AM BST

PDB ID	:	7OIZ
EMDB ID	:	EMD-12936
Title	:	Cryo-EM structure of 70S ribosome stalled with TnaC peptide
Authors	:	Su, T.; Kudva, R.; Becker, T.; Berninghausen, O.; Heijne, G.; Cheng, J.; Beckmann, R.
Deposited on	:	2021-05-13
Resolution	:	2.90 Å(reported)

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

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

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

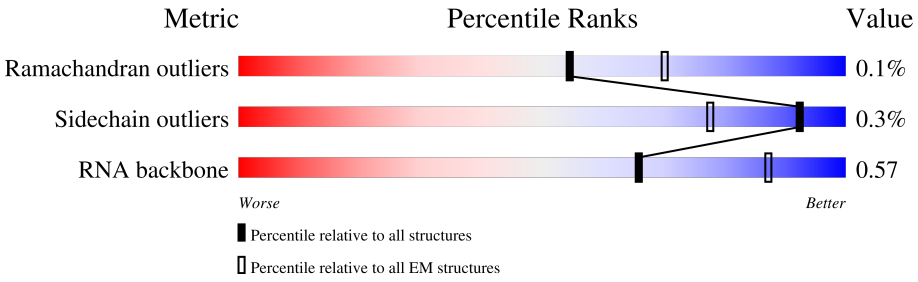
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	A	1519	84% 16% ·
2	B	241	92% · 7%
3	C	233	88% 12%
4	D	206	100%
5	E	167	93% · 7%
6	F	135	76% 24%
7	G	179	85% · 15%
8	H	130	98% ··
9	I	130	96% · ·

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Mol	Chain	Length	Quality of chain
10	J	103	94% 5%
11	K	129	89% 9%
12	L	124	98%
13	M	118	97%
14	N	101	98%
15	O	89	99%
16	P	82	99%
17	Q	84	94% 6%
18	R	75	88% 12%
19	S	92	89% 9%
20	T	87	99%
21	U	71	97%
22	a	2753	85% 15%
23	b	119	85% 15%
24	c	273	99%
25	d	209	99%
26	e	201	100%
27	f	179	99%
28	g	177	99%
29	h	149	28% 72%
30	i	142	100%
31	j	123	99%
32	k	144	99%
33	l	136	97%
34	m	127	93% 7%

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Mol	Chain	Length	Quality of chain
35	n	117	99%
36	o	115	99%
37	p	118	99%
38	q	103	99%
39	r	110	100%
40	s	100	93% 7%
41	t	104	97%
42	u	94	100%
43	v	85	92% 8%
44	w	78	99%
45	x	63	97%
46	y	59	98%
47	z	57	98%
48	0	55	91% 7%
49	1	46	98%
50	2	65	98%
51	3	38	97%
52	4	66	91% 9%
53	X	6	50% 33% 17%
54	7	16	100%
55	V	75	72% 27%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 140295 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1519	32611	14551	5986	10555	1519	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1753	1109	315	321	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	103	839	530	151	151	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	ASP	ASN	conflict	UNP A0A6D2X4T2

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 23 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

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

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	6	Total	C	N	O	P	0	0
			125	56	21	42	6		

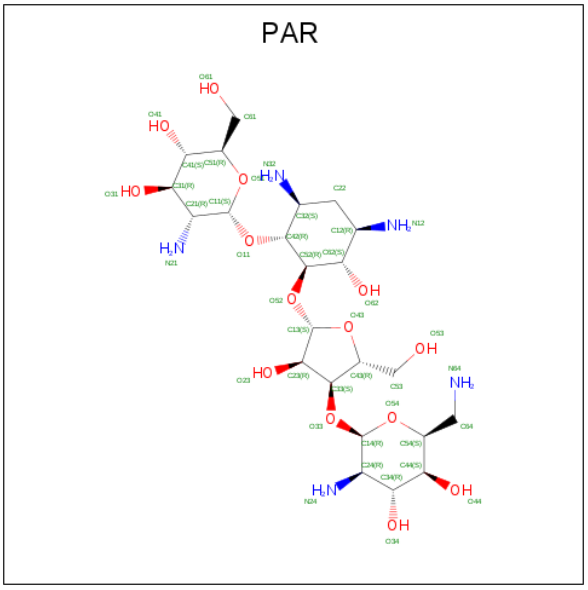
- Molecule 54 is a protein called TnaC.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	7	16	Total	C	N	O	0	0
			139	89	26	24		

- Molecule 55 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	V	75	Total	C	N	O	P	0	0
			1609	715	292	527	75		

- Molecule 56 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).

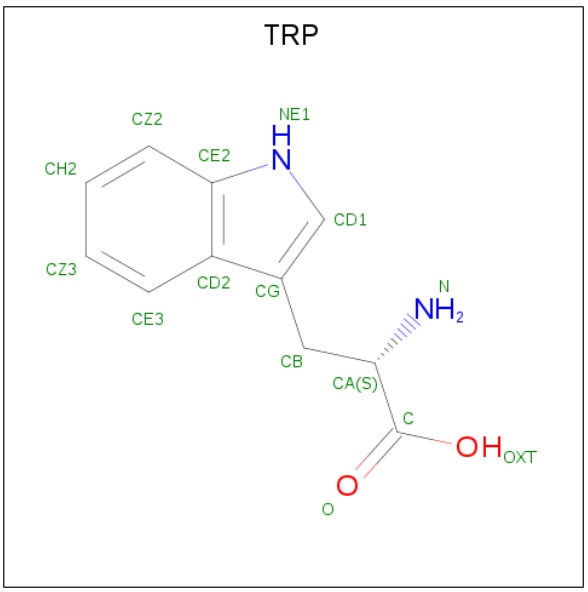


Mol	Chain	Residues	Atoms				AltConf
56	A	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	93	Total	Mg	0
			93	93	
57	a	205	Total	Mg	0
			205	205	
57	b	5	Total	Mg	0
			5	5	
57	c	1	Total	Mg	0
			1	1	
57	k	1	Total	Mg	0
			1	1	
57	m	2	Total	Mg	0
			2	2	
57	V	1	Total	Mg	0
			1	1	

- Molecule 58 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
58	a	1	15	11	2	2	0

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

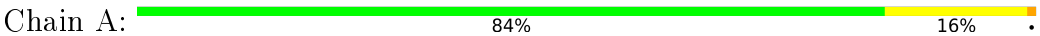
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	3	1	1	1	0
			Total	Zn	
59	4	1	1	1	0

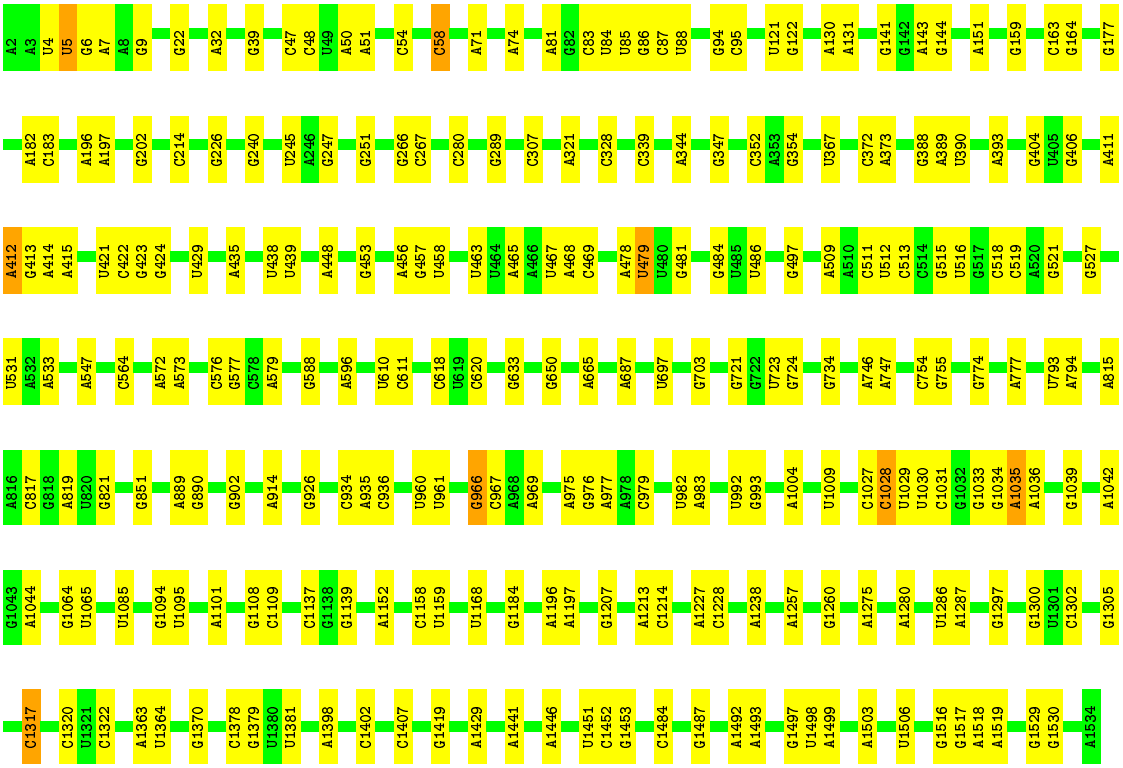
3 Residue-property plots (i)

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: 16S rRNA

Chain A:





- Molecule 2: 30S ribosomal protein S2

Chain B:

- Molecule 3: 30S ribosomal protein S3

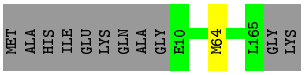
Chain C:

• Molecule 4: 30S ribosomal protein S4

Chain D:

• Molecule 5: 30S ribosomal protein S5

Chain E:



• Molecule 6: 30S ribosomal protein S6, fully modified isoform

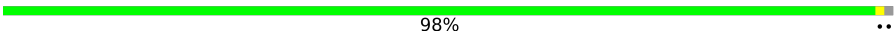
Chain F:

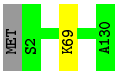
• Molecule 7: 30S ribosomal protein S7

Chain G:

• Molecule 8: 30S ribosomal protein S8

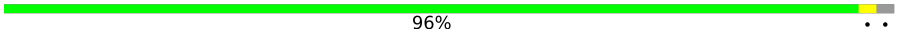
Chain H:

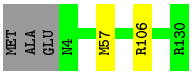




• Molecule 9: 30S ribosomal protein S9

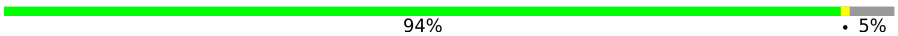
Chain I:





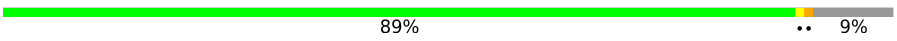
• Molecule 10: 30S ribosomal protein S10

Chain J:



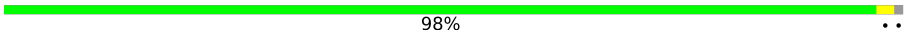
• Molecule 11: 30S ribosomal protein S11

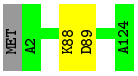
Chain K:



- Molecule 12: 30S ribosomal protein S12

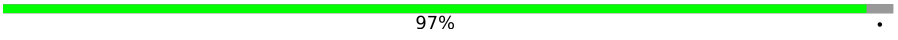
Chain L:

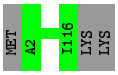




- Molecule 13: 30S ribosomal protein S13

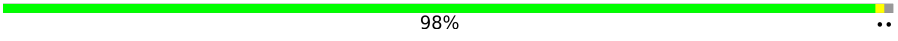
Chain M:

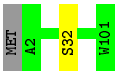




- Molecule 14: 30S ribosomal protein S14

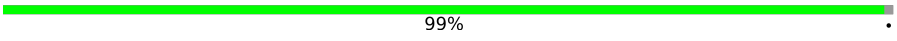
Chain N:





