



Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 06:34 pm GMT

PDB ID : 7NWT
EMDB ID : EMD-12635
Title : Initiated 70S ribosome in complex with 2A protein from encephalomyocarditis virus (EMCV)
Authors : Hill, C.H.; Naphine, S.; Pekarek, L.; Kibe, A.; Firth, A.E.; Graham, S.C.; Caliskan, N.; Brierley, I.
Deposited on : 2021-03-17
Resolution : 2.66 Å (reported)
Based on initial model : 5MDZ

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

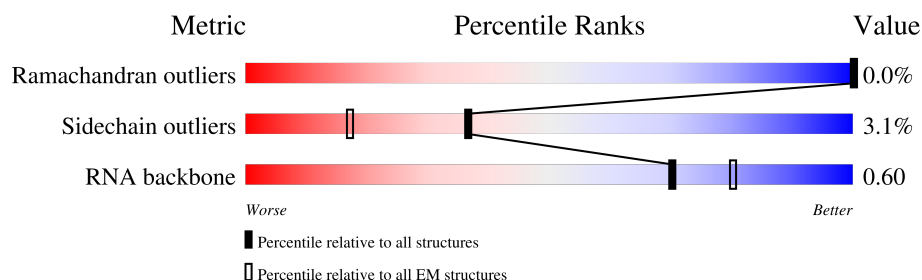
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.66 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.



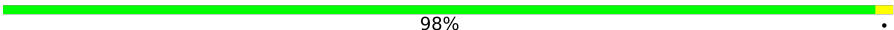
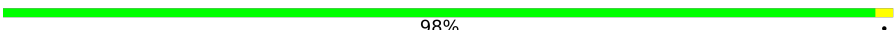
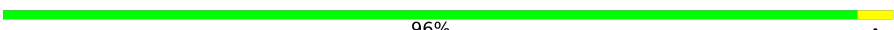

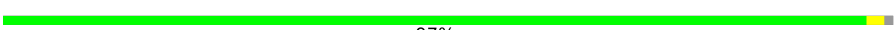





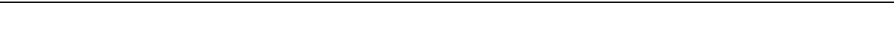

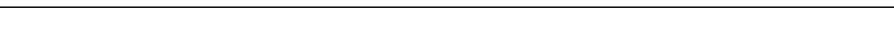
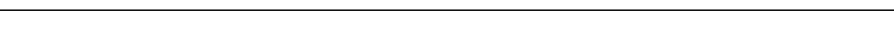
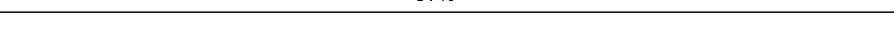
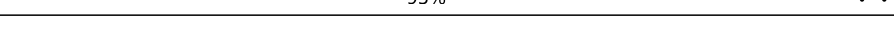
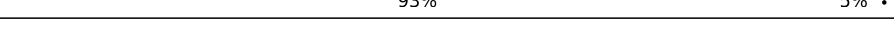





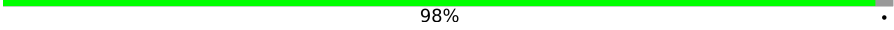
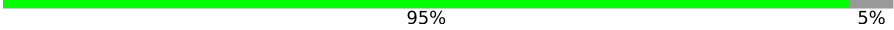

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	273	97% ..
2	C	209	98% .
3	D	201	98% .
4	E	179	94% 5% .
5	F	177	95% ..
6	G	149	95% 5%
7	H	165	74% 5% 21%
8	I	142	87% 8% 5%
9	J	142	99% .

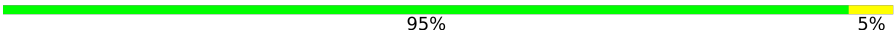


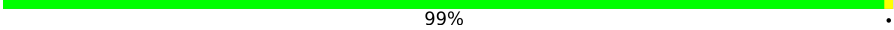



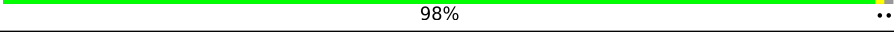
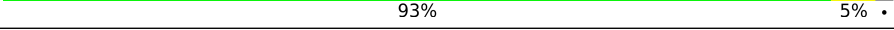


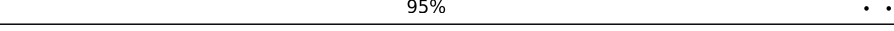
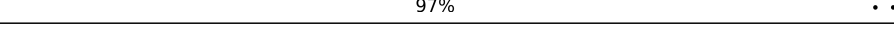
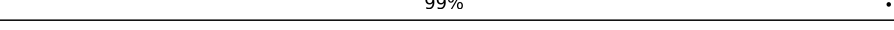
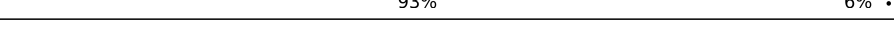
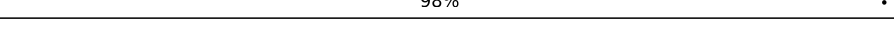
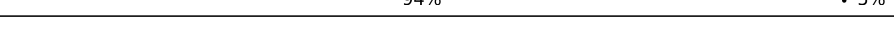


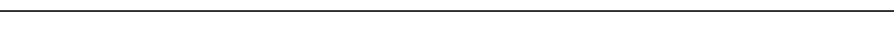

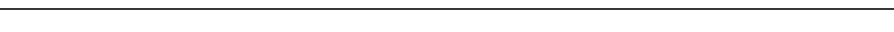
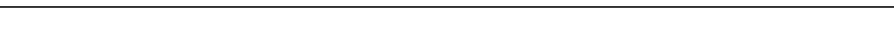


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Mol	Chain	Length	Quality of chain
10	K	123	 98% .
11	L	144	 98% .
12	M	136	 96% .
13	N	127	 92% . 6%
14	O	117	 97% ..
15	P	115	 97% ..
16	Q	118	 97% ..
17	R	103	 96% .
18	S	110	 95% 5%
19	T	100	 92% . 6%
20	U	104	 98% ..
21	V	94	 98% .
22	W	85	 89% 11%
23	X	78	 97% ..
24	Y	63	 95% ..
25	Z	59	 93% 5% .
26	1	2904	 82% 17% .
27	2	1534	 85% 14%
28	3	120	 90% 10%
29	5	77	 75% 19% ..
30	a	70	 90% . 6%
31	b	57	 98% .
32	c	55	 95% 5%
33	d	46	 100%
34	e	65	 95% ..

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Mol	Chain	Length	Quality of chain
35	f	38	 95% 5%
36	g	241	 92% 7%
37	h	233	 89% 11%
38	i	206	 99%
39	j	167	 91% 7%
40	k	135	 74% 23%
41	l	179	 83% 16%
42	m	130	 98% ..
43	n	130	 93% 5%
44	o	103	 91% 5%
45	p	129	 89% 9%
46	q	124	 95% ..
47	r	118	 97% ..
48	s	101	 99% .
49	t	89	 93% 6%
50	u	82	 98% .
51	v	84	 94% 5%
52	w	75	 87% 12%
53	x	92	 86% 10%
54	y	87	 99% .
55	z	71	 92% 7%
56	XX	117	 5% 93%
57	AA	152	 84% 16%
57	BB	152	 85% 14%
57	CC	152	 82% 18%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 149932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

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

- Molecule 8 is a protein called 50S ribosomal protein L11.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 27 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 29 is a RNA chain called fMet-NH-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	5	76	Total	C	N	O	P	S	0	0
			1622	725	292	528	76	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	8	4SU	G	conflict	GB 1317722521

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

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

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

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

- Molecule 33 is a protein called 50S ribosomal protein L34.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a protein called 30S ribosomal protein S2.

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

- Molecule 37 is a protein called 30S ribosomal protein S3.

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

- Molecule 38 is a protein called 30S ribosomal protein S4.

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

- Molecule 39 is a protein called 30S ribosomal protein S5.

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

- Molecule 40 is a protein called 30S ribosomal protein S6.

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

- Molecule 41 is a protein called 30S ribosomal protein S7.

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

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

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

- Molecule 45 is a protein called 30S ribosomal protein S11.

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

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

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

- Molecule 48 is a protein called 30S ribosomal protein S14.

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

- Molecule 49 is a protein called 30S ribosomal protein S15.

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

- Molecule 50 is a protein called 30S ribosomal protein S16.

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

- Molecule 51 is a protein called 30S ribosomal protein S17.

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

- Molecule 52 is a protein called 30S ribosomal protein S18.

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

- Molecule 53 is a protein called 30S ribosomal protein S19.

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

- Molecule 54 is a protein called 30S ribosomal protein S20.

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

- Molecule 55 is a protein called 30S ribosomal protein S21.