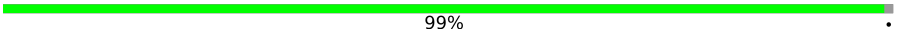
- Molecule 15: 30S ribosomal protein S15

Chain O:



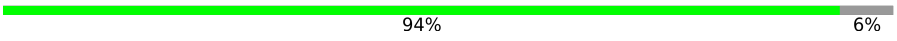
- Molecule 16: 30S ribosomal protein S16

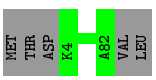
Chain P:



- Molecule 17: 30S ribosomal protein S17

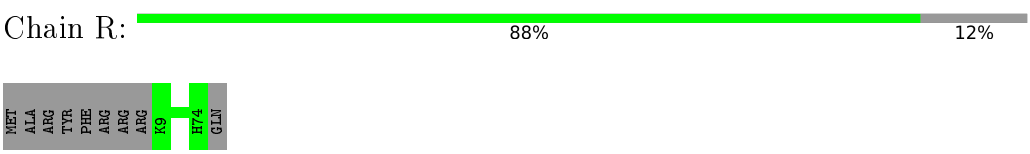
Chain Q:





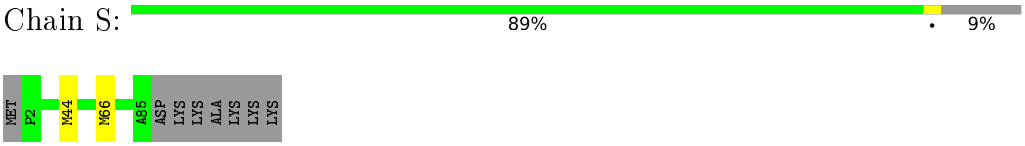
- Molecule 18: 30S ribosomal protein S18

Chain R:



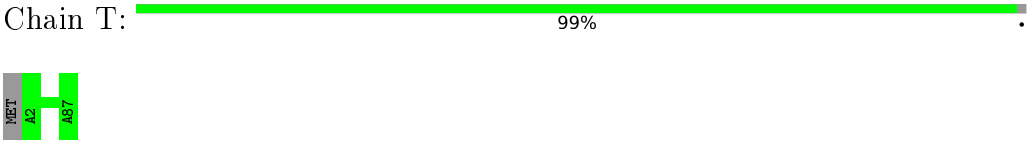
• Molecule 19: 30S ribosomal protein S19

Chain S:



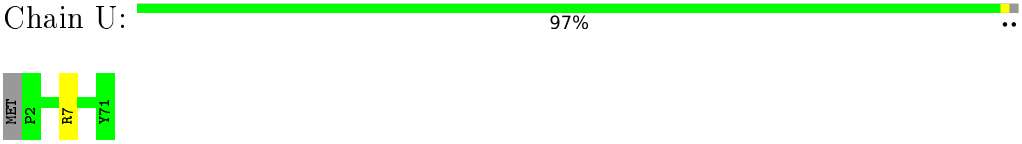
• Molecule 20: 30S ribosomal protein S20

Chain T:



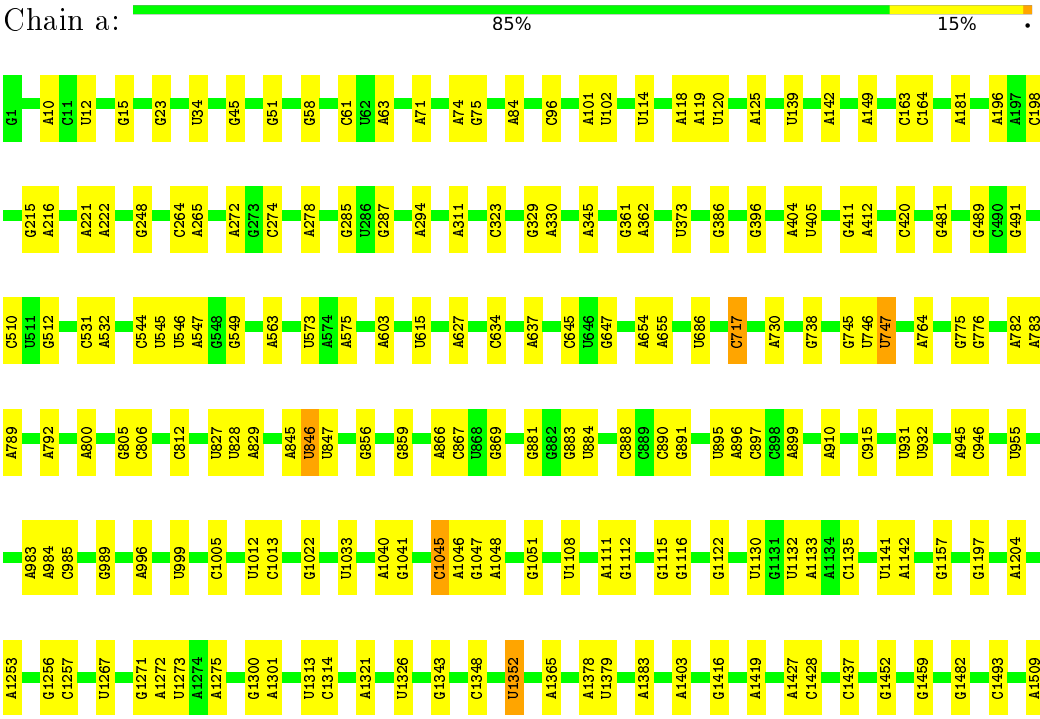
• Molecule 21: 30S ribosomal protein S21

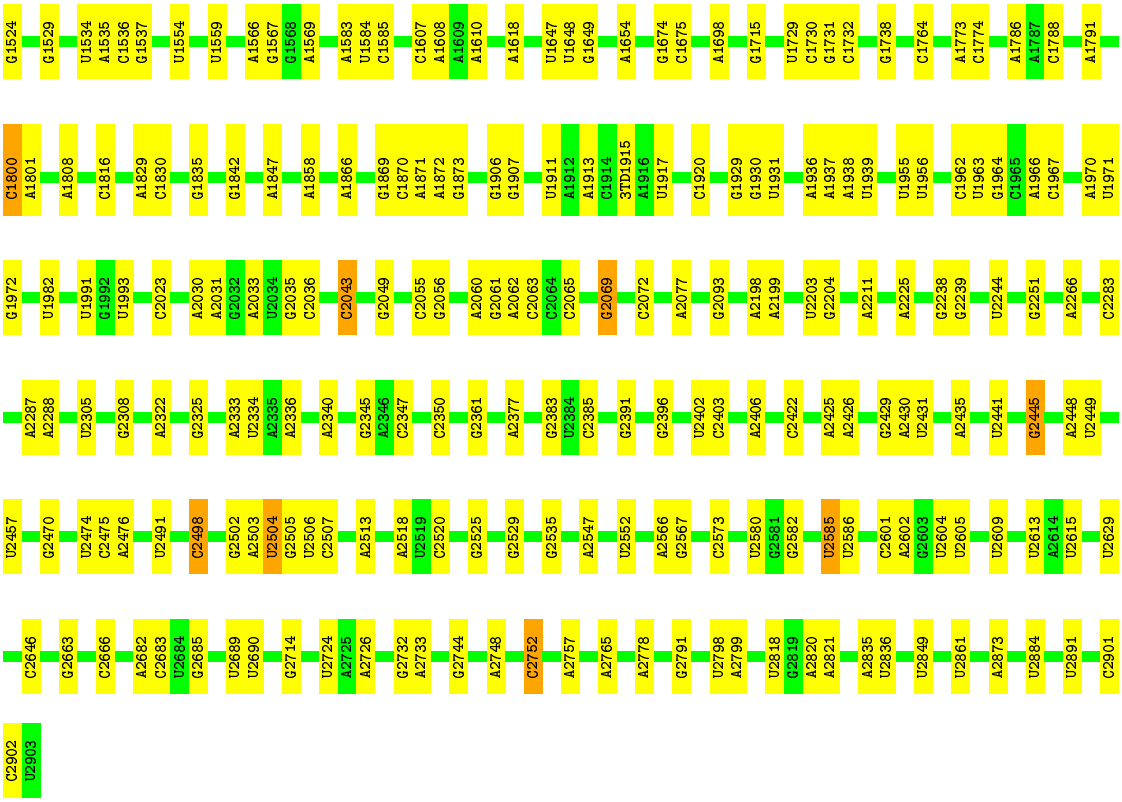
Chain U:



• Molecule 22: 23S rRNA

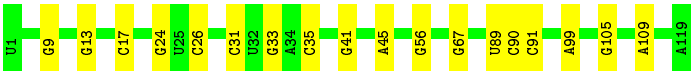
Chain a:





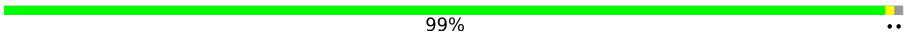
- Molecule 23: 16S rRNA

Chain b:



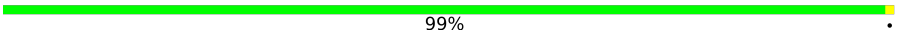
- Molecule 24: 50S ribosomal protein L2

Chain c:



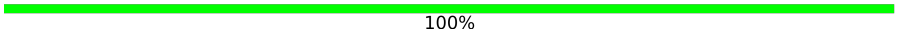
- Molecule 25: 50S ribosomal protein L3

Chain d:



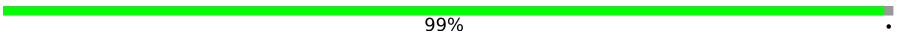
- Molecule 26: 50S ribosomal protein L4

Chain e:



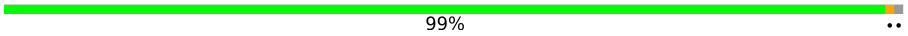
• Molecule 27: 50S ribosomal protein L5

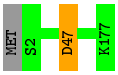
Chain f:



• Molecule 28: 50S ribosomal protein L6

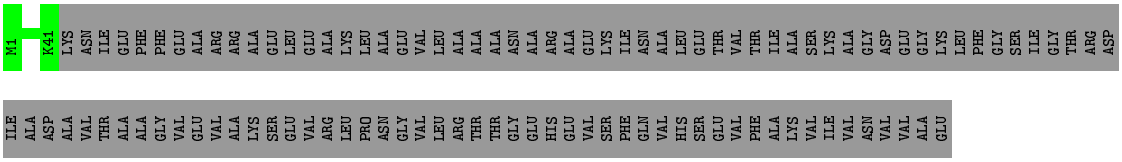
Chain g:





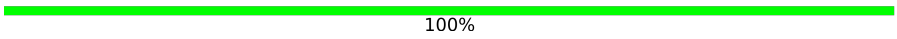
• Molecule 29: 50S ribosomal protein L9

Chain h:



• Molecule 30: 50S ribosomal protein L13

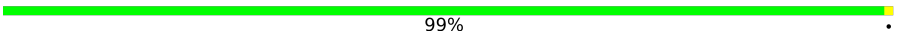
Chain i:



There are no outlier residues recorded for this chain.

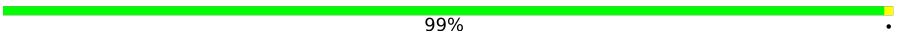
• Molecule 31: 50S ribosomal protein L14

Chain j:



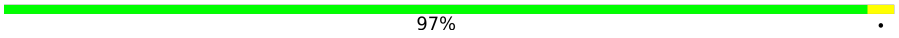
• Molecule 32: 50S ribosomal protein L15

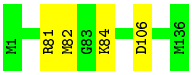
Chain k:



• Molecule 33: 50S ribosomal protein L16

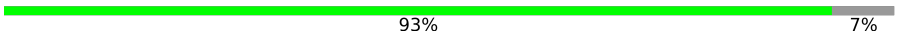
Chain l:





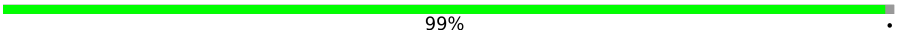
• Molecule 34: 50S ribosomal protein L17

Chain m:



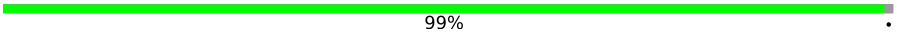
• Molecule 35: 50S ribosomal protein L18

Chain n:



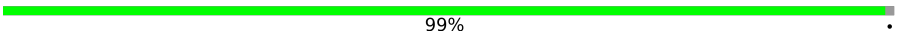
• Molecule 36: 50S ribosomal protein L19

Chain o:



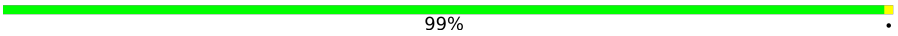
• Molecule 37: 50S ribosomal protein L20

Chain p:



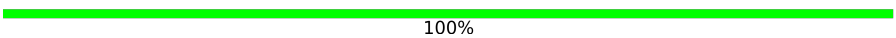
• Molecule 38: 50S ribosomal protein L21

Chain q:



• Molecule 39: 50S ribosomal protein L22

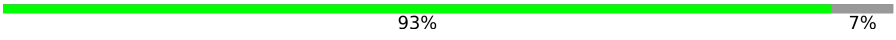
Chain r:



There are no outlier residues recorded for this chain.

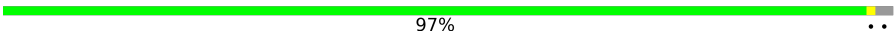
• Molecule 40: 50S ribosomal protein L23

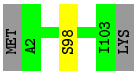
Chain s:



- Molecule 41: 50S ribosomal protein L24

Chain t:





- Molecule 42: 50S ribosomal protein L25

Chain u:

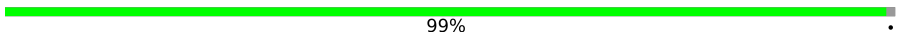
There are no outlier residues recorded for this chain.

- Molecule 43: 50S ribosomal protein L27

Chain v:

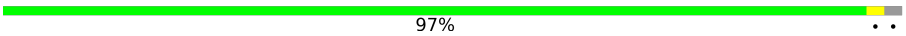
- Molecule 44: 50S ribosomal protein L28

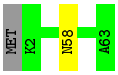
Chain w:



- Molecule 45: 50S ribosomal protein L29

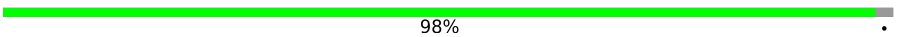
Chain x:





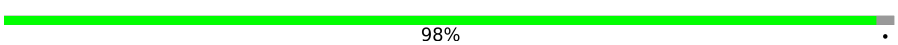
- Molecule 46: 50S ribosomal protein L30

Chain y:



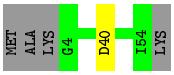
- Molecule 47: 50S ribosomal protein L32

Chain z:



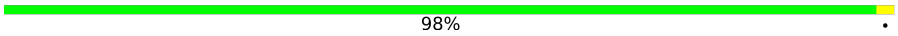
• Molecule 48: 50S ribosomal protein L33

Chain 0:



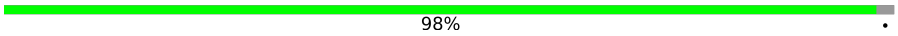
• Molecule 49: 50S ribosomal protein L34

Chain 1:



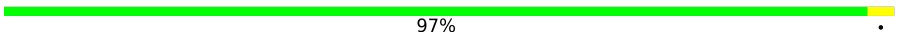
• Molecule 50: 50S ribosomal protein L35

Chain 2:



• Molecule 51: 50S ribosomal protein L36

Chain 3:

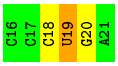


• Molecule 52: 50S ribosomal protein L31

Chain 4:

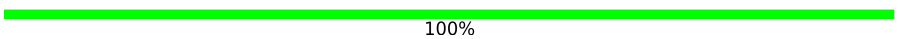
• Molecule 53: mRNA

Chain X:



• Molecule 54: TnaC

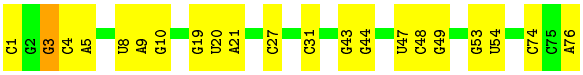
Chain 7:



There are no outlier residues recorded for this chain.

• Molecule 55: tRNA

Chain V:


C1
G2
G3
C4
A5
U8
A9
G10
G19
U20
A21
C27
C31
G43
G44
U47
C48
G49
G53
U54
C74
C75
A76

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	459171	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 ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, G7M, OMC, UR3, 1MG, 5MC, MG, MEQ, 5MU, 4OC, OMG, MA6, PSU, 2MG, 6MZ, PAR, OMU, ZN, 3TD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.55	0/36262	0.93	43/56561 (0.1%)
2	B	0.32	0/1784	0.64	1/2403 (0.0%)
3	C	0.30	0/1651	0.63	0/2225
4	D	0.34	0/1665	0.63	0/2227
5	E	0.35	0/1165	0.62	1/1568 (0.1%)
6	F	0.34	0/858	0.59	0/1160
7	G	0.34	0/1219	0.69	1/1635 (0.1%)
8	H	0.32	0/989	0.59	0/1326
9	I	0.30	0/1034	0.68	1/1375 (0.1%)
10	J	0.33	0/796	0.70	0/1077
11	K	0.36	0/893	0.65	0/1205
12	L	0.38	0/969	0.67	0/1300
13	M	0.29	0/900	0.62	0/1204
14	N	0.30	0/817	0.64	0/1088
15	O	0.31	0/722	0.58	0/964
16	P	0.30	0/653	0.62	0/877
17	Q	0.33	0/650	0.60	0/871
18	R	0.32	0/553	0.59	0/742
19	S	0.36	0/685	0.67	1/922 (0.1%)
20	T	0.31	0/676	0.52	0/895
21	U	0.31	0/597	0.64	0/792
22	a	0.90	7/65673 (0.0%)	0.98	89/102447 (0.1%)
23	b	0.74	0/2850	1.00	5/4444 (0.1%)
24	c	0.47	0/2121	0.67	1/2852 (0.0%)
25	d	0.49	0/1576	0.62	0/2119
26	e	0.42	0/1571	0.62	0/2113
27	f	0.36	0/1434	0.65	0/1926
28	g	0.39	0/1343	0.67	0/1816
29	h	0.34	0/306	0.68	0/413
30	i	0.47	0/1152	0.60	0/1551
31	j	0.48	0/955	0.74	1/1279 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	k	0.43	0/1062	0.65	1/1413 (0.1%)
33	l	0.51	0/1093	0.68	1/1460 (0.1%)
34	m	0.48	0/958	0.68	0/1281
35	n	0.40	0/902	0.65	0/1209
36	o	0.47	0/929	0.67	0/1242
37	p	0.53	0/960	0.60	0/1278
38	q	0.42	0/829	0.65	1/1107 (0.1%)
39	r	0.40	0/864	0.59	0/1156
40	s	0.38	0/744	0.61	0/994
41	t	0.35	0/787	0.65	1/1051 (0.1%)
42	u	0.42	0/766	0.60	0/1025
43	v	0.48	0/593	0.59	0/785
44	w	0.45	0/635	0.63	0/848
45	x	0.30	0/502	0.59	0/667
46	y	0.44	0/453	0.64	0/605
47	z	0.41	0/450	0.64	0/599
48	0	0.49	0/424	0.65	1/565 (0.2%)
49	1	0.46	0/380	0.72	0/498
50	2	0.43	0/513	0.67	0/676
51	3	0.52	0/303	0.62	0/397
52	4	0.28	0/488	0.55	0/649
53	X	1.01	2/138 (1.4%)	1.08	1/212 (0.5%)
54	7	0.38	0/143	0.56	0/193
55	V	0.59	1/1775 (0.1%)	1.06	9/2764 (0.3%)
All	All	0.69	10/151210 (0.0%)	0.89	159/226051 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	1
25	d	0	1
28	g	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2449	U	C5-C6	16.64	1.49	1.34
22	a	2449	U	C2-N3	15.75	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	1	C	OP3-P	-10.83	1.48	1.61
22	a	2449	U	N1-C2	8.59	1.46	1.38
22	a	2449	U	N3-C4	7.42	1.45	1.38
22	a	2449	U	N1-C6	7.37	1.44	1.38
22	a	2449	U	C4-O4	-6.94	1.18	1.23
53	X	20	G	C1'-N9	-5.97	1.38	1.46
53	X	19	U	C1'-N1	5.25	1.56	1.48
22	a	2449	U	C4-C5	5.21	1.48	1.43