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

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	XX	8	Total	C	N	O	P	0	0
			176	78	34	56	8		

- Molecule 57 is a protein called Protein 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AA	127	Total	C	N	O	S	0	0
			1067	690	192	182	3		
57	BB	130	Total	C	N	O	S	2	0
			1111	716	204	188	3		
57	CC	125	Total	C	N	O	S	0	0
			1048	677	190	178	3		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	144	GLY	-	expression tag	UNP P12296
AA	145	SER	-	expression tag	UNP P12296
AA	146	LYS	-	expression tag	UNP P12296
AA	147	HIS	-	expression tag	UNP P12296
AA	148	HIS	-	expression tag	UNP P12296
AA	149	HIS	-	expression tag	UNP P12296
AA	150	HIS	-	expression tag	UNP P12296
AA	151	HIS	-	expression tag	UNP P12296
AA	152	HIS	-	expression tag	UNP P12296
BB	144	GLY	-	expression tag	UNP P12296
BB	145	SER	-	expression tag	UNP P12296
BB	146	LYS	-	expression tag	UNP P12296
BB	147	HIS	-	expression tag	UNP P12296
BB	148	HIS	-	expression tag	UNP P12296
BB	149	HIS	-	expression tag	UNP P12296
BB	150	HIS	-	expression tag	UNP P12296
BB	151	HIS	-	expression tag	UNP P12296
BB	152	HIS	-	expression tag	UNP P12296
CC	144	GLY	-	expression tag	UNP P12296
CC	145	SER	-	expression tag	UNP P12296
CC	146	LYS	-	expression tag	UNP P12296

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Chain	Residue	Modelled	Actual	Comment	Reference
CC	147	HIS	-	expression tag	UNP P12296
CC	148	HIS	-	expression tag	UNP P12296
CC	149	HIS	-	expression tag	UNP P12296
CC	150	HIS	-	expression tag	UNP P12296
CC	151	HIS	-	expression tag	UNP P12296
CC	152	HIS	-	expression tag	UNP P12296

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	B	1	Total 1	Mg 1	0
58	C	1	Total 1	Mg 1	0
58	M	1	Total 1	Mg 1	0
58	N	1	Total 1	Mg 1	0
58	Q	1	Total 1	Mg 1	0
58	1	290	Total 290	Mg 290	0
58	2	128	Total 128	Mg 128	0
58	3	8	Total 8	Mg 8	0
58	5	3	Total 3	Mg 3	0
58	b	1	Total 1	Mg 1	0
58	i	1	Total 1	Mg 1	0
58	BB	1	Total 1	Mg 1	0

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
59	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	B	2	Total	O	0
			2	2	

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: 50S ribosomal protein L2

Chain B:  97% ..



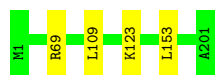
- Molecule 2: 50S ribosomal protein L3

Chain C:  98% .



- Molecule 3: 50S ribosomal protein L4

Chain D:  98% .



- Molecule 4: 50S ribosomal protein L5

Chain E:  94% 5% .



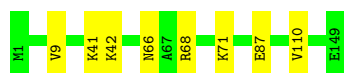
- Molecule 5: 50S ribosomal protein L6

Chain F:  95% ..



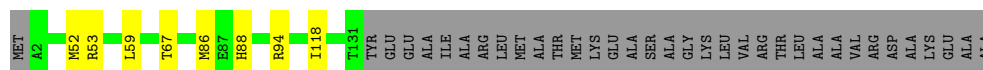
- Molecule 6: 50S ribosomal protein L9

Chain G:  95% 5%



- Molecule 7: 50S ribosomal protein L10

Chain H: 74% 5% 21%



- Molecule 8: 50S ribosomal protein L11

Chain I: 87% 8% 5%



- Molecule 9: 50S ribosomal protein L13

Chain J: 99%



- Molecule 10: 50S ribosomal protein L14

Chain K: 98%



- Molecule 11: 50S ribosomal protein L15

Chain L: 98%



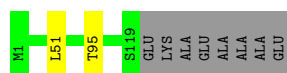
- Molecule 12: 50S ribosomal protein L16

Chain M: 96%



- Molecule 13: 50S ribosomal protein L17

Chain N: 92% 6%



- Molecule 14: 50S ribosomal protein L18

Chain O: 97% ..



- Molecule 15: 50S ribosomal protein L19

Chain P: 97% ..



- Molecule 16: 50S ribosomal protein L20

Chain Q: 97% ..



- Molecule 17: 50S ribosomal protein L21

Chain R: 96% .



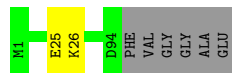
- Molecule 18: 50S ribosomal protein L22

Chain S: 95% 5%



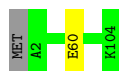
- Molecule 19: 50S ribosomal protein L23

Chain T: 92% . 6%



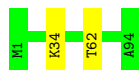
- Molecule 20: 50S ribosomal protein L24

Chain U: 98% ..



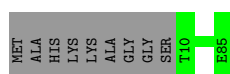
- Molecule 21: 50S ribosomal protein L25

Chain V: 98%



- Molecule 22: 50S ribosomal protein L27

Chain W: 89%



- Molecule 23: 50S ribosomal protein L28

Chain X: 97%



- Molecule 24: 50S ribosomal protein L29

Chain Y: 95%



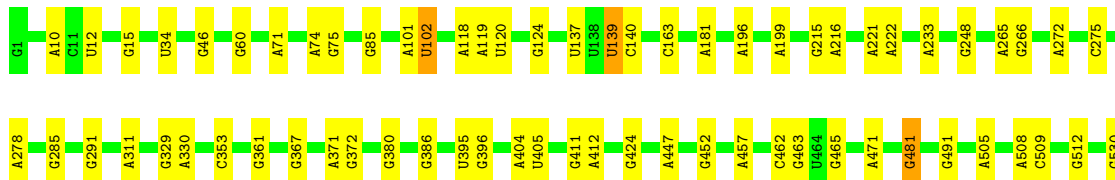
- Molecule 25: 50S ribosomal protein L30