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	2449	U	C5-C4-O4	-11.25	119.15	125.90
22	a	2449	U	C2-N3-C4	-11.20	120.28	127.00
22	a	1313	U	C2-N1-C1'	9.99	129.69	117.70
22	a	1313	U	N3-C2-O2	-9.76	115.36	122.20
22	a	2449	U	N3-C4-C5	9.44	120.26	114.60
22	a	1313	U	N1-C2-O2	9.05	129.13	122.80
22	a	1045	C	N1-C2-O2	9.03	124.31	118.90
22	a	1045	C	N3-C2-O2	-8.96	115.63	121.90
22	a	2902	C	N3-C2-O2	-8.89	115.68	121.90
22	a	512	G	O4'-C1'-N9	8.69	115.15	108.20
22	a	1314	C	C2-N1-C1'	8.64	128.30	118.80
22	a	1045	C	C6-N1-C2	-8.18	117.03	120.30
55	V	27	C	N3-C2-O2	-8.00	116.30	121.90
22	a	1045	C	C2-N1-C1'	7.85	127.43	118.80
22	a	2449	U	N1-C2-N3	7.82	119.59	114.90
1	A	961	U	N3-C2-O2	-7.34	117.06	122.20
22	a	2063	C	C2-N1-C1'	7.31	126.84	118.80
22	a	1348	C	N1-C2-O2	7.22	123.23	118.90
1	A	1028	C	N3-C2-O2	-7.00	117.00	121.90
22	a	1963	U	N3-C2-O2	-6.90	117.37	122.20
55	V	27	C	N1-C2-O2	6.88	123.03	118.90
1	A	1028	C	C6-N1-C2	-6.81	117.58	120.30
22	a	1774	C	C6-N1-C2	-6.77	117.59	120.30
22	a	198	C	C6-N1-C2	-6.67	117.63	120.30
1	A	214	C	C2-N1-C1'	6.61	126.07	118.80
23	b	17	C	N1-C2-O2	6.60	122.86	118.90
1	A	54	C	N3-C2-O2	-6.58	117.29	121.90
55	V	19	G	O4'-C1'-N9	-6.54	102.97	108.20
23	b	31	C	C2-N1-C1'	6.52	125.98	118.80
1	A	439	U	C2-N1-C1'	6.51	125.51	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	846	U	C2-N1-C1'	6.46	125.45	117.70
1	A	1029	U	N1-C2-O2	6.45	127.31	122.80
1	A	979	C	N1-C2-O2	6.42	122.75	118.90
9	I	57	MET	CA-CB-CG	6.38	124.14	113.30
22	a	1314	C	N1-C2-O2	6.33	122.70	118.90
1	A	979	C	C2-N1-C1'	6.30	125.73	118.80
22	a	1313	U	C6-N1-C1'	-6.28	112.41	121.20
1	A	993	G	C4-N9-C1'	6.26	134.64	126.50
24	c	98	ASP	CB-CG-OD1	6.25	123.93	118.30
22	a	1314	C	C6-N1-C1'	-6.25	113.30	120.80
22	a	2063	C	C6-N1-C2	-6.22	117.81	120.30
22	a	915	C	C2-N1-C1'	6.18	125.60	118.80
1	A	1158	C	C2-N1-C1'	6.17	125.59	118.80
1	A	618	C	N1-C2-O2	6.13	122.58	118.90
1	A	993	G	N3-C4-N9	6.12	129.67	126.00
22	a	2063	C	N1-C2-O2	6.11	122.57	118.90
22	a	2585	U	O4'-C1'-N1	6.08	113.06	108.20
1	A	979	C	N3-C2-O2	-6.08	117.64	121.90
23	b	17	C	N3-C2-O2	-6.05	117.67	121.90
22	a	1348	C	N3-C2-O2	-6.03	117.68	121.90
1	A	1035	A	P-O3'-C3'	6.00	126.91	119.70
22	a	1920	C	C5-C6-N1	5.99	123.99	121.00
1	A	979	C	C6-N1-C2	-5.97	117.91	120.30
1	A	515	G	N3-C4-C5	-5.96	125.62	128.60
1	A	54	C	N1-C2-O2	5.95	122.47	118.90
22	a	12	U	N3-C2-O2	-5.94	118.04	122.20
22	a	2683	C	N1-C2-O2	5.93	122.46	118.90
38	q	51	VAL	CG1-CB-CG2	-5.92	101.43	110.90
1	A	479	U	N1-C2-O2	5.92	126.94	122.80
22	a	198	C	C5-C6-N1	5.89	123.95	121.00
22	a	1774	C	C5-C6-N1	5.89	123.94	121.00
22	a	867	C	N1-C2-O2	5.89	122.43	118.90
22	a	114	U	C2-N1-C1'	5.88	124.76	117.70
22	a	846	U	N1-C2-O2	5.85	126.90	122.80
22	a	1343	G	C4-N9-C1'	5.83	134.08	126.50
22	a	1956	U	N1-C2-O2	5.83	126.88	122.80
1	A	1029	U	N3-C2-O2	-5.80	118.14	122.20
22	a	1788	C	C6-N1-C2	-5.80	117.98	120.30
22	a	784	G	P-O3'-C3'	5.79	126.65	119.70
55	V	44	G	C5-C6-O6	5.79	132.07	128.60
22	a	2430	A	C2-N3-C4	5.78	113.49	110.60
1	A	439	U	N1-C2-O2	5.76	126.83	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	412	A	O4'-C1'-N9	5.73	112.79	108.20
22	a	1931	U	N1-C2-O2	5.72	126.81	122.80
22	a	783	A	C2-N3-C4	5.71	113.45	110.60
22	a	1830	C	C5-C6-N1	5.70	123.85	121.00
22	a	1348	C	C2-N1-C1'	5.67	125.04	118.80
22	a	1800	C	C6-N1-C2	-5.66	118.03	120.30
22	a	2043	C	C5-C6-N1	5.66	123.83	121.00
1	A	307	C	N1-C2-O2	5.66	122.29	118.90
1	A	993	G	C8-N9-C1'	-5.65	119.66	127.00
55	V	44	G	N1-C6-O6	-5.63	116.52	119.90
22	a	2646	C	C5-C6-N1	5.62	123.81	121.00
5	E	64	MET	CA-CB-CG	5.62	122.86	113.30
22	a	1314	C	C5-C6-N1	5.61	123.81	121.00
1	A	610	U	N1-C2-O2	5.60	126.72	122.80
22	a	985	C	C2-N1-C1'	5.59	124.95	118.80
1	A	610	U	N3-C2-O2	-5.58	118.30	122.20
22	a	2449	U	N1-C2-O2	-5.57	118.90	122.80
22	a	404	A	P-O3'-C3'	5.56	126.37	119.70
22	a	1931	U	N3-C2-O2	-5.56	118.31	122.20
48	0	40	ASP	CB-CG-OD1	5.55	123.29	118.30
19	S	66	MET	CA-CB-CG	5.50	122.64	113.30
55	V	3	G	N3-C4-N9	5.49	129.29	126.00
1	A	439	U	N3-C2-O2	-5.48	118.37	122.20
1	A	339	C	C2-N1-C1'	5.48	124.82	118.80
22	a	2063	C	N3-C2-O2	-5.48	118.07	121.90
41	t	98	SER	C-N-CA	5.46	135.35	121.70
1	A	936	C	N1-C2-O2	5.46	122.17	118.90
32	k	117	THR	C-N-CA	5.46	135.34	121.70
22	a	1343	G	C8-N9-C1'	-5.44	119.93	127.00
22	a	1267	U	C2-N1-C1'	5.43	124.22	117.70
22	a	2666	C	N1-C2-O2	5.42	122.16	118.90
22	a	1830	C	C6-N1-C2	-5.41	118.13	120.30
22	a	867	C	N3-C2-O2	-5.40	118.12	121.90
22	a	1326	U	N3-C2-O2	-5.38	118.44	122.20
23	b	26	C	N1-C2-O2	5.38	122.13	118.90
31	j	12	ASP	CB-CG-OD1	5.38	123.14	118.30
22	a	2474	U	N1-C2-O2	5.36	126.55	122.80
1	A	936	C	C2-N1-C1'	5.36	124.69	118.80
22	a	2902	C	C6-N1-C2	-5.35	118.16	120.30
1	A	515	G	N3-C4-N9	5.34	129.21	126.00
1	A	479	U	C2-N1-C1'	5.34	124.11	117.70
1	A	1109	C	N1-C2-O2	5.34	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	59	LEU	CA-CB-CG	5.33	127.56	115.30
22	a	1931	U	C2-N1-C1'	5.33	124.10	117.70
22	a	2065	C	C6-N1-C2	-5.33	118.17	120.30
1	A	611	C	N1-C2-O2	5.32	122.09	118.90
22	a	1956	U	N3-C2-O2	-5.28	118.50	122.20
22	a	2072	C	C5-C6-N1	5.28	123.64	121.00
55	V	43	G	N3-C4-N9	5.27	129.16	126.00
1	A	1317	C	N1-C2-O2	5.27	122.06	118.90
22	a	717	C	N1-C2-O2	5.27	122.06	118.90
53	X	18	C	C2-N1-C1'	-5.27	113.01	118.80
22	a	1313	U	C6-N1-C2	-5.26	117.84	121.00
22	a	1348	C	C6-N1-C2	-5.25	118.20	120.30
22	a	510	C	N1-C2-O2	5.24	122.05	118.90
22	a	1314	C	C6-N1-C2	-5.24	118.20	120.30
1	A	1029	U	C2-N1-C1'	5.23	123.98	117.70
1	A	754	C	C2-N1-C1'	5.22	124.54	118.80
22	a	2506	U	N3-C2-O2	-5.22	118.55	122.20
2	B	151	ILE	CG1-CB-CG2	-5.21	99.94	111.40
23	b	31	C	C6-N1-C2	-5.21	118.22	120.30
1	A	961	U	C2-N3-C4	-5.20	123.88	127.00
22	a	404	A	OP2-P-O3'	5.17	116.58	105.20
22	a	1197	G	C5-C6-O6	5.17	131.70	128.60
33	l	106	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	515	G	C4-N9-C1'	5.17	133.22	126.50
22	a	1920	C	C6-N1-C2	-5.16	118.23	120.30
55	V	31	C	C2-N1-C1'	5.16	124.47	118.80
1	A	697	U	N3-C2-O2	-5.15	118.59	122.20
22	a	1352	U	N3-C2-O2	-5.14	118.60	122.20
22	a	2752	C	N1-C2-O2	5.14	121.99	118.90
1	A	5	U	P-O3'-C3'	5.14	125.87	119.70
22	a	373	U	N3-C2-O2	-5.09	118.63	122.20
22	a	323	C	C2-N1-C1'	5.09	124.39	118.80
22	a	510	C	C2-N1-C1'	5.09	124.40	118.80
22	a	2582	G	N3-C4-N9	5.09	129.05	126.00
22	a	984	A	O4'-C1'-N9	5.08	112.27	108.20
22	a	2901	C	N1-C2-O2	5.08	121.94	118.90
1	A	58	C	C6-N1-C2	-5.07	118.27	120.30
22	a	1157	G	C4-N9-C1'	5.06	133.07	126.50
22	a	2902	C	N1-C2-N3	5.06	122.74	119.20
22	a	2043	C	C2-N1-C1'	5.05	124.36	118.80
55	V	3	G	C4-N9-C1'	5.04	133.05	126.50
1	A	151	A	N1-C6-N6	-5.03	115.58	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	2244	U	N3-C4-O4	5.03	122.92	119.40
22	a	2474	U	N3-C2-O2	-5.03	118.68	122.20
22	a	999	U	N3-C2-O2	-5.03	118.68	122.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	32	SER	Peptide
25	d	16	THR	Peptide
28	g	47	ASP	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
3	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
4	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
5	E	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
6	F	101/135 (75%)	98 (97%)	3 (3%)	0	100	100
7	G	151/179 (84%)	143 (95%)	8 (5%)	0	100	100
8	H	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
9	I	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
10	J	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	15	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	K	115/129 (89%)	110 (96%)	3 (3%)	2 (2%)	9 31
12	L	121/124 (98%)	115 (95%)	4 (3%)	2 (2%)	9 31
13	M	113/118 (96%)	110 (97%)	3 (3%)	0	100 100
14	N	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
15	O	86/89 (97%)	85 (99%)	1 (1%)	0	100 100
16	P	79/82 (96%)	77 (98%)	2 (2%)	0	100 100
17	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100 100
18	R	64/75 (85%)	60 (94%)	4 (6%)	0	100 100
19	S	82/92 (89%)	75 (92%)	7 (8%)	0	100 100
20	T	84/87 (97%)	84 (100%)	0	0	100 100
21	U	68/71 (96%)	68 (100%)	0	0	100 100
24	c	269/273 (98%)	259 (96%)	10 (4%)	0	100 100
25	d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	29 61
26	e	199/201 (99%)	197 (99%)	2 (1%)	0	100 100
27	f	175/179 (98%)	167 (95%)	8 (5%)	0	100 100
28	g	174/177 (98%)	157 (90%)	16 (9%)	1 (1%)	25 58
29	h	39/149 (26%)	34 (87%)	5 (13%)	0	100 100
30	i	140/142 (99%)	137 (98%)	3 (2%)	0	100 100
31	j	121/123 (98%)	119 (98%)	2 (2%)	0	100 100
32	k	142/144 (99%)	138 (97%)	4 (3%)	0	100 100
33	l	134/136 (98%)	130 (97%)	4 (3%)	0	100 100
34	m	116/127 (91%)	110 (95%)	6 (5%)	0	100 100
35	n	114/117 (97%)	109 (96%)	5 (4%)	0	100 100
36	o	112/115 (97%)	107 (96%)	5 (4%)	0	100 100
37	p	115/118 (98%)	115 (100%)	0	0	100 100
38	q	101/103 (98%)	99 (98%)	2 (2%)	0	100 100
39	r	108/110 (98%)	108 (100%)	0	0	100 100
40	s	91/100 (91%)	85 (93%)	6 (7%)	0	100 100
41	t	100/104 (96%)	93 (93%)	7 (7%)	0	100 100
42	u	92/94 (98%)	90 (98%)	2 (2%)	0	100 100
43	v	76/85 (89%)	74 (97%)	2 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
45	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
48	0	49/55 (89%)	49 (100%)	0	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/66 (85%)	53 (95%)	3 (5%)	0	100	100
54	7	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
All	All	5500/5925 (93%)	5301 (96%)	192 (4%)	7 (0%)	54	82

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	g	47	ASP
10	J	57	VAL
12	L	89	ASP
25	d	149	ASN
11	K	120	GLY
11	K	119	ASP
12	L	88	LYS

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	
2	B	186/199 (94%)	185 (100%)	1 (0%)	88	96
3	C	170/190 (90%)	169 (99%)	1 (1%)	86	96
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	103 (99%)	1 (1%)	76	92
9	I	105/107 (98%)	104 (99%)	1 (1%)	76	92
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	90/99 (91%)	89 (99%)	1 (1%)	73	92
12	L	103/104 (99%)	103 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	71 (99%)	1 (1%)	67	89
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	59 (98%)	1 (2%)	60	86
24	c	216/218 (99%)	215 (100%)	1 (0%)	88	96
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	164 (99%)	1 (1%)	86	96
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	137/138 (99%)	137 (100%)	0	100	100
29	h	32/114 (28%)	32 (100%)	0	100	100
30	i	116/116 (100%)	116 (100%)	0	100	100
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	109/109 (100%)	106 (97%)	3 (3%)	43	76
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	86 (100%)	0	100	100
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	r	93/93 (100%)	93 (100%)	0	100 100
40	s	80/84 (95%)	80 (100%)	0	100 100
41	t	83/85 (98%)	83 (100%)	0	100 100
42	u	78/78 (100%)	78 (100%)	0	100 100
43	v	58/63 (92%)	58 (100%)	0	100 100
44	w	67/68 (98%)	67 (100%)	0	100 100
45	x	54/55 (98%)	53 (98%)	1 (2%)	57 84
46	y	48/49 (98%)	48 (100%)	0	100 100
47	z	47/48 (98%)	47 (100%)	0	100 100
48	0	46/49 (94%)	46 (100%)	0	100 100
49	1	38/38 (100%)	37 (97%)	1 (3%)	46 77
50	2	51/52 (98%)	51 (100%)	0	100 100
51	3	34/34 (100%)	33 (97%)	1 (3%)	42 76
52	4	55/59 (93%)	55 (100%)	0	100 100
54	7	16/16 (100%)	16 (100%)	0	100 100
All	All	4592/4842 (95%)	4577 (100%)	15 (0%)	92 98

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	128	LYS
3	C	127	ARG
8	H	69	LYS
9	I	106	ARG
11	K	119	ASP
19	S	44	MET
21	U	7	ARG
24	c	214	ARG
26	e	88	ARG
33	l	81	ARG
33	l	82	MET
33	l	84	LYS
45	x	58	ASN
49	1	25	LYS
51	3	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
9	I	126	GLN
16	P	63	GLN
45	x	58	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1519 (99%)	218 (14%)	4 (0%)
22	a	2745/2753 (99%)	362 (13%)	0
23	b	118/119 (99%)	15 (12%)	0
53	X	5/6 (83%)	1 (20%)	0
55	V	73/75 (97%)	14 (19%)	0
All	All	4454/4472 (99%)	610 (13%)	4 (0%)

All (610) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	7	A
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	58	C
1	A	71	A
1	A	74	A
1	A	81	A
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	87	C
1	A	88	U
1	A	94	G
1	A	95	C

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Mol	Chain	Res	Type
1	A	121	U
1	A	122	G
1	A	130	A
1	A	131	A
1	A	141	G
1	A	143	A
1	A	144	G
1	A	159	G
1	A	163	C
1	A	164	G
1	A	177	G
1	A	182	A
1	A	183	C
1	A	197	A
1	A	202	G
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	344	A
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	388	G
1	A	389	A
1	A	390	U
1	A	393	A
1	A	404	G
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G

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Mol	Chain	Res	Type
1	A	414	A
1	A	415	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	435	A
1	A	438	U
1	A	448	A
1	A	453	G
1	A	456	A
1	A	457	G
1	A	458	U
1	A	463	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	497	G
1	A	509	A
1	A	511	C
1	A	512	U
1	A	513	C
1	A	518	C
1	A	519	C
1	A	521	G
1	A	527	G
1	A	531	U
1	A	533	A
1	A	547	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A

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Mol	Chain	Res	Type
1	A	588	G
1	A	596	A
1	A	620	C
1	A	633	G
1	A	650	G
1	A	665	A
1	A	687	A
1	A	703	G
1	A	721	G
1	A	723	U
1	A	724	G
1	A	734	G
1	A	746	A
1	A	747	A
1	A	755	G
1	A	774	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	851	G
1	A	889	A
1	A	890	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	983	A
1	A	992	U
1	A	1004	A
1	A	1009	U

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Mol	Chain	Res	Type
1	A	1027	C
1	A	1028	C
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1039	G
1	A	1042	A
1	A	1044	A
1	A	1064	G
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1108	G
1	A	1137	C
1	A	1139	G
1	A	1152	A
1	A	1159	U
1	A	1168	U
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1257	A
1	A	1260	G
1	A	1275	A
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1297	G
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1317	C
1	A	1320	C

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Mol	Chain	Res	Type
1	A	1322	C
1	A	1363	A
1	A	1364	U
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1398	A
1	A	1419	G
1	A	1429	A
1	A	1441	A
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1484	C
1	A	1487	G
1	A	1492	A
1	A	1493	A
1	A	1497	G
1	A	1499	A
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
22	a	10	A
22	a	15	G
22	a	23	G
22	a	34	U
22	a	45	G
22	a	51	G
22	a	58	G
22	a	61	C
22	a	63	A
22	a	71	A
22	a	74	A
22	a	75	G
22	a	84	A
22	a	96	C
22	a	101	A
22	a	102	U

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Mol	Chain	Res	Type
22	a	118	A
22	a	119	A
22	a	120	U
22	a	125	A
22	a	139	U
22	a	142	A
22	a	149	A
22	a	163	C
22	a	164	C
22	a	181	A
22	a	196	A
22	a	199	A
22	a	200	U
22	a	204	A
22	a	215	G
22	a	216	A
22	a	221	A
22	a	222	A
22	a	248	G
22	a	264	C
22	a	265	A
22	a	272	A
22	a	274	C
22	a	278	A
22	a	285	G
22	a	287	G
22	a	294	A
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	361	G
22	a	362	A
22	a	386	G
22	a	396	G
22	a	405	U
22	a	411	G
22	a	412	A
22	a	420	C
22	a	481	G
22	a	489	G
22	a	491	G

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Mol	Chain	Res	Type
22	a	504	A
22	a	505	A
22	a	509	C
22	a	531	C
22	a	532	A
22	a	544	C
22	a	545	U
22	a	546	U
22	a	547	A
22	a	549	G
22	a	563	A
22	a	573	U
22	a	575	A
22	a	603	A
22	a	615	U
22	a	627	A
22	a	634	C
22	a	637	A
22	a	645	C
22	a	647	G
22	a	654	A
22	a	655	A
22	a	686	U
22	a	717	C
22	a	730	A
22	a	738	G
22	a	747	5MU
22	a	764	A
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	788	A
22	a	789	A
22	a	792	A
22	a	800	A
22	a	805	G
22	a	806	C
22	a	812	C
22	a	827	U
22	a	828	U

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Mol	Chain	Res	Type
22	a	829	A
22	a	845	A
22	a	846	U
22	a	847	U
22	a	856	G
22	a	859	G
22	a	866	A
22	a	869	G
22	a	881	G
22	a	883	G
22	a	884	U
22	a	888	C
22	a	890	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	897	C
22	a	899	A
22	a	910	A
22	a	931	U
22	a	932	U
22	a	945	A
22	a	946	C
22	a	961	C
22	a	973	A
22	a	974	G
22	a	983	A
22	a	989	G
22	a	996	A
22	a	1005	C
22	a	1012	U
22	a	1013	C
22	a	1022	G
22	a	1033	U
22	a	1040	A
22	a	1041	G
22	a	1045	C
22	a	1046	A
22	a	1047	G
22	a	1048	A
22	a	1051	G
22	a	1108	U

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Mol	Chain	Res	Type
22	a	1111	A
22	a	1112	G
22	a	1115	G
22	a	1116	G
22	a	1122	G
22	a	1130	U
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1141	U
22	a	1142	A
22	a	1204	A
22	a	1236	G
22	a	1250	G
22	a	1253	A
22	a	1256	G
22	a	1257	C
22	a	1271	G
22	a	1272	A
22	a	1273	U
22	a	1275	A
22	a	1300	G
22	a	1301	A
22	a	1321	A
22	a	1352	U
22	a	1365	A
22	a	1378	A
22	a	1379	U
22	a	1383	A
22	a	1403	A
22	a	1416	G
22	a	1419	A
22	a	1427	A
22	a	1428	C
22	a	1437	C
22	a	1452	G
22	a	1459	G
22	a	1482	G
22	a	1493	C
22	a	1509	A
22	a	1510	G
22	a	1515	A

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Mol	Chain	Res	Type
22	a	1524	G
22	a	1529	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1554	U
22	a	1559	U
22	a	1566	A
22	a	1567	G
22	a	1569	A
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1607	C
22	a	1608	A
22	a	1610	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1654	A
22	a	1674	G
22	a	1675	C
22	a	1698	A
22	a	1715	G
22	a	1729	U
22	a	1730	C
22	a	1731	G
22	a	1732	C
22	a	1738	G
22	a	1764	C
22	a	1773	A
22	a	1786	A
22	a	1791	A
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1842	G
22	a	1847	A
22	a	1858	A

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Mol	Chain	Res	Type
22	a	1866	A
22	a	1869	G
22	a	1870	C
22	a	1871	A
22	a	1872	A
22	a	1873	G
22	a	1906	G
22	a	1907	G
22	a	1913	A
22	a	1929	G
22	a	1930	G
22	a	1936	A
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1964	G
22	a	1966	A
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1982	U
22	a	1991	U
22	a	1993	U
22	a	2023	C
22	a	2031	A
22	a	2033	A
22	a	2035	G
22	a	2036	C
22	a	2043	C
22	a	2049	G
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2077	A
22	a	2093	G
22	a	2198	A
22	a	2199	A
22	a	2203	U

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Mol	Chain	Res	Type
22	a	2204	G
22	a	2211	A
22	a	2225	A
22	a	2238	G
22	a	2239	G
22	a	2266	A
22	a	2283	C
22	a	2287	A
22	a	2288	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2334	U
22	a	2336	A
22	a	2340	A
22	a	2345	G
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2377	A
22	a	2383	G
22	a	2385	C
22	a	2391	G
22	a	2396	G
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2422	C
22	a	2425	A
22	a	2426	A
22	a	2429	G
22	a	2431	U
22	a	2435	A
22	a	2441	U
22	a	2445	2MG
22	a	2448	A
22	a	2470	G
22	a	2475	C
22	a	2476	A
22	a	2491	U

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Mol	Chain	Res	Type
22	a	2498	OMC
22	a	2502	G
22	a	2504	PSU
22	a	2505	G
22	a	2507	C
22	a	2513	A
22	a	2518	A
22	a	2520	C
22	a	2525	G
22	a	2529	G
22	a	2535	G
22	a	2547	A
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2585	U
22	a	2586	U
22	a	2601	C
22	a	2602	A
22	a	2609	U
22	a	2613	U
22	a	2615	U
22	a	2629	U
22	a	2663	G
22	a	2682	A
22	a	2685	G
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2724	U
22	a	2726	A
22	a	2732	G
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2752	C
22	a	2757	A
22	a	2765	A
22	a	2778	A
22	a	2791	G
22	a	2798	U
22	a	2799	A