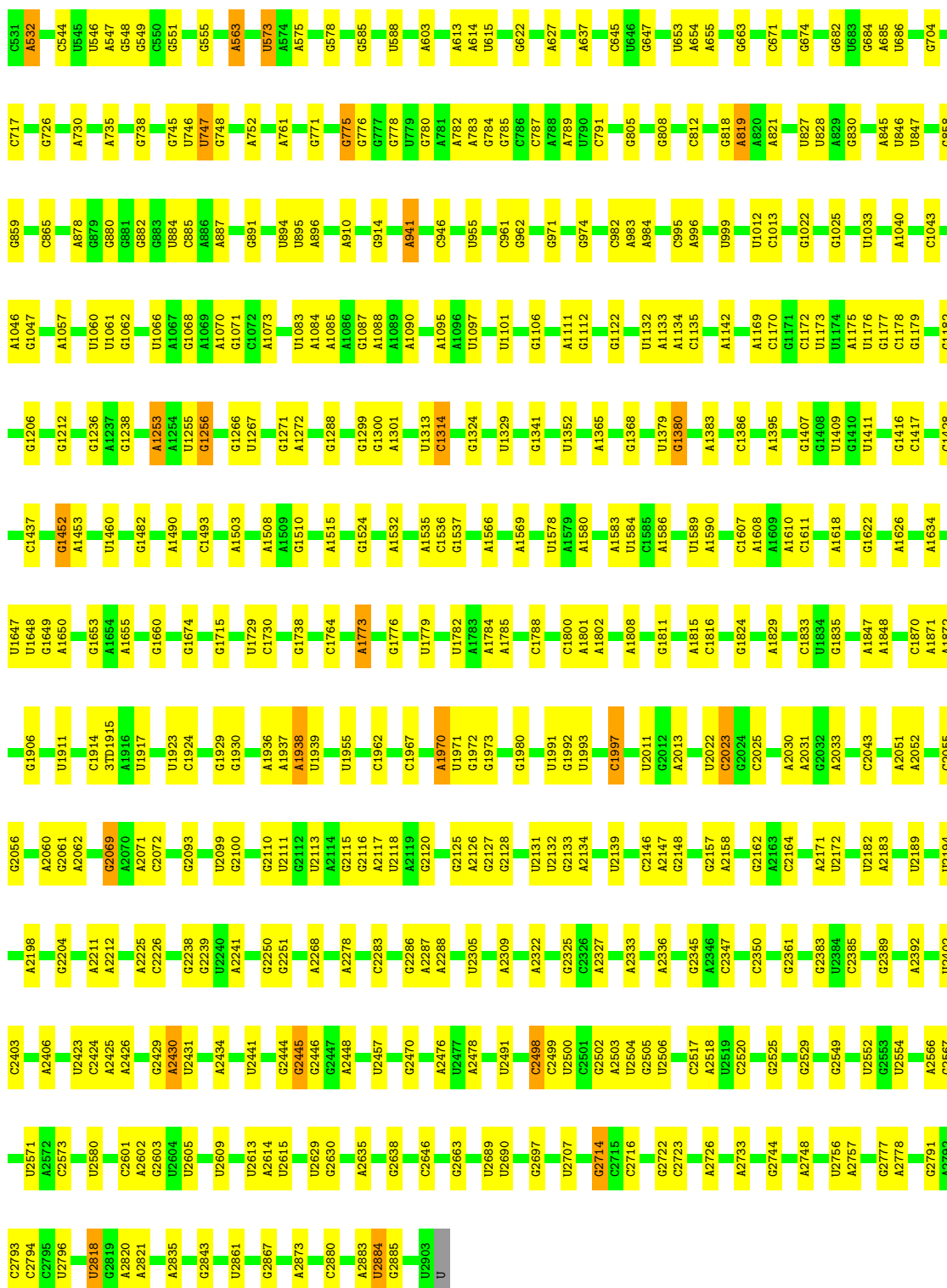
Chain Z: 93%



- Molecule 26: 23S ribosomal RNA

Chain 1: 82%

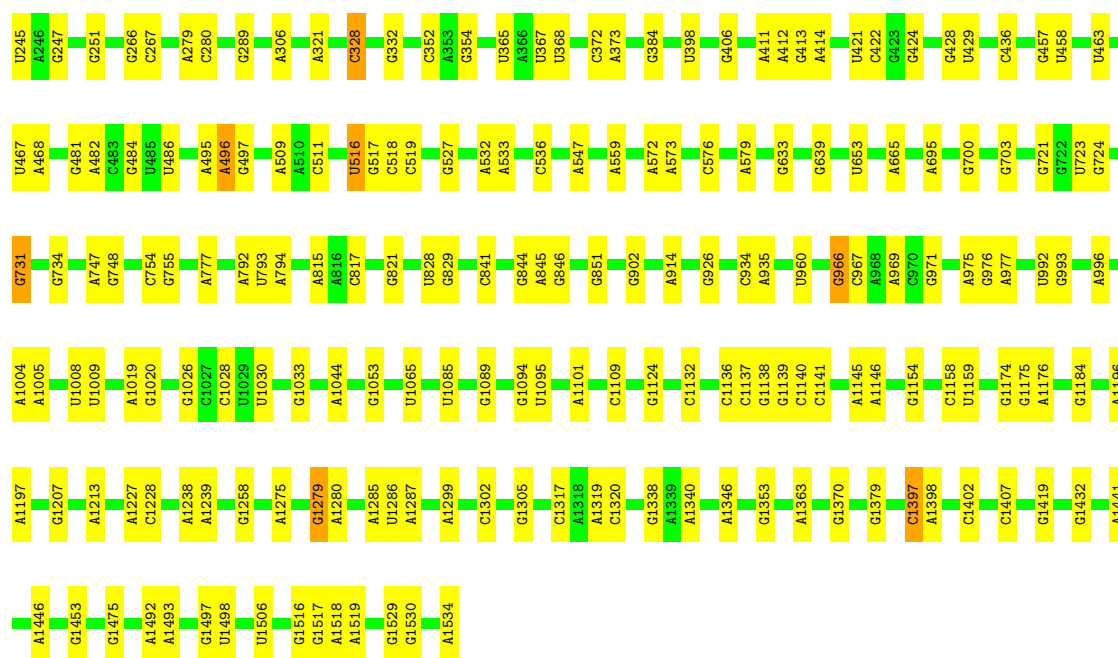




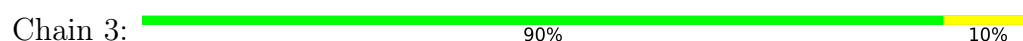
● Molecule 27: 16S ribosomal RNA

Chain 2: 85% 14%





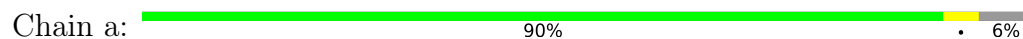
• Molecule 28: 5S ribosomal RNA



• Molecule 29: fMet-NH-tRNA(fMet)



• Molecule 30: 50S ribosomal protein L31



• Molecule 31: 50S ribosomal protein L32



• Molecule 32: 50S ribosomal protein L33

Chain c:  95% 5%



- Molecule 33: 50S ribosomal protein L34

Chain d:  100%

There are no outlier residues recorded for this chain.

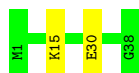
- Molecule 34: 50S ribosomal protein L35

Chain e:  95% . .



- Molecule 35: 50S ribosomal protein L36

Chain f:  95% 5%




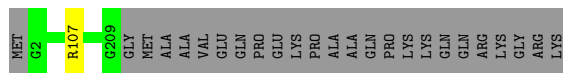
- Molecule 36: 30S ribosomal protein S2

Chain g:  92% . 7%



- Molecule 37: 30S ribosomal protein S3

Chain h:  89% 11%




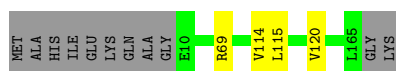
- Molecule 38: 30S ribosomal protein S4

Chain i:  99% .



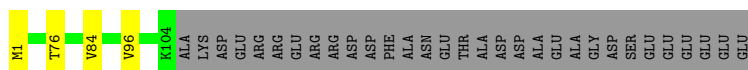
- Molecule 39: 30S ribosomal protein S5

Chain j:  91% . 7%



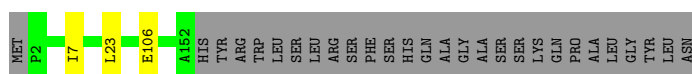
- Molecule 40: 30S ribosomal protein S6

Chain k: 74% 23%



- Molecule 41: 30S ribosomal protein S7

Chain l: 83% 16%



- Molecule 42: 30S ribosomal protein S8

Chain m: 98% ..



- Molecule 43: 30S ribosomal protein S9

Chain n: 93% 5% .



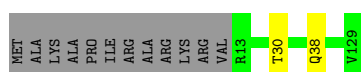
- Molecule 44: 30S ribosomal protein S10

Chain o: 91% 5% .



- Molecule 45: 30S ribosomal protein S11

Chain p: 89% . 9%



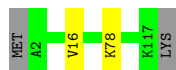
- Molecule 46: 30S ribosomal protein S12

Chain q: 95% ..



- Molecule 47: 30S ribosomal protein S13

Chain r: 97% ..



- Molecule 48: 30S ribosomal protein S14

Chain s: 99% .



- Molecule 49: 30S ribosomal protein S15

Chain t: 93% 6% .



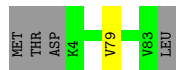
- Molecule 50: 30S ribosomal protein S16

Chain u: 98% .



- Molecule 51: 30S ribosomal protein S17

Chain v: 94% 5% .



- Molecule 52: 30S ribosomal protein S18

Chain w: 87% 12% .



- Molecule 53: 30S ribosomal protein S19

Chain x: 86% 10% .

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	120749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The contrast transfer function (CTF) was estimated per-image using CtfFind4. All further phase+amplitude correction was performed internally in Relion. Per-particle CTF refinement was done after polishing	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (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: 2MG, 4SU, 3TD, 5MC, 6MZ, PSU, ZN, MG, H2U, FME, 7MG, UR3, 1MG, MA6, 8AN, G7M, OMU, OMG, 2MA, OMC, 5MU, 0TD, 4OC

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	B	0.54	0/2121	0.68	0/2852
2	C	0.50	0/1586	0.59	0/2134
3	D	0.47	0/1571	0.56	0/2113
4	E	0.40	0/1434	0.53	0/1926
5	F	0.36	0/1333	0.52	0/1805
6	G	0.32	0/1122	0.52	0/1515
7	H	0.26	0/993	0.54	0/1340
8	I	0.25	0/998	0.48	0/1348
9	J	0.53	0/1152	0.55	0/1551
10	K	0.49	0/955	0.63	0/1279
11	L	0.44	0/1062	0.65	0/1413
12	M	0.49	0/1093	0.60	0/1460
13	N	0.51	0/964	0.65	0/1289
14	O	0.43	0/902	0.55	0/1209
15	P	0.52	0/929	0.59	0/1242
16	Q	0.58	0/960	0.61	0/1278
17	R	0.52	0/829	0.59	0/1107
18	S	0.49	0/864	0.62	0/1156
19	T	0.46	0/752	0.54	0/1005
20	U	0.45	0/796	0.57	0/1062
21	V	0.44	0/766	0.52	0/1025
22	W	0.51	0/589	0.62	0/779
23	X	0.48	0/635	0.62	0/848
24	Y	0.35	0/502	0.52	0/667
25	Z	0.43	0/452	0.62	0/605
26	1	1.33	41/69286 (0.1%)	1.00	84/108087 (0.1%)
27	2	1.14	0/36588	0.86	21/57066 (0.0%)
28	3	1.01	0/2872	0.80	0/4478
29	5	0.81	0/1672	0.81	0/2603
30	a	0.35	0/531	0.53	0/709
31	b	0.47	0/450	0.63	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.47	0/433	0.56	0/576
33	d	0.49	0/380	0.72	0/498
34	e	0.51	0/513	0.63	0/676
35	f	0.46	0/303	0.61	0/397
36	g	0.35	0/1791	0.48	0/2413
37	h	0.42	0/1663	0.55	0/2241
38	i	0.46	0/1665	0.55	0/2227
39	j	0.45	0/1165	0.59	0/1568
40	k	0.42	0/867	0.52	0/1171
41	l	0.36	0/1195	0.54	0/1602
42	m	0.47	0/989	0.55	0/1326
43	n	0.43	0/1034	0.59	0/1375
44	o	0.41	1/800 (0.1%)	0.61	0/1082
45	p	0.42	0/893	0.58	0/1205
46	q	0.50	0/960	0.64	0/1286
47	r	0.39	0/909	0.60	0/1215
48	s	0.41	0/817	0.56	0/1088
49	t	0.41	0/722	0.55	0/964
50	u	0.50	0/659	0.59	0/884
51	v	0.45	0/657	0.58	0/881
52	w	0.50	0/553	0.58	0/743
53	x	0.39	0/680	0.55	0/915
54	y	0.39	0/675	0.50	0/895
55	z	0.42	0/597	0.60	0/792
56	XX	1.11	0/197	0.77	0/306
57	AA	0.37	0/1102	0.58	0/1498
57	BB	0.42	0/1146	0.61	0/1555
57	CC	0.31	0/1082	0.56	0/1469
All	All	1.07	42/161206 (0.0%)	0.86	105/240398 (0.0%)