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Mol	Chain	Res	Type
22	a	2818	U
22	a	2820	A
22	a	2821	A
22	a	2835	A
22	a	2836	U
22	a	2849	U
22	a	2861	U
22	a	2873	A
22	a	2884	U
22	a	2891	U
23	b	9	G
23	b	13	G
23	b	24	G
23	b	33	G
23	b	35	C
23	b	41	G
23	b	45	A
23	b	56	G
23	b	67	G
23	b	89	U
23	b	90	C
23	b	91	C
23	b	99	A
23	b	105	G
23	b	109	A
53	X	19	U
55	V	3	G
55	V	4	C
55	V	5	A
55	V	8	U
55	V	9	A
55	V	10	G
55	V	20	U
55	V	21	A
55	V	47	U
55	V	48	C
55	V	49	G
55	V	53	G
55	V	74	C
55	V	76	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	196	A
1	A	411	A
1	A	1035	A

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

35 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	5MC	A	1407	1	15,22,23	2.80	5 (33%)	19,32,35	1.40	4 (21%)
22	5MC	a	1962	22	15,22,23	2.73	5 (33%)	19,32,35	1.35	2 (10%)
25	MEQ	d	150	25	8,9,10	0.90	0	5,10,12	0.81	0
1	MA6	A	1519	1	19,26,27	1.10	1 (5%)	18,38,41	4.85	3 (16%)
1	PSU	A	516	1,57	17,21,22	1.02	2 (11%)	20,30,33	3.26	4 (20%)
1	MA6	A	1518	1	19,26,27	1.16	2 (10%)	18,38,41	4.66	3 (16%)
22	3TD	a	1915	22	17,22,23	3.17	8 (47%)	19,32,35	1.37	3 (15%)
22	PSU	a	1917	22	17,21,22	1.05	2 (11%)	20,30,33	3.14	5 (25%)
22	OMG	a	2251	22,55	18,26,27	3.28	8 (44%)	20,38,41	2.32	4 (20%)
1	5MC	A	967	1	15,22,23	2.94	5 (33%)	19,32,35	1.35	4 (21%)
22	PSU	a	2504	22	17,21,22	1.16	3 (17%)	20,30,33	3.34	6 (30%)
1	2MG	A	1516	1	19,26,27	3.93	8 (42%)	21,38,41	2.40	7 (33%)
22	PSU	a	2457	22	17,21,22	1.36	3 (17%)	20,30,33	2.88	5 (25%)
22	PSU	a	2605	22	17,21,22	1.18	3 (17%)	20,30,33	3.01	5 (25%)
22	PSU	a	1911	22	17,21,22	1.05	2 (11%)	20,30,33	3.00	5 (25%)
22	6MZ	a	1618	22	18,25,26	1.92	2 (11%)	16,36,39	2.11	3 (18%)
22	OMU	a	2552	22	14,22,23	2.86	5 (35%)	14,31,34	0.71	0
22	OMC	a	2498	22,57	15,22,23	2.97	6 (40%)	17,31,34	1.44	1 (5%)
1	4OC	A	1402	1	16,23,24	3.23	6 (37%)	17,32,35	1.57	1 (5%)
22	2MG	a	1835	22	19,26,27	3.77	9 (47%)	21,38,41	2.83	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	5MU	a	1939	22	15,22,23	5.60	5 (33%)	16,32,35	2.00	2 (12%)
22	2MA	a	2503	22,57	17,25,26	3.40	5 (29%)	19,37,40	1.92	3 (15%)
22	PSU	a	955	22	17,21,22	1.19	3 (17%)	20,30,33	2.94	5 (25%)
22	5MU	a	747	22	15,22,23	5.68	5 (33%)	16,32,35	2.20	2 (12%)
1	UR3	A	1498	1	14,22,23	2.64	4 (28%)	15,32,35	0.71	0
22	PSU	a	2604	22	17,21,22	1.17	3 (17%)	20,30,33	2.99	6 (30%)
22	PSU	a	746	22,57	17,21,22	1.13	2 (11%)	20,30,33	3.13	7 (35%)
22	6MZ	a	2030	22	18,25,26	1.99	2 (11%)	16,36,39	2.40	3 (18%)
1	2MG	A	1207	1	19,26,27	4.16	8 (42%)	21,38,41	2.41	8 (38%)
22	G7M	a	2069	22	20,26,27	3.61	8 (40%)	20,39,42	1.97	4 (20%)
22	2MG	a	2445	22	19,26,27	3.74	9 (47%)	21,38,41	2.61	7 (33%)
55	5MU	V	54	55	14,21,23	7.41	5 (35%)	14,30,35	0.67	0
22	PSU	a	2580	22	17,21,22	1.32	3 (17%)	20,30,33	3.06	7 (35%)
1	2MG	A	966	1	19,26,27	4.14	8 (42%)	21,38,41	2.48	8 (38%)
22	1MG	a	745	22	18,26,27	3.62	6 (33%)	19,39,42	1.91	3 (15%)

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	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
22	5MC	a	1962	22	-	2/5/25/26	0/2/2/2
25	MEQ	d	150	25	-	5/8/9/11	-
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3
1	PSU	A	516	1,57	-	1/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
22	3TD	a	1915	22	-	2/7/25/26	0/2/2/2
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
22	OMG	a	2251	22,55	-	1/5/27/28	0/3/3/3
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
22	PSU	a	2504	22	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMU	a	2552	22	-	0/7/27/28	0/2/2/2
22	OMC	a	2498	22,57	-	3/7/27/28	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
22	2MG	a	1835	22	-	0/5/27/28	0/3/3/3
22	5MU	a	1939	22	-	0/5/25/26	0/2/2/2
22	2MA	a	2503	22,57	-	1/3/25/26	0/3/3/3
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
22	5MU	a	747	22	-	0/5/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	a	746	22,57	-	3/7/25/26	0/2/2/2
22	6MZ	a	2030	22	-	2/5/27/28	0/3/3/3
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
22	G7M	a	2069	22	-	2/3/25/26	0/3/3/3
22	2MG	a	2445	22	-	2/5/27/28	0/3/3/3
55	5MU	V	54	55	-	0/5/25/26	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	2/5/27/28	0/3/3/3
22	1MG	a	745	22	-	0/3/25/26	0/3/3/3

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	54	5MU	C6-N1	24.24	1.65	1.35
22	a	747	5MU	C4-C5	17.49	1.78	1.41
22	a	1939	5MU	C4-C5	17.17	1.78	1.41
1	A	1207	2MG	C2-N2	13.13	1.45	1.34
1	A	966	2MG	C2-N2	12.98	1.45	1.34
1	A	1516	2MG	C2-N2	12.44	1.44	1.34
22	a	1835	2MG	C2-N2	11.57	1.43	1.34
22	a	2445	2MG	C2-N2	11.56	1.43	1.34
55	V	54	5MU	C6-C5	-9.45	1.17	1.38
22	a	747	5MU	C4-N3	-8.92	1.17	1.33
22	a	745	1MG	C4-N3	8.79	1.49	1.35
22	a	1939	5MU	C6-C5	-8.67	1.16	1.40
22	a	1939	5MU	C4-N3	-8.51	1.18	1.33
22	a	747	5MU	C6-C5	-8.47	1.16	1.40
22	a	2069	G7M	C4-N3	8.41	1.48	1.35
22	a	2251	OMG	C4-N3	8.09	1.48	1.35
55	V	54	5MU	C4-N3	-8.06	1.19	1.33
22	a	745	1MG	C2-N3	8.04	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C6-N1	7.61	1.45	1.35
22	a	2503	2MA	C6-C5	7.55	1.53	1.41
22	a	2069	G7M	C2-N2	7.50	1.48	1.33
22	a	2503	2MA	C4-N3	7.34	1.47	1.35
22	a	1915	3TD	C6-C5	7.22	1.49	1.38
1	A	966	2MG	C4-N3	7.06	1.46	1.35
1	A	1207	2MG	C4-N3	7.00	1.46	1.35
22	a	2030	6MZ	C6-N6	6.97	1.46	1.35
22	a	2069	G7M	C6-C5	6.91	1.53	1.41
1	A	967	5MC	C4-N3	6.90	1.44	1.35
1	A	1498	UR3	C6-N1	6.83	1.44	1.35
22	a	745	1MG	C6-C5	6.83	1.52	1.41
22	a	2498	OMC	C6-N1	6.80	1.44	1.35
22	a	1618	6MZ	C6-N6	6.78	1.46	1.35
22	a	1962	5MC	C4-N3	6.66	1.44	1.35
1	A	1407	5MC	C4-N3	6.33	1.44	1.35
22	a	2069	G7M	C6-N1	6.21	1.43	1.33
1	A	1516	2MG	C4-N3	6.16	1.45	1.35
22	a	2251	OMG	C6-C5	6.12	1.51	1.41
22	a	2552	OMU	C4-N3	6.01	1.43	1.33
22	a	1835	2MG	C4-N3	5.99	1.45	1.35
22	a	2503	2MA	C2-N1	5.99	1.44	1.34
22	a	2445	2MG	C4-N3	5.92	1.44	1.35
22	a	2503	2MA	C2-N3	5.91	1.44	1.34
1	A	966	2MG	C6-C5	5.84	1.51	1.41
1	A	1207	2MG	C6-C5	5.82	1.51	1.41
1	A	966	2MG	C6-N1	5.81	1.43	1.33
1	A	1207	2MG	C6-N1	5.79	1.43	1.33
22	a	1835	2MG	C6-N1	5.75	1.43	1.33
1	A	1516	2MG	C6-C5	5.66	1.51	1.41
1	A	1516	2MG	C6-N1	5.61	1.42	1.33
22	a	1835	2MG	C6-C5	5.57	1.50	1.41
22	a	2445	2MG	C6-C5	5.48	1.50	1.41
22	a	1915	3TD	C6-N1	5.33	1.45	1.34
22	a	1915	3TD	C4-N3	5.29	1.46	1.38
22	a	2445	2MG	C6-N1	5.28	1.42	1.33
22	a	2251	OMG	C6-N1	5.26	1.42	1.33
1	A	967	5MC	C2-N3	5.25	1.48	1.38
22	a	745	1MG	C2-N2	5.20	1.44	1.33
22	a	2552	OMU	C2-N3	5.20	1.48	1.38
22	a	2251	OMG	C2-N2	5.17	1.44	1.33
1	A	1402	4OC	C6-C5	5.10	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C2-N1	5.07	1.48	1.38
22	a	1962	5MC	C2-N3	5.06	1.48	1.38
1	A	1402	4OC	C4-N3	4.99	1.44	1.34
1	A	1407	5MC	C2-N3	4.98	1.48	1.38
1	A	1402	4OC	C2-N3	4.97	1.48	1.38
22	a	2069	G7M	C2-N1	4.94	1.44	1.35
22	a	2552	OMU	C6-N1	4.89	1.41	1.35
22	a	2498	OMC	C2-N3	4.83	1.47	1.38
1	A	1498	UR3	C6-C5	4.78	1.48	1.38
22	a	2498	OMC	C6-C5	4.74	1.48	1.38
22	a	2498	OMC	C4-N3	4.60	1.43	1.35
1	A	967	5MC	C5-C4	4.55	1.48	1.41
22	a	2552	OMU	C6-C5	4.48	1.48	1.38
1	A	1407	5MC	C5-C4	4.42	1.48	1.41
1	A	967	5MC	C4-N4	4.41	1.45	1.34
1	A	1407	5MC	C4-N4	4.38	1.45	1.34
55	V	54	5MU	C2-N3	4.37	1.46	1.38
22	a	1962	5MC	C4-N4	4.29	1.44	1.34
1	A	1498	UR3	C4-N3	4.27	1.44	1.38
22	a	2251	OMG	C2-N1	4.08	1.42	1.35
22	a	747	5MU	C2-N3	4.06	1.46	1.38
1	A	1402	4OC	C4-N4	4.06	1.44	1.36
22	a	1939	5MU	C2-N3	3.98	1.46	1.38
22	a	1915	3TD	C4-C5	3.95	1.49	1.41
1	A	966	2MG	C2-N3	3.95	1.46	1.34
1	A	1402	4OC	C5-C4	3.90	1.48	1.39
1	A	1207	2MG	C2-N3	3.89	1.46	1.34
22	a	1962	5MC	C5-C4	3.59	1.47	1.41
1	A	1516	2MG	C2-N3	3.42	1.45	1.34
1	A	967	5MC	C6-C5	3.39	1.49	1.40
22	a	2445	2MG	C2-N3	3.25	1.44	1.34
1	A	1407	5MC	C6-C5	3.25	1.49	1.40
22	a	1835	2MG	C2-N3	3.13	1.44	1.34
22	a	2457	PSU	C5-C1'	-3.12	1.49	1.52
22	a	2030	6MZ	C5-C4	-3.10	1.32	1.40
22	a	2498	OMC	C4-N4	3.08	1.44	1.35
1	A	516	PSU	C4-N3	3.08	1.38	1.33
1	A	1207	2MG	CM2-N2	3.01	1.50	1.45
1	A	1519	MA6	C5-C4	-2.96	1.33	1.40
22	a	1917	PSU	C4-N3	2.91	1.38	1.33
22	a	1962	5MC	C6-C5	2.91	1.48	1.40
22	a	1618	6MZ	C5-C4	-2.88	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2580	PSU	O4'-C1'	-2.84	1.40	1.44
1	A	1516	2MG	CM2-N2	2.83	1.50	1.45
22	a	1915	3TD	C5-C1'	-2.83	1.49	1.52
1	A	1518	MA6	C5-C4	-2.82	1.33	1.40
1	A	966	2MG	CM2-N2	2.82	1.50	1.45
22	a	2580	PSU	C5-C1'	-2.78	1.49	1.52
22	a	1835	2MG	CM2-N2	2.78	1.49	1.45
22	a	745	1MG	O6-C6	-2.73	1.17	1.24
22	a	1939	5MU	O4-C4	-2.64	1.17	1.24
22	a	2445	2MG	CM2-N2	2.62	1.49	1.45
22	a	2251	OMG	O6-C6	-2.62	1.18	1.24
22	a	1911	PSU	C4-N3	2.61	1.37	1.33
22	a	2445	2MG	O6-C6	-2.60	1.18	1.24
22	a	747	5MU	O4-C4	-2.58	1.18	1.24
22	a	1835	2MG	O6-C6	-2.55	1.18	1.24
22	a	2503	2MA	C6-N1	2.54	1.40	1.35
22	a	2069	G7M	C5-C4	-2.51	1.36	1.39
22	a	2498	OMC	C5-C4	2.50	1.47	1.41
1	A	1498	UR3	O4-C4	-2.50	1.18	1.24
1	A	966	2MG	C2-N1	2.50	1.42	1.34
1	A	1516	2MG	O6-C6	-2.49	1.18	1.24
22	a	955	PSU	C5-C1'	-2.47	1.50	1.52
55	V	54	5MU	O4-C4	-2.46	1.18	1.24
1	A	1207	2MG	C2-N1	2.46	1.42	1.34
22	a	2069	G7M	O6-C6	-2.44	1.18	1.24
1	A	966	2MG	O6-C6	-2.43	1.18	1.24
22	a	1915	3TD	O4-C4	-2.43	1.18	1.24
1	A	1207	2MG	O6-C6	-2.43	1.18	1.24
22	a	2457	PSU	O4'-C1'	-2.40	1.41	1.44
22	a	2605	PSU	C4-N3	2.35	1.37	1.33
22	a	2504	PSU	C4-N3	2.33	1.37	1.33
22	a	2069	G7M	C2-N3	2.33	1.45	1.34
22	a	2604	PSU	C5-C1'	-2.33	1.50	1.52
22	a	2457	PSU	C4-N3	2.33	1.37	1.33
22	a	746	PSU	O4'-C1'	-2.33	1.41	1.44
1	A	1516	2MG	C2-N1	2.30	1.41	1.34
22	a	2605	PSU	C5-C1'	-2.26	1.50	1.52
22	a	955	PSU	O4'-C1'	-2.26	1.41	1.44
22	a	955	PSU	C4-N3	2.26	1.37	1.33
22	a	2552	OMU	O4-C4	-2.25	1.18	1.24
22	a	2504	PSU	O4'-C1'	-2.25	1.41	1.44
22	a	2604	PSU	C4-N3	2.25	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2251	OMG	C5-C4	-2.24	1.35	1.40
22	a	1835	2MG	C2-N1	2.22	1.41	1.34
22	a	2445	2MG	C2-N1	2.20	1.41	1.34
22	a	1911	PSU	O4'-C1'	-2.19	1.41	1.44
22	a	2251	OMG	C2-N3	2.19	1.45	1.34
22	a	2504	PSU	C5-C1'	-2.19	1.50	1.52
22	a	2445	2MG	C5-C4	-2.18	1.35	1.40
22	a	1835	2MG	C5-C4	-2.17	1.35	1.40
1	A	1518	MA6	C2-N3	2.14	1.35	1.32
22	a	1917	PSU	O4'-C1'	-2.11	1.41	1.44
1	A	516	PSU	O4'-C1'	-2.11	1.41	1.44
22	a	2580	PSU	C4-N3	2.10	1.36	1.33
22	a	1915	3TD	O4'-C1'	-2.09	1.41	1.44
22	a	746	PSU	C4-N3	2.08	1.36	1.33
22	a	2604	PSU	O4'-C1'	-2.07	1.41	1.44
22	a	745	1MG	C6-N1	2.07	1.41	1.38
22	a	2605	PSU	O4'-C1'	-2.01	1.41	1.44