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
6	G	0	1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	585	G	C8-N7	-7.00	1.26	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	778	G	C8-N7	-6.48	1.27	1.30
26	1	578	G	C8-N7	-6.32	1.27	1.30
26	1	1973	G	C8-N7	-6.27	1.27	1.30
26	1	685	A	C8-N7	-6.24	1.27	1.31
26	1	684	G	C8-N7	-6.06	1.27	1.30
26	1	2722	G	C8-N7	-6.00	1.27	1.30
26	1	2051	A	N7-C5	-5.70	1.35	1.39
26	1	821	A	N7-C5	-5.65	1.35	1.39
26	1	780	G	C8-N7	-5.60	1.27	1.30
26	1	1784	A	C8-N7	-5.51	1.27	1.31
26	1	1773	A	N7-C5	-5.49	1.35	1.39
26	1	1824	G	C5-C4	-5.43	1.34	1.38
26	1	462	C	N3-C4	-5.41	1.30	1.33
26	1	735	A	C8-N7	-5.40	1.27	1.31
26	1	971	G	C8-N7	-5.35	1.27	1.30
26	1	2241	A	N7-C5	-5.35	1.36	1.39
26	1	124	G	C8-N7	-5.33	1.27	1.30
26	1	563	A	C8-N7	-5.30	1.27	1.31
26	1	2071	A	N7-C5	-5.20	1.36	1.39
26	1	465	G	C8-N7	-5.20	1.27	1.30
26	1	1256	G	C8-N7	-5.20	1.27	1.30
26	1	573	U	C2-N3	-5.20	1.34	1.37
26	1	2013	A	N9-C8	-5.19	1.33	1.37
26	1	2392	A	N7-C5	-5.17	1.36	1.39
26	1	452	G	C8-N7	-5.17	1.27	1.30
26	1	2430	A	N7-C5	-5.13	1.36	1.39
26	1	2052	A	C8-N7	-5.13	1.27	1.31
26	1	819	A	N7-C5	-5.10	1.36	1.39
26	1	2444	G	C8-N7	-5.08	1.27	1.30
26	1	808	G	C8-N7	-5.08	1.27	1.30
26	1	1299	G	C8-N7	-5.08	1.27	1.30
26	1	2392	A	C8-N7	-5.08	1.27	1.31
26	1	682	G	C8-N7	-5.08	1.27	1.30
26	1	982	C	N3-C4	-5.08	1.30	1.33
44	o	53	ILE	C-N	-5.06	1.22	1.34
26	1	463	G	C5-C4	-5.06	1.34	1.38
26	1	1776	G	C8-N7	-5.06	1.27	1.30
26	1	2571	U	C2-N3	-5.05	1.34	1.37
26	1	2714	G	C8-N7	-5.03	1.27	1.30
26	1	962	G	C5-C4	-5.02	1.34	1.38
26	1	1380	G	C8-N7	-5.01	1.27	1.30

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	512	G	O4'-C1'-N9	10.32	116.45	108.20
26	1	1779	U	N3-C2-O2	-9.18	115.77	122.20
27	2	1158	C	C2-N1-C1'	7.94	127.53	118.80
26	1	139	U	C2-N1-C1'	7.64	126.87	117.70
27	2	328	C	N1-C2-O2	7.64	123.48	118.90
27	2	328	C	C2-N1-C1'	7.57	127.13	118.80
26	1	1452	G	N3-C4-C5	7.37	132.28	128.60
27	2	1397	C	C2-N1-C1'	7.22	126.74	118.80
26	1	139	U	N1-C2-O2	7.13	127.79	122.80
26	1	2614	A	N1-C6-N6	-7.03	114.38	118.60
26	1	748	G	O4'-C1'-N9	6.93	113.74	108.20
26	1	2884	U	N3-C2-O2	-6.92	117.36	122.20
26	1	1611	C	C5-C4-N4	6.71	124.90	120.20
26	1	102	U	C2-N1-C1'	6.61	125.64	117.70
26	1	1452	G	N3-C4-N9	-6.59	122.05	126.00
26	1	1655	A	N1-C6-N6	-6.59	114.64	118.60
27	2	328	C	N3-C2-O2	-6.58	117.29	121.90
26	1	671	C	N1-C2-O2	6.49	122.79	118.90
26	1	671	C	N3-C2-O2	-6.38	117.43	121.90
27	2	1397	C	N1-C2-O2	6.36	122.72	118.90
26	1	2614	A	C5-C6-N6	6.29	128.73	123.70
26	1	1779	U	C4-C5-C6	6.27	123.46	119.70
26	1	1779	U	N1-C2-N3	6.27	118.66	114.90
26	1	1313	U	N1-C2-O2	6.24	127.17	122.80
26	1	1653	G	N1-C6-O6	-6.21	116.18	119.90
27	2	1158	C	N1-C2-O2	6.19	122.61	118.90
26	1	139	U	N3-C2-O2	-6.15	117.89	122.20
26	1	12	U	C2-N1-C1'	6.04	124.95	117.70
26	1	984	A	C8-N9-C4	-6.02	103.39	105.80
27	2	1279	G	N7-C8-N9	5.97	116.08	113.10
26	1	2025	C	C6-N1-C2	-5.96	117.92	120.30
27	2	368	U	C2-N1-C1'	5.95	124.84	117.70
27	2	792	A	O4'-C1'-N9	5.94	112.95	108.20
26	1	102	U	N1-C2-O2	5.93	126.95	122.80
26	1	984	A	O4'-C1'-N9	5.90	112.92	108.20
26	1	2446	G	N1-C6-O6	-5.90	116.36	119.90
26	1	2499	C	C6-N1-C2	-5.88	117.95	120.30
26	1	2052	A	N9-C4-C5	-5.88	103.45	105.80
26	1	2023	C	N1-C2-O2	5.88	122.43	118.90
26	1	1313	U	C2-N1-C1'	5.87	124.74	117.70
26	1	1788	C	C6-N1-C2	-5.84	117.96	120.30
26	1	1785	A	N1-C6-N6	-5.84	115.10	118.60
27	2	754	C	C2-N1-C1'	5.82	125.20	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	1288	G	C8-N9-C4	-5.81	104.08	106.40
26	1	775	G	O4'-C1'-N9	5.80	112.84	108.20
26	1	2517	C	C6-N1-C2	-5.80	117.98	120.30
26	1	674	G	N1-C6-O6	-5.77	116.44	119.90
26	1	2697	G	N1-C6-O6	-5.76	116.44	119.90
26	1	532	A	N1-C6-N6	-5.76	115.15	118.60
26	1	748	G	N3-C4-N9	-5.74	122.56	126.00
26	1	783	A	C8-N9-C4	-5.74	103.50	105.80
26	1	1314	C	C6-N1-C2	-5.72	118.01	120.30
26	1	1980	G	N3-C4-C5	-5.70	125.75	128.60
26	1	1650	A	N1-C6-N6	-5.68	115.19	118.60
27	2	1158	C	C6-N1-C1'	-5.68	113.99	120.80
26	1	1815	A	N1-C6-N6	-5.65	115.21	118.60
26	1	818	G	N1-C6-O6	-5.63	116.52	119.90
26	1	1313	U	N3-C2-O2	-5.63	118.26	122.20
27	2	328	C	C6-N1-C1'	-5.63	114.05	120.80
26	1	1395	A	O4'-C1'-N9	5.58	112.66	108.20
26	1	12	U	N3-C2-O2	-5.56	118.31	122.20
26	1	787	C	N3-C4-N4	-5.55	114.11	118.00
26	1	1255	U	N3-C4-O4	-5.54	115.52	119.40
26	1	941	A	O5'-P-OP1	-5.52	100.73	105.70
27	2	1397	C	C6-N1-C1'	-5.49	114.21	120.80
26	1	1622	G	N3-C4-N9	5.47	129.28	126.00
26	1	585	G	N9-C4-C5	-5.46	103.22	105.40
27	2	496	A	C8-N9-C4	-5.44	103.62	105.80
26	1	771	G	N1-C6-O6	-5.44	116.64	119.90
26	1	780	G	N9-C4-C5	-5.39	103.25	105.40
26	1	704	G	O4'-C1'-N9	5.37	112.49	108.20
26	1	1324	G	O4'-C1'-N9	5.37	112.49	108.20
26	1	1970	A	C8-N9-C4	-5.35	103.66	105.80
26	1	761	A	N1-C6-N6	-5.33	115.40	118.60
26	1	1938	A	C8-N9-C4	-5.33	103.67	105.80
26	1	1937	A	O4'-C1'-N9	5.32	112.46	108.20
26	1	2072	C	C6-N1-C2	-5.32	118.17	120.30
26	1	1776	G	N9-C4-C5	-5.30	103.28	105.40
26	1	2723	C	C6-N1-C2	-5.29	118.19	120.30
27	2	108	G	C4-C5-N7	5.28	112.91	110.80
26	1	1025	G	C8-N9-C4	-5.26	104.30	106.40
26	1	752	A	C5-N7-C8	-5.25	101.27	103.90
26	1	685	A	N9-C4-C5	-5.20	103.72	105.80
26	1	671	C	C5-C4-N4	5.20	123.84	120.20
26	1	2500	U	O4'-C1'-N1	5.20	112.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	395	U	O4'-C1'-N1	5.18	112.35	108.20
26	1	555	G	N3-C4-N9	5.18	129.11	126.00
26	1	1267	U	O5'-P-OP2	-5.17	101.05	105.70
26	1	1660	G	C5-C6-O6	5.17	131.70	128.60
26	1	1992	G	N1-C6-O6	-5.12	116.83	119.90
26	1	481	G	O4'-C1'-N9	5.12	112.30	108.20
26	1	2011	U	N3-C4-O4	-5.12	115.82	119.40
26	1	787	C	N1-C2-O2	5.10	121.96	118.90
26	1	2818	U	N3-C2-O2	-5.10	118.63	122.20
26	1	1253	A	O4'-C1'-N9	-5.10	104.12	108.20
27	2	1279	G	C8-N9-C4	-5.10	104.36	106.40
27	2	365	U	O4'-C1'-N1	5.08	112.27	108.20
27	2	368	U	N3-C2-O2	-5.08	118.64	122.20
26	1	663	G	N1-C6-O6	-5.07	116.86	119.90
26	1	748	G	C8-N9-C1'	5.06	133.57	127.00
26	1	1997	C	N3-C2-O2	-5.02	118.39	121.90
26	1	139	U	C6-N1-C1'	-5.01	114.18	121.20
27	2	1279	G	C5-N7-C8	-5.01	101.79	104.30
26	1	1611	C	N3-C4-N4	-5.01	114.49	118.00
27	2	731	G	O5'-P-OP2	-5.01	101.19	105.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	G	71	LYS	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	
1	B	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
2	C	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
3	D	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
4	E	175/179 (98%)	173 (99%)	2 (1%)	0	100	100
5	F	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
6	G	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
7	H	128/165 (78%)	108 (84%)	20 (16%)	0	100	100
8	I	133/142 (94%)	121 (91%)	12 (9%)	0	100	100
9	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
10	K	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
11	L	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
12	M	134/136 (98%)	134 (100%)	0	0	100	100
13	N	117/127 (92%)	114 (97%)	3 (3%)	0	100	100
14	O	114/117 (97%)	114 (100%)	0	0	100	100
15	P	112/115 (97%)	112 (100%)	0	0	100	100
16	Q	115/118 (98%)	115 (100%)	0	0	100	100
17	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
18	S	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
19	T	92/100 (92%)	91 (99%)	1 (1%)	0	100	100
20	U	101/104 (97%)	97 (96%)	4 (4%)	0	100	100
21	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
22	W	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
23	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
24	Y	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
25	Z	56/59 (95%)	56 (100%)	0	0	100	100
30	a	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
31	b	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
32	c	50/55 (91%)	50 (100%)	0	0	100	100
33	d	44/46 (96%)	44 (100%)	0	0	100	100
34	e	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
35	f	36/38 (95%)	36 (100%)	0	0	100	100
36	g	223/241 (92%)	218 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	h	206/233 (88%)	201 (98%)	5 (2%)	0	100	100
38	i	203/206 (98%)	203 (100%)	0	0	100	100
39	j	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
40	k	102/135 (76%)	102 (100%)	0	0	100	100
41	l	149/179 (83%)	146 (98%)	3 (2%)	0	100	100
42	m	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
43	n	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
44	o	97/103 (94%)	88 (91%)	9 (9%)	0	100	100
45	p	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
46	q	120/124 (97%)	117 (98%)	3 (2%)	0	100	100
47	r	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
48	s	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
49	t	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
50	u	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
51	v	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
52	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
53	x	81/92 (88%)	81 (100%)	0	0	100	100
54	y	84/87 (97%)	84 (100%)	0	0	100	100
55	z	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
57	AA	125/152 (82%)	119 (95%)	6 (5%)	0	100	100
57	BB	130/152 (86%)	125 (96%)	5 (4%)	0	100	100
57	CC	123/152 (81%)	119 (97%)	3 (2%)	1 (1%)	16	28
All	All	6247/6676 (94%)	6085 (97%)	161 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	CC	71	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	216/218 (99%)	209 (97%)	7 (3%)	34	54
2	C	164/164 (100%)	159 (97%)	5 (3%)	36	56
3	D	165/165 (100%)	161 (98%)	4 (2%)	44	65
4	E	148/150 (99%)	139 (94%)	9 (6%)	15	27
5	F	136/138 (99%)	130 (96%)	6 (4%)	24	40
6	G	114/114 (100%)	107 (94%)	7 (6%)	15	27
7	H	99/123 (80%)	91 (92%)	8 (8%)	9	16
8	I	104/110 (94%)	93 (89%)	11 (11%)	5	9
9	J	116/116 (100%)	114 (98%)	2 (2%)	56	75
10	K	104/104 (100%)	101 (97%)	3 (3%)	37	58
11	L	103/103 (100%)	100 (97%)	3 (3%)	37	58
12	M	109/109 (100%)	104 (95%)	5 (5%)	23	38
13	N	99/103 (96%)	97 (98%)	2 (2%)	50	71
14	O	86/87 (99%)	84 (98%)	2 (2%)	45	67
15	P	99/100 (99%)	97 (98%)	2 (2%)	50	71
16	Q	89/90 (99%)	86 (97%)	3 (3%)	32	51
17	R	84/84 (100%)	80 (95%)	4 (5%)	21	36
18	S	93/93 (100%)	88 (95%)	5 (5%)	18	32
19	T	81/84 (96%)	79 (98%)	2 (2%)	42	64
20	U	84/85 (99%)	83 (99%)	1 (1%)	67	82
21	V	78/78 (100%)	76 (97%)	2 (3%)	41	63
22	W	58/63 (92%)	58 (100%)	0	100	100
23	X	67/68 (98%)	66 (98%)	1 (2%)	60	77
24	Y	54/55 (98%)	52 (96%)	2 (4%)	29	48
25	Z	48/49 (98%)	45 (94%)	3 (6%)	15	25
30	a	59/62 (95%)	56 (95%)	3 (5%)	20	34
31	b	47/48 (98%)	47 (100%)	0	100	100
32	c	47/49 (96%)	47 (100%)	0	100	100
33	d	38/38 (100%)	38 (100%)	0	100	100
34	e	51/52 (98%)	49 (96%)	2 (4%)	27	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	f	34/34 (100%)	32 (94%)	2 (6%)	16	28
36	g	187/199 (94%)	183 (98%)	4 (2%)	48	70
37	h	171/190 (90%)	170 (99%)	1 (1%)	84	92
38	i	172/173 (99%)	170 (99%)	2 (1%)	67	82
39	j	119/126 (94%)	115 (97%)	4 (3%)	32	51
40	k	91/116 (78%)	87 (96%)	4 (4%)	24	40
41	l	124/147 (84%)	121 (98%)	3 (2%)	44	65
42	m	104/105 (99%)	103 (99%)	1 (1%)	73	85
43	n	105/107 (98%)	99 (94%)	6 (6%)	17	29
44	o	86/90 (96%)	82 (95%)	4 (5%)	22	37
45	p	90/99 (91%)	88 (98%)	2 (2%)	47	68
46	q	102/103 (99%)	98 (96%)	4 (4%)	27	45
47	r	94/96 (98%)	92 (98%)	2 (2%)	48	70
48	s	83/84 (99%)	83 (100%)	0	100	100
49	t	76/77 (99%)	71 (93%)	5 (7%)	14	23
50	u	65/65 (100%)	63 (97%)	2 (3%)	35	55
51	v	74/78 (95%)	73 (99%)	1 (1%)	62	79
52	w	57/65 (88%)	56 (98%)	1 (2%)	54	73
53	x	72/79 (91%)	68 (94%)	4 (6%)	17	30
54	y	65/66 (98%)	65 (100%)	0	100	100
55	z	60/61 (98%)	55 (92%)	5 (8%)	9	15
57	AA	115/138 (83%)	115 (100%)	0	100	100
57	BB	120/138 (87%)	119 (99%)	1 (1%)	79	89
57	CC	113/138 (82%)	113 (100%)	0	100	100
All	All	5219/5476 (95%)	5057 (97%)	162 (3%)	37	55

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	VAL
1	B	35	GLU
1	B	38	SER
1	B	139	SER
1	B	156	ARG

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Mol	Chain	Res	Type
1	B	180	GLU
1	B	202	LEU
2	C	59	ARG
2	C	104	VAL
2	C	105	LYS
2	C	151	THR
2	C	170	VAL
3	D	69	ARG
3	D	109	LEU
3	D	123	LYS
3	D	153	LEU
4	E	5	HIS
4	E	17	MET
4	E	28	VAL
4	E	105	THR
4	E	132	VAL
4	E	140	GLU
4	E	152	LEU
4	E	174	ASP
4	E	176	PRO
5	F	11	VAL
5	F	20	ASN
5	F	42	GLU
5	F	49	THR
5	F	99	LYS
5	F	127	THR
6	G	9	VAL
6	G	41	LYS
6	G	42	LYS
6	G	66	ASN
6	G	68	ARG
6	G	87	GLU
6	G	110	VAL
7	H	52	MET
7	H	53	ARG
7	H	59	LEU
7	H	67	THR
7	H	86	MET
7	H	88	HIS
7	H	94	ARG
7	H	118	ILE
8	I	9	LYS