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1519	MA6	N1-C6-N6	-17.46	98.68	117.06
1	A	1518	MA6	N1-C6-N6	-16.41	99.78	117.06
1	A	516	PSU	N1-C2-N3	-11.61	119.20	128.43
22	a	2504	PSU	N1-C2-N3	-11.21	119.52	128.43
22	a	1917	PSU	N1-C2-N3	-10.88	119.78	128.43
22	a	2605	PSU	N1-C2-N3	-10.32	120.22	128.43
22	a	746	PSU	N1-C2-N3	-10.25	120.28	128.43
22	a	1911	PSU	N1-C2-N3	-10.25	120.28	128.43
22	a	2580	PSU	N1-C2-N3	-10.09	120.41	128.43
22	a	2457	PSU	N1-C2-N3	-9.97	120.50	128.43
22	a	955	PSU	N1-C2-N3	-9.94	120.53	128.43
22	a	2604	PSU	N1-C2-N3	-9.93	120.53	128.43
1	A	1518	MA6	C1'-N9-C4	-9.42	110.09	126.64
1	A	1519	MA6	C1'-N9-C4	-8.87	111.06	126.64
22	a	747	5MU	C5-C6-N1	-7.82	113.76	122.19
22	a	1939	5MU	C5-C6-N1	-7.16	114.48	122.19
1	A	966	2MG	C1'-N9-C4	6.96	138.87	126.64
22	a	1835	2MG	CM2-N2-C2	-6.76	115.43	123.59
22	a	1835	2MG	N2-C2-N1	6.69	123.38	116.96
22	a	2504	PSU	C4-N3-C2	6.66	120.77	115.14
1	A	1207	2MG	C1'-N9-C4	6.50	138.05	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	2503	2MA	C2-N3-C4	6.35	120.68	115.52
22	a	2445	2MG	CM2-N2-C2	-6.31	115.98	123.59
22	a	2251	OMG	C1'-N9-C4	-6.29	115.58	126.64
22	a	2030	6MZ	C9-N6-C6	-6.21	117.52	122.87
22	a	1917	PSU	C4-N3-C2	6.09	120.28	115.14
1	A	516	PSU	C4-N3-C2	6.06	120.26	115.14
22	a	1618	6MZ	N3-C2-N1	-5.77	119.67	128.68
1	A	1519	MA6	N3-C2-N1	-5.75	119.69	128.68
22	a	2580	PSU	C4-N3-C2	5.68	119.94	115.14
1	A	1402	4OC	CM4-N4-C4	-5.65	118.11	122.97
22	a	2069	G7M	N3-C2-N1	-5.64	119.70	127.22
22	a	955	PSU	C4-N3-C2	5.59	119.87	115.14
22	a	2445	2MG	N2-C2-N1	5.59	122.33	116.96
22	a	2030	6MZ	N3-C2-N1	-5.51	120.06	128.68
22	a	2251	OMG	N3-C2-N1	-5.48	119.91	127.22
22	a	745	1MG	C1'-N9-C4	5.48	136.26	126.64
22	a	2604	PSU	C4-N3-C2	5.44	119.73	115.14
22	a	1911	PSU	C4-N3-C2	5.41	119.71	115.14
1	A	1518	MA6	N3-C2-N1	-5.15	120.63	128.68
22	a	2605	PSU	C4-N3-C2	5.12	119.46	115.14
1	A	1516	2MG	CM2-N2-C2	-5.03	117.52	123.59
22	a	1835	2MG	C1'-N9-C4	5.01	135.44	126.64
22	a	2445	2MG	C1'-N9-C4	4.92	135.29	126.64
22	a	746	PSU	C4-N3-C2	4.87	119.25	115.14
1	A	1516	2MG	N2-C2-N1	4.78	121.55	116.96
1	A	1516	2MG	C1'-N9-C4	4.77	135.03	126.64
22	a	2498	OMC	C2-N3-C4	4.66	121.07	116.34
22	a	2457	PSU	C4-N3-C2	4.56	118.99	115.14
22	a	2251	OMG	C2-N3-C4	4.54	120.55	115.36
22	a	2504	PSU	C5-C4-N3	-4.54	119.51	125.36
22	a	1835	2MG	C2-N3-C4	4.38	120.25	115.28
1	A	1207	2MG	C2-N3-C4	4.34	120.20	115.28
22	a	2580	PSU	C5-C4-N3	-4.31	119.81	125.36
22	a	746	PSU	C5-C1'-C2'	-4.30	107.65	115.32
22	a	955	PSU	C5-C4-N3	-4.24	119.90	125.36
22	a	745	1MG	C2-N3-C4	4.22	120.18	115.36
22	a	1917	PSU	C5-C4-N3	-4.22	119.93	125.36
22	a	2604	PSU	C5-C4-N3	-4.22	119.93	125.36
22	a	1618	6MZ	C9-N6-C6	-4.12	119.32	122.87
22	a	2069	G7M	C2-N3-C4	4.06	119.99	115.36
22	a	1911	PSU	C5-C4-N3	-4.03	120.16	125.36
1	A	966	2MG	C2-N3-C4	4.00	119.82	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	2457	PSU	C5-C4-N3	-3.96	120.26	125.36
1	A	1516	2MG	C2-N3-C4	3.89	119.70	115.28
22	a	1618	6MZ	C2-N1-C6	3.88	119.92	116.59
22	a	1962	5MC	C2-N3-C4	3.83	120.64	116.02
1	A	1207	2MG	N3-C2-N1	-3.81	120.20	126.23
1	A	516	PSU	C5-C4-N3	-3.77	120.51	125.36
1	A	966	2MG	N3-C2-N1	-3.73	120.34	126.23
22	a	2030	6MZ	C2-N1-C6	3.71	119.77	116.59
1	A	966	2MG	CM2-N2-C2	-3.69	119.14	123.59
22	a	1835	2MG	N3-C2-N1	-3.63	120.50	126.23
22	a	2445	2MG	C2-N3-C4	3.61	119.38	115.28
22	a	746	PSU	C5-C4-N3	-3.60	120.72	125.36
1	A	1516	2MG	N3-C2-N1	-3.54	120.63	126.23
22	a	2605	PSU	C5-C4-N3	-3.52	120.82	125.36
22	a	2445	2MG	N3-C2-N1	-3.51	120.68	126.23
22	a	746	PSU	O4'-C1'-C5	3.46	115.28	109.93
1	A	1207	2MG	CM2-N2-C2	-3.41	119.48	123.59
22	a	1915	3TD	C5-C6-N1	-3.39	120.27	124.44
1	A	1207	2MG	N2-C2-N1	3.39	120.21	116.96
1	A	967	5MC	C2-N3-C4	3.35	120.07	116.02
22	a	2504	PSU	C5-C1'-C2'	-3.33	109.38	115.32
22	a	745	1MG	N2-C2-N3	3.30	122.75	117.40
22	a	2605	PSU	C5-C6-N1	-3.28	120.41	124.44
22	a	2457	PSU	C5-C6-N1	-3.27	120.42	124.44
22	a	746	PSU	C5-C6-N1	-3.23	120.47	124.44
22	a	2503	2MA	N3-C2-N1	-3.22	119.80	125.72
1	A	1407	5MC	C2-N3-C4	3.21	119.89	116.02
22	a	2457	PSU	C6-N1-C2	3.15	120.55	115.36
1	A	966	2MG	N2-C2-N1	3.14	119.98	116.96
1	A	516	PSU	C6-N1-C2	3.12	120.50	115.36
22	a	746	PSU	C6-N1-C2	3.07	120.43	115.36
22	a	2604	PSU	C5-C6-N1	-3.06	120.67	124.44
22	a	2580	PSU	C5-C1'-C2'	3.03	120.72	115.32
22	a	747	5MU	C4-N3-C2	2.99	117.67	115.14
22	a	2605	PSU	C6-N1-C2	2.96	120.25	115.36
22	a	1917	PSU	C6-N1-C2	2.93	120.19	115.36
22	a	1911	PSU	C5-C6-N1	-2.93	120.84	124.44
22	a	2604	PSU	C6-N1-C2	2.93	120.19	115.36
22	a	1911	PSU	C6-N1-C2	2.90	120.14	115.36
22	a	2504	PSU	C6-N1-C2	2.89	120.12	115.36
1	A	966	2MG	N2-C2-N3	2.84	119.69	116.96
22	a	1962	5MC	N4-C4-N3	2.82	121.02	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	1915	3TD	C5-C1'-C2'	-2.79	110.35	115.32
1	A	1207	2MG	N2-C2-N3	2.74	119.59	116.96
22	a	2580	PSU	C6-N1-C2	2.71	119.83	115.36
22	a	2580	PSU	C5-C6-N1	-2.66	121.17	124.44
22	a	1939	5MU	C4-N3-C2	2.66	117.39	115.14
22	a	1915	3TD	C6-N1-C2	2.62	119.69	115.36
1	A	1516	2MG	C5-C6-N1	-2.59	119.89	123.43
1	A	966	2MG	C5-C6-N1	-2.58	119.91	123.43
22	a	955	PSU	C6-N1-C2	2.58	119.61	115.36
22	a	2069	G7M	C5-C6-N1	-2.56	119.93	123.43
22	a	2503	2MA	C5-C6-N1	-2.54	120.39	123.06
22	a	2069	G7M	C6-N1-C2	2.53	119.95	115.93
22	a	2445	2MG	C5-C6-N1	-2.46	120.07	123.43
1	A	966	2MG	C6-N1-C2	2.43	119.53	115.18
22	a	2504	PSU	C5-C6-N1	-2.43	121.45	124.44
1	A	1407	5MC	CM5-C5-C4	-2.36	119.33	121.72
1	A	1207	2MG	C5-C6-N1	-2.34	120.24	123.43
22	a	2580	PSU	O4'-C1'-C2'	2.33	108.44	104.66
22	a	1917	PSU	C5-C6-N1	-2.33	121.58	124.44
1	A	967	5MC	CM5-C5-C4	-2.32	119.38	121.72
1	A	967	5MC	N4-C4-N3	2.31	120.30	117.03
1	A	1207	2MG	C6-N1-C2	2.30	119.30	115.18
22	a	955	PSU	C5-C6-N1	-2.30	121.61	124.44
1	A	1407	5MC	N4-C4-N3	2.28	120.26	117.03
22	a	1835	2MG	C5-C6-N1	-2.25	120.35	123.43
1	A	1516	2MG	C6-N1-C2	2.24	119.20	115.18
22	a	2445	2MG	C6-N1-C2	2.24	119.18	115.18
1	A	1407	5MC	C5-C6-N1	-2.20	119.83	122.19
22	a	2604	PSU	O2'-C2'-C1'	-2.16	106.81	111.94
22	a	1835	2MG	C4-C5-N7	-2.09	107.22	109.40
1	A	967	5MC	C5-C6-N1	-2.08	119.95	122.19
22	a	2251	OMG	C6-N1-C2	2.06	119.20	115.93