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Mol	Chain	Res	Type
8	I	10	LEU
8	I	16	MET
8	I	44	LYS
8	I	49	GLU
8	I	61	TYR
8	I	63	ASP
8	I	102	ARG
8	I	117	THR
8	I	124	MET
8	I	135	MET
9	J	30	THR
9	J	81	ILE
10	K	1	MET
10	K	58	LEU
10	K	76	VAL
11	L	60	ARG
11	L	86	GLU
11	L	115	GLU
12	M	70	ASP
12	M	75	GLU
12	M	88	ASN
12	M	112	LEU
12	M	118	LYS
13	N	51	LEU
13	N	95	THR
14	O	25	ARG
14	O	94	ARG
15	P	40	LEU
15	P	81	VAL
16	Q	51	ARG
16	Q	89	GLU
16	Q	92	ARG
17	R	10	LYS
17	R	51	VAL
17	R	58	VAL
17	R	86	GLN
18	S	7	HIS
18	S	19	LEU
18	S	97	LEU
18	S	107	VAL
18	S	109	ASP
19	T	25	GLU

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Mol	Chain	Res	Type
19	T	26	LYS
20	U	60	GLU
21	V	34	LYS
21	V	62	THR
23	X	11	ARG
24	Y	8	GLU
24	Y	24	GLU
25	Z	32	ILE
25	Z	36	VAL
25	Z	37	GLU
30	a	59	ARG
30	a	62	LYS
30	a	64	PHE
34	e	31	HIS
34	e	33	LEU
35	f	15	LYS
35	f	30	GLU
36	g	7	ARG
36	g	23	TRP
36	g	50	PHE
36	g	56	GLU
37	h	107	ARG
38	i	30	THR
38	i	143	VAL
39	j	69	ARG
39	j	114	VAL
39	j	115	LEU
39	j	120	VAL
40	k	1	MET
40	k	76	THR
40	k	84	VAL
40	k	96	VAL
41	l	7	ILE
41	l	23	LEU
41	l	106	GLU
42	m	51	VAL
43	n	18	ARG
43	n	25	ASN
43	n	43	THR
43	n	58	VAL
43	n	116	VAL
43	n	123	ARG

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Mol	Chain	Res	Type
44	o	17	LEU
44	o	20	GLN
44	o	31	ARG
44	o	74	VAL
45	p	30	THR
45	p	38	GLN
46	q	4	VAL
46	q	52	VAL
46	q	74	LEU
46	q	110	ARG
47	r	16	VAL
47	r	78	LYS
49	t	17	ARG
49	t	18	ASP
49	t	22	THR
49	t	39	LEU
49	t	67	LEU
50	u	2	VAL
50	u	3	THR
51	v	79	VAL
52	w	74	HIS
53	x	20	GLU
53	x	28	LYS
53	x	56	GLN
53	x	81	ARG
55	z	7	ARG
55	z	16	LEU
55	z	17	ARG
55	z	58	LYS
55	z	66	ARG
57	BB	73	LYS

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

Mol	Chain	Res	Type
24	Y	39	GLN
36	g	39	HIS
44	o	20	GLN
57	AA	105	GLN
57	CC	105	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	1	2898/2904 (99%)	411 (14%)	7 (0%)
27	2	1527/1534 (99%)	209 (13%)	4 (0%)
28	3	119/120 (99%)	12 (10%)	0
29	5	73/77 (94%)	14 (19%)	2 (2%)
56	XX	7/117 (5%)	2 (28%)	0
All	All	4624/4752 (97%)	648 (14%)	13 (0%)

All (648) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	1	10	A
26	1	15	G
26	1	34	U
26	1	46	G
26	1	60	G
26	1	71	A
26	1	74	A
26	1	75	G
26	1	85	G
26	1	101	A
26	1	102	U
26	1	118	A
26	1	119	A
26	1	120	U
26	1	137	U
26	1	139	U
26	1	140	C
26	1	163	C
26	1	181	A
26	1	196	A
26	1	199	A
26	1	215	G
26	1	216	A
26	1	221	A
26	1	222	A
26	1	233	A
26	1	248	G
26	1	265	A
26	1	266	G
26	1	272	A
26	1	275	C

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Mol	Chain	Res	Type
26	1	278	A
26	1	285	G
26	1	291	G
26	1	311	A
26	1	329	G
26	1	330	A
26	1	353	C
26	1	361	G
26	1	367	G
26	1	371	A
26	1	372	G
26	1	380	G
26	1	386	G
26	1	396	G
26	1	405	U
26	1	411	G
26	1	412	A
26	1	424	G
26	1	447	A
26	1	457	A
26	1	471	A
26	1	481	G
26	1	491	G
26	1	505	A
26	1	508	A
26	1	509	C
26	1	530	G
26	1	532	A
26	1	544	C
26	1	546	U
26	1	547	A
26	1	548	G
26	1	549	G
26	1	551	G
26	1	563	A
26	1	573	U
26	1	575	A
26	1	588	U
26	1	603	A
26	1	613	A
26	1	614	A
26	1	615	U

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Mol	Chain	Res	Type
26	1	622	G
26	1	627	A
26	1	637	A
26	1	645	C
26	1	647	G
26	1	653	U
26	1	654	A
26	1	655	A
26	1	686	U
26	1	717	C
26	1	726	G
26	1	730	A
26	1	738	G
26	1	747	5MU
26	1	775	G
26	1	776	G
26	1	782	A
26	1	784	G
26	1	785	G
26	1	789	A
26	1	791	C
26	1	805	G
26	1	812	C
26	1	819	A
26	1	827	U
26	1	828	U
26	1	830	G
26	1	845	A
26	1	846	U
26	1	847	U
26	1	858	G
26	1	859	G
26	1	865	C
26	1	878	A
26	1	880	G
26	1	882	G
26	1	884	U
26	1	885	C
26	1	887	A
26	1	891	G
26	1	895	U
26	1	896	A

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Mol	Chain	Res	Type
26	1	910	A
26	1	914	G
26	1	941	A
26	1	946	C
26	1	961	C
26	1	974	G
26	1	983	A
26	1	995	C
26	1	996	A
26	1	999	U
26	1	1012	U
26	1	1013	C
26	1	1022	G
26	1	1033	U
26	1	1040	A
26	1	1043	C
26	1	1046	A
26	1	1047	G
26	1	1057	A
26	1	1060	U
26	1	1061	U
26	1	1062	G
26	1	1066	U
26	1	1068	G
26	1	1070	A
26	1	1071	G
26	1	1073	A
26	1	1083	U
26	1	1084	A
26	1	1085	A
26	1	1087	G
26	1	1088	A
26	1	1090	A
26	1	1095	A
26	1	1097	U
26	1	1101	U
26	1	1106	G
26	1	1111	A
26	1	1112	G
26	1	1122	G
26	1	1132	U
26	1	1133	A

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Mol	Chain	Res	Type
26	1	1134	A
26	1	1135	C
26	1	1142	A
26	1	1169	A
26	1	1170	C
26	1	1172	C
26	1	1173	U
26	1	1175	A
26	1	1176	U
26	1	1177	G
26	1	1178	C
26	1	1179	G
26	1	1182	G
26	1	1206	G
26	1	1212	G
26	1	1236	G
26	1	1238	G
26	1	1253	A
26	1	1256	G
26	1	1266	G
26	1	1271	G
26	1	1272	A
26	1	1300	G
26	1	1301	A
26	1	1314	C
26	1	1329	U
26	1	1341	G
26	1	1352	U
26	1	1365	A
26	1	1368	G
26	1	1379	U
26	1	1380	G
26	1	1383	A
26	1	1386	C
26	1	1407	G
26	1	1409	U
26	1	1411	U
26	1	1416	G
26	1	1417	C
26	1	1428	C
26	1	1437	C
26	1	1452	G

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Mol	Chain	Res	Type
26	1	1453	A
26	1	1460	U
26	1	1482	G
26	1	1490	A
26	1	1493	C
26	1	1503	A
26	1	1508	A
26	1	1510	G
26	1	1515	A
26	1	1524	G
26	1	1532	A
26	1	1535	A
26	1	1536	C
26	1	1537	G
26	1	1566	A
26	1	1569	A
26	1	1578	U
26	1	1580	A
26	1	1583	A
26	1	1584	U
26	1	1586	A
26	1	1589	U
26	1	1590	A
26	1	1607	C
26	1	1608	A
26	1	1610	A
26	1	1626	A
26	1	1634	A
26	1	1647	U
26	1	1648	U
26	1	1649	G
26	1	1674	G
26	1	1715	G
26	1	1729	U
26	1	1730	C
26	1	1738	G
26	1	1764	C
26	1	1773	A
26	1	1782	U
26	1	1800	C
26	1	1801	A
26	1	1802	A

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Mol	Chain	Res	Type
26	1	1808	A
26	1	1811	G
26	1	1816	C
26	1	1829	A
26	1	1833	C
26	1	1847	A
26	1	1848	A
26	1	1870	C
26	1	1871	A
26	1	1872	A
26	1	1906	G
26	1	1914	C
26	1	1923	U
26	1	1924	C
26	1	1929	G
26	1	1930	G
26	1	1936	A
26	1	1938	A
26	1	1955	U
26	1	1967	C
26	1	1970	A
26	1	1971	U
26	1	1972	G
26	1	1991	U
26	1	1993	U
26	1	1997	C
26	1	2022	U
26	1	2023	C
26	1	2031	A
26	1	2033	A
26	1	2043	C
26	1	2055	C
26	1	2056	G
26	1	2060	A
26	1	2061	G
26	1	2062	A
26	1	2069	G7M
26	1	2093	G
26	1	2099	U
26	1	2100	G
26	1	2110	G
26	1	2111	U

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Mol	Chain	Res	Type
26	1	2113	U
26	1	2115	G
26	1	2116	G
26	1	2117	A
26	1	2118	U
26	1	2120	G
26	1	2125	G
26	1	2126	A
26	1	2127	G
26	1	2128	G
26	1	2131	U
26	1	2132	U
26	1	2133	G
26	1	2134	A
26	1	2139	U
26	1	2146	C
26	1	2147	A
26	1	2148	G
26	1	2157	G
26	1	2158	A
26	1	2162	G
26	1	2164	C
26	1	2171	A
26	1	2172	U
26	1	2182	U
26	1	2183	A
26	1	2189	U
26	1	2194	U
26	1	2198	A
26	1	2204	G
26	1	2211	A
26	1	2212	A
26	1	2225	A
26	1	2226	C
26	1	2238	G
26	1	2239	G
26	1	2250	G
26	1	2268	A
26	1	2278	A
26	1	2283	C
26	1	2286	G
26	1	2287	A

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Mol	Chain	Res	Type
26	1	2288	A
26	1	2305	U
26	1	2309	A
26	1	2322	A
26	1	2325	G
26	1	2327	A
26	1	2333	A
26	1	2336	A
26	1	2345	G
26	1	2347	C
26	1	2350	C
26	1	2361	G
26	1	2383	G
26	1	2385	C
26	1	2389	G
26	1	2402	U
26	1	2403	C
26	1	2406	A
26	1	2423	U
26	1	2424	C
26	1	2425	A
26	1	2426	A
26	1	2429	G
26	1	2430	A
26	1	2431	U
26	1	2434	A
26	1	2441	U
26	1	2445	2MG
26	1	2448	A
26	1	2470	G
26	1	2476	A
26	1	2478	A
26	1	2491	U
26	1	2498	OMC
26	1	2502	G
26	1	2505	G
26	1	2506	U
26	1	2518	A
26	1	2520	C
26	1	2525	G
26	1	2529	G
26	1	2549	G

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Mol	Chain	Res	Type
26	1	2554	U
26	1	2566	A
26	1	2567	G
26	1	2573	C
26	1	2601	C
26	1	2602	A
26	1	2603	G
26	1	2609	U
26	1	2613	U
26	1	2615	U
26	1	2629	U
26	1	2630	G
26	1	2635	A
26	1	2638	G
26	1	2646	C
26	1	2663	G
26	1	2689	U
26	1	2690	U
26	1	2707	U
26	1	2714	G
26	1	2716	C
26	1	2726	A
26	1	2733	A
26	1	2744	G
26	1	2748	A
26	1	2757	A
26	1	2777	G
26	1	2778	A
26	1	2791	G
26	1	2793	C
26	1	2794	C
26	1	2796	U
26	1	2818	U
26	1	2820	A
26	1	2821	A
26	1	2835	A
26	1	2843	G
26	1	2861	U
26	1	2867	G
26	1	2873	A
26	1	2880	C
26	1	2883	A

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Mol	Chain	Res	Type
26	1	2884	U
26	1	2885	G
27	2	9	G
27	2	32	A
27	2	39	G
27	2	47	C
27	2	48	C
27	2	50	A
27	2	51	A
27	2	54	C
27	2	68	G
27	2	70	U
27	2	72	A
27	2	73	C
27	2	74	A
27	2	77	A
27	2	78	A
27	2	83	C
27	2	84	U
27	2	85	U
27	2	87	C
27	2	94	G
27	2	95	C
27	2	100	G
27	2	120	A
27	2	121	U
27	2	128	G
27	2	130	A
27	2	131	A
27	2	141	G
27	2	181	A
27	2	182	A
27	2	204	G
27	2	209	U
27	2	211	G
27	2	212	G
27	2	245	U
27	2	247	G
27	2	251	G
27	2	266	G
27	2	267	C
27	2	279	A

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Mol	Chain	Res	Type
27	2	280	C
27	2	289	G
27	2	306	A
27	2	321	A
27	2	328	C
27	2	332	G
27	2	352	C
27	2	354	G
27	2	367	U
27	2	372	C
27	2	373	A
27	2	384	G
27	2	398	U
27	2	406	G
27	2	411	A
27	2	412	A
27	2	413	G
27	2	414	A
27	2	421	U
27	2	422	C
27	2	424	G
27	2	429	U
27	2	436	C
27	2	457	G
27	2	458	U
27	2	463	U
27	2	467	U
27	2	468	A
27	2	481	G
27	2	482	A
27	2	484	G
27	2	486	U
27	2	495	A
27	2	496	A
27	2	497	G
27	2	509	A
27	2	511	C
27	2	517	G
27	2	518	C
27	2	519	C
27	2	532	A
27	2	533	A

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Mol	Chain	Res	Type
27	2	536	C
27	2	547	A
27	2	559	A
27	2	572	A
27	2	573	A
27	2	576	C
27	2	579	A
27	2	633	G
27	2	639	G
27	2	653	U
27	2	665	A
27	2	695	A
27	2	700	G
27	2	703	G
27	2	721	G
27	2	723	U
27	2	724	G
27	2	731	G
27	2	734	G
27	2	747	A
27	2	748	G
27	2	755	G
27	2	777	A
27	2	793	U
27	2	794	A
27	2	815	A
27	2	817	C
27	2	821	G
27	2	828	U
27	2	829	G
27	2	841	C
27	2	844	G
27	2	845	A
27	2	846	G
27	2	851	G
27	2	902	G
27	2	914	A
27	2	926	G
27	2	934	C
27	2	935	A
27	2	960	U
27	2	966	2MG

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Mol	Chain	Res	Type
27	2	969	A
27	2	971	G
27	2	975	A
27	2	976	G
27	2	977	A
27	2	992	U
27	2	993	G
27	2	996	A
27	2	1004	A
27	2	1005	A
27	2	1008	U
27	2	1009	U
27	2	1019	A
27	2	1020	G
27	2	1026	G
27	2	1028	C
27	2	1030	U
27	2	1033	G
27	2	1044	A
27	2	1053	G
27	2	1065	U
27	2	1085	U
27	2	1089	G
27	2	1094	G
27	2	1095	U
27	2	1101	A
27	2	1124	G
27	2	1132	C
27	2	1136	C
27	2	1137	C
27	2	1138	G
27	2	1139	G
27	2	1140	C
27	2	1141	C
27	2	1145	A
27	2	1146	A
27	2	1154	G
27	2	1159	U
27	2	1174	G
27	2	1175	G
27	2	1176	A
27	2	1184	G

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Mol	Chain	Res	Type
27	2	1196	A
27	2	1197	A
27	2	1213	A
27	2	1227	A
27	2	1228	C
27	2	1238	A
27	2	1239	A
27	2	1258	G
27	2	1275	A
27	2	1279	G
27	2	1280	A
27	2	1285	A
27	2	1286	U
27	2	1287	A
27	2	1299	A
27	2	1302	C
27	2	1305	G
27	2	1317	C
27	2	1319	A
27	2	1320	C
27	2	1338	G
27	2	1340	A
27	2	1346	A
27	2	1353	G
27	2	1363	A
27	2	1370	G
27	2	1379	G
27	2	1397	C
27	2	1398	A
27	2	1419	G
27	2	1432	G
27	2	1441	A
27	2	1446	A
27	2	1453	G
27	2	1475	G
27	2	1492	A
27	2	1493	A
27	2	1497	G
27	2	1506	U
27	2	1517	G
27	2	1529	G
27	2	1530	G

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Mol	Chain	Res	Type
27	2	1534	A
28	3	2	G
28	3	13	G
28	3	24	G
28	3	25	U
28	3	35	C
28	3	51	G
28	3	56	G
28	3	84	G
28	3	89	U
28	3	90	C
28	3	99	A
28	3	109	A
29	5	2	C
29	5	8	4SU
29	5	13	A
29	5	16	C
29	5	18	G
29	5	19	G
29	5	20	H2U
29	5	21	A
29	5	22	G
29	5	47	U
29	5	48	C
29	5	54	5MU
29	5	58	A
29	5	74	C
56	XX	5	G
56	XX	8	G

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1	404	A
26	1	784	G
26	1	894	U
26	1	1379	U
26	1	2146	C
26	1	2602	A
26	1	2756	U
27	2	428	G
27	2	516	PSU