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	d	150	MEQ	O-C-CA-CB
22	a	746	PSU	O4'-C1'-C5-C6
22	a	1962	5MC	O4'-C1'-N1-C6
22	a	1962	5MC	C2'-C1'-N1-C6
22	a	2251	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
22	a	2445	2MG	C3'-C4'-C5'-O5'
22	a	2498	OMC	O4'-C1'-N1-C6
1	A	1519	MA6	O4'-C4'-C5'-O5'
22	a	1915	3TD	O4'-C4'-C5'-O5'
22	a	2030	6MZ	O4'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
22	a	2069	G7M	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
22	a	2069	G7M	C3'-C4'-C5'-O5'
1	A	966	2MG	C3'-C4'-C5'-O5'
22	a	1915	3TD	C3'-C4'-C5'-O5'
1	A	966	2MG	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
22	a	2445	2MG	O4'-C4'-C5'-O5'
22	a	2498	OMC	O4'-C4'-C5'-O5'
25	d	150	MEQ	N-CA-CB-CG
25	d	150	MEQ	C-CA-CB-CG
22	a	746	PSU	C2'-C1'-C5-C6
22	a	746	PSU	O4'-C1'-C5-C4
1	A	516	PSU	C2'-C1'-C5-C6
25	d	150	MEQ	OE1-CD-CG-CB
22	a	2498	OMC	C3'-C4'-C5'-O5'
25	d	150	MEQ	NE2-CD-CG-CB
22	a	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 312 ligands modelled in this entry, 310 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	PAR	A	1601	-	45,45,45	3.33	9 (20%)	64,67,67	1.41	9 (14%)
58	TRP	a	6206	-	12,16,16	0.80	0	12,22,22	0.89	0

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
56	PAR	A	1601	-	-	10/18/94/94	0/4/4/4
58	TRP	a	6206	-	-	0/3/8/8	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	A	1601	PAR	C13-C23	-14.15	1.34	1.52
56	A	1601	PAR	O43-C13	12.32	1.63	1.41
56	A	1601	PAR	O43-C43	-6.04	1.31	1.45
56	A	1601	PAR	O51-C11	4.11	1.52	1.41
56	A	1601	PAR	C31-C21	-4.06	1.48	1.53
56	A	1601	PAR	O33-C33	-3.51	1.34	1.43
56	A	1601	PAR	O54-C14	3.48	1.50	1.41
56	A	1601	PAR	C34-C24	-3.30	1.49	1.53
56	A	1601	PAR	C33-C43	2.70	1.60	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	A	1601	PAR	C13-O52-C52	-4.31	107.31	117.96
56	A	1601	PAR	C14-O33-C33	-3.35	109.67	117.96
56	A	1601	PAR	C44-C34-C24	3.31	116.77	111.07
56	A	1601	PAR	C11-O51-C51	3.22	120.01	113.69
56	A	1601	PAR	C34-C44-C54	2.92	115.45	110.24
56	A	1601	PAR	O51-C51-C41	2.81	114.79	109.69
56	A	1601	PAR	O51-C11-C21	2.77	116.30	110.06
56	A	1601	PAR	C13-C23-C33	2.19	104.74	102.10
56	A	1601	PAR	C14-O54-C54	-2.04	109.69	113.69

There are no chirality outliers.

All (10) torsion outliers are listed below:

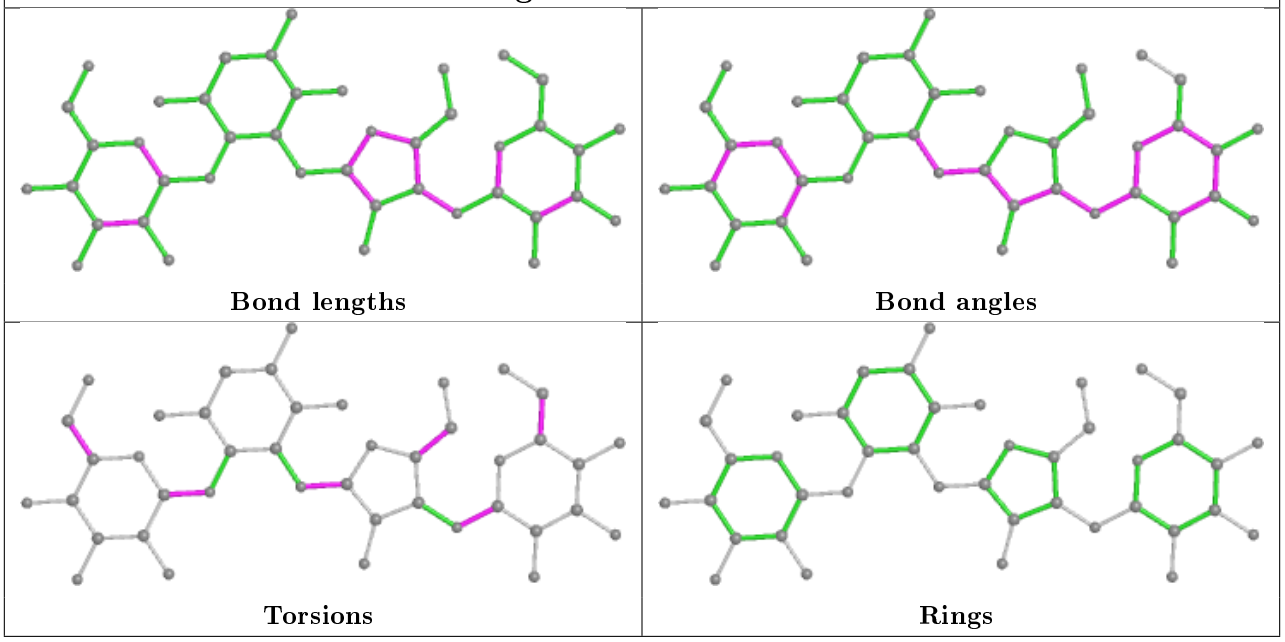
Mol	Chain	Res	Type	Atoms
56	A	1601	PAR	C23-C13-O52-C52
56	A	1601	PAR	C24-C14-O33-C33
56	A	1601	PAR	O51-C11-O11-C42
56	A	1601	PAR	O51-C51-C61-O61
56	A	1601	PAR	C33-C43-C53-O53
56	A	1601	PAR	C41-C51-C61-O61
56	A	1601	PAR	O43-C43-C53-O53
56	A	1601	PAR	O43-C13-O52-C52
56	A	1601	PAR	O54-C14-O33-C33
56	A	1601	PAR	C44-C54-C64-N64

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PAR A 1601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	a	3
1	A	2
55	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	2098:U	O3'	2191:A	P	17.56
1	A	840:C	O3'	846:G	P	17.24
1	a	1052:C	O3'	1107:G	P	17.19
1	A	204:G	O3'	214:C	P	17.13
1	a	1172:C	O3'	1177:G	P	16.62
1	V	16:C	O3'	18:G	P	6.84