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Mol	Chain	Res	Type
27	2	1109	C
27	2	1145	A
29	5	17	U
29	5	47	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
26	3TD	1	1915	26	18,22,23	4.49	7 (38%)	22,32,35	1.71	3 (13%)
26	6MZ	1	1618	26	18,25,26	1.77	5 (27%)	16,36,39	1.89	3 (18%)
27	5MC	2	1407	27	18,22,23	3.19	7 (38%)	26,32,35	1.12	1 (3%)
26	6MZ	1	2030	26	18,25,26	1.70	5 (27%)	16,36,39	2.96	5 (31%)
26	5MU	1	747	26	19,22,23	4.78	7 (36%)	28,32,35	3.41	8 (28%)
26	OMC	1	2498	26,58	19,22,23	2.69	8 (42%)	26,31,34	0.97	1 (3%)
29	8AN	5	76	29,58,59	19,24,25	5.61	8 (42%)	13,35,38	3.10	3 (23%)
27	MA6	2	1518	27	18,26,27	1.37	2 (11%)	19,38,41	3.27	2 (10%)
26	PSU	1	1917	26	18,21,22	1.02	2 (11%)	22,30,33	1.66	4 (18%)
26	2MG	1	1835	26	18,26,27	2.09	7 (38%)	16,38,41	1.41	4 (25%)
26	2MG	1	2445	26	18,26,27	2.25	6 (33%)	16,38,41	1.48	4 (25%)
26	PSU	1	955	26	18,21,22	1.15	1 (5%)	22,30,33	2.02	4 (18%)
26	PSU	1	2504	26	18,21,22	1.02	1 (5%)	22,30,33	1.87	4 (18%)
29	5MU	5	54	29	19,22,23	4.75	7 (36%)	28,32,35	3.65	9 (32%)
29	4OC	5	32	29	20,23,24	2.83	8 (40%)	26,32,35	0.97	2 (7%)
27	2MG	2	1207	27	18,26,27	2.35	7 (38%)	16,38,41	1.47	4 (25%)
26	5MC	1	1962	26	18,22,23	3.23	7 (38%)	26,32,35	1.05	2 (7%)
27	2MG	2	966	27	18,26,27	2.26	7 (38%)	16,38,41	1.41	3 (18%)
46	0TD	q	89	46	7,9,10	1.47	0	6,11,13	2.30	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	1MG	1	745	26	18,26,27	2.46	5 (27%)	19,39,42	1.65	4 (21%)
26	OMG	1	2251	29,26	18,26,27	2.34	8 (44%)	19,38,41	1.44	3 (15%)
26	G7M	1	2069	26	20,26,27	1.72	5 (25%)	17,39,42	1.31	3 (17%)
29	PSU	5	55	29	18,21,22	1.04	1 (5%)	22,30,33	1.78	5 (22%)
27	4OC	2	1402	27	20,23,24	2.84	8 (40%)	26,32,35	0.95	1 (3%)
27	UR3	2	1498	27	19,22,23	2.43	6 (31%)	26,32,35	1.44	2 (7%)
29	4SU	5	8	29	18,21,22	3.64	8 (44%)	26,30,33	2.22	5 (19%)
26	5MU	1	1939	26,58	19,22,23	4.68	7 (36%)	28,32,35	3.87	12 (42%)
26	PSU	1	2580	26,58	18,21,22	1.31	3 (16%)	22,30,33	1.89	4 (18%)
29	H2U	5	20	29,58	18,21,22	3.54	3 (16%)	21,30,33	2.02	5 (23%)
26	PSU	1	2457	26	18,21,22	1.15	1 (5%)	22,30,33	2.13	5 (22%)
26	OMU	1	2552	26	19,22,23	2.65	7 (36%)	26,31,34	2.10	7 (26%)
26	PSU	1	1911	26	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
27	PSU	2	516	27,58	18,21,22	1.08	1 (5%)	22,30,33	1.81	3 (13%)
27	MA6	2	1519	27	18,26,27	1.37	2 (11%)	19,38,41	3.41	2 (10%)
27	5MC	2	967	27	18,22,23	3.33	7 (38%)	26,32,35	1.06	2 (7%)
26	2MA	1	2503	26,58	19,25,26	3.17	7 (36%)	21,37,40	1.94	3 (14%)
26	PSU	1	2605	26	18,21,22	1.15	2 (11%)	22,30,33	1.64	4 (18%)
26	PSU	1	746	26	18,21,22	1.09	1 (5%)	22,30,33	1.70	4 (18%)
27	2MG	2	1516	27	18,26,27	2.21	7 (38%)	16,38,41	1.60	4 (25%)
27	7MG	2	527	27	22,26,27	3.26	10 (45%)	29,39,42	1.95	8 (27%)

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
26	3TD	1	1915	26	-	5/7/25/26	0/2/2/2
26	6MZ	1	1618	26	-	2/5/27/28	0/3/3/3
27	5MC	2	1407	27	-	0/7/25/26	0/2/2/2
26	6MZ	1	2030	26	-	2/5/27/28	0/3/3/3
26	5MU	1	747	26	-	0/7/25/26	0/2/2/2
26	OMC	1	2498	26,58	-	1/9/27/28	0/2/2/2
29	8AN	5	76	29,58,59	-	3/3/25/26	0/3/3/3
27	MA6	2	1518	27	-	0/7/29/30	0/3/3/3
26	PSU	1	1917	26	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	2MG	1	1835	26	-	0/5/27/28	0/3/3/3
26	2MG	1	2445	26	-	2/5/27/28	0/3/3/3
26	PSU	1	955	26	-	0/7/25/26	0/2/2/2
26	PSU	1	2504	26	-	0/7/25/26	0/2/2/2
29	5MU	5	54	29	-	2/7/25/26	0/2/2/2
29	4OC	5	32	29	-	0/9/29/30	0/2/2/2
27	2MG	2	1207	27	-	0/5/27/28	0/3/3/3
26	5MC	1	1962	26	-	0/7/25/26	0/2/2/2
27	2MG	2	966	27	-	2/5/27/28	0/3/3/3
46	0TD	q	89	46	-	1/7/12/14	-
26	1MG	1	745	26	-	0/3/25/26	0/3/3/3
26	OMG	1	2251	29,26	-	1/5/27/28	0/3/3/3
26	G7M	1	2069	26	-	1/3/25/26	0/3/3/3
29	PSU	5	55	29	-	0/7/25/26	0/2/2/2
27	4OC	2	1402	27	-	2/9/29/30	0/2/2/2
27	UR3	2	1498	27	-	0/7/25/26	0/2/2/2
29	4SU	5	8	29	-	4/7/25/26	0/2/2/2
26	5MU	1	1939	26,58	-	0/7/25/26	0/2/2/2
26	PSU	1	2580	26,58	-	0/7/25/26	0/2/2/2
29	H2U	5	20	29,58	-	5/7/38/39	0/2/2/2
26	PSU	1	2457	26	-	0/7/25/26	0/2/2/2
26	OMU	1	2552	26	-	1/9/27/28	0/2/2/2
26	PSU	1	1911	26	-	0/7/25/26	0/2/2/2
27	PSU	2	516	27,58	-	2/7/25/26	0/2/2/2
27	MA6	2	1519	27	-	0/7/29/30	0/3/3/3
27	5MC	2	967	27	-	0/7/25/26	0/2/2/2
26	2MA	1	2503	26,58	-	2/3/25/26	0/3/3/3
26	PSU	1	2605	26	-	0/7/25/26	0/2/2/2
26	PSU	1	746	26	-	2/7/25/26	0/2/2/2
27	2MG	2	1516	27	-	0/5/27/28	0/3/3/3
27	7MG	2	527	27	-	2/7/37/38	0/3/3/3

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	76	8AN	C2'-C1'	-15.41	1.30	1.53
29	5	76	8AN	O4'-C1'	15.38	1.62	1.41
26	1	1915	3TD	C6-C5	14.20	1.51	1.35
29	5	20	H2U	C2-N1	12.18	1.53	1.35
29	5	54	5MU	C2-N1	10.92	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	747	5MU	C2-N1	10.79	1.55	1.38
26	1	747	5MU	C6-N1	10.50	1.56	1.38
29	5	54	5MU	C6-N1	10.25	1.55	1.38
26	1	1939	5MU	C2-N1	10.15	1.54	1.38
29	5	54	5MU	C4-C5	9.75	1.61	1.44
26	1	1939	5MU	C4-C5	9.49	1.60	1.44
26	1	1939	5MU	C4-N3	-9.13	1.21	1.38
26	1	1939	5MU	C6-N1	9.05	1.53	1.38
26	1	747	5MU	C4-C5	9.01	1.59	1.44
26	1	1962	5MC	C6-C5	8.70	1.48	1.34
26	1	1915	3TD	C2-N1	8.60	1.48	1.37
27	2	967	5MC	C6-C5	8.51	1.48	1.34
27	2	1407	5MC	C6-C5	8.42	1.48	1.34
26	1	747	5MU	C4-N3	-8.22	1.23	1.38
29	5	76	8AN	O4'-C4'	-7.98	1.27	1.45
26	1	2503	2MA	C4-N3	7.96	1.48	1.35
29	5	8	4SU	C4-N3	7.95	1.46	1.37
29	5	54	5MU	C4-N3	-7.94	1.24	1.38
27	2	527	7MG	C8-N9	7.83	1.50	1.46
27	2	527	7MG	C5-N7	7.44	1.44	1.35
26	1	2503	2MA	C2-N3	6.78	1.46	1.34
29	5	8	4SU	C2-N3	6.74	1.50	1.38
29	5	20	H2U	C2-N3	6.50	1.49	1.38
29	5	8	4SU	C2-N1	6.09	1.48	1.38
27	2	1402	4OC	C4-N3	6.08	1.43	1.32
29	5	32	4OC	C4-N3	6.05	1.43	1.32
26	1	2552	OMU	C2-N3	6.05	1.48	1.38
26	1	2552	OMU	C2-N1	5.93	1.48	1.38
27	2	1402	4OC	C6-C5	5.91	1.48	1.35
26	1	747	5MU	C6-C5	5.89	1.44	1.34
27	2	1498	UR3	C2-N1	5.84	1.46	1.38
26	1	1915	3TD	C2-N3	5.81	1.51	1.38
27	2	967	5MC	C4-N3	5.80	1.43	1.34
29	5	32	4OC	C6-C5	5.77	1.48	1.35
27	2	967	5MC	C2-N3	5.64	1.47	1.36
29	5	8	4SU	C6-C5	5.57	1.48	1.35
29	5	54	5MU	C6-C5	5.54	1.43	1.34
26	1	2503	2MA	C2-N1	5.53	1.43	1.34
26	1	745	1MG	C2-N2	5.51	1.44	1.34
26	1	2498	OMC	C6-C5	5.42	1.47	1.35
26	1	1962	5MC	C4-N3	5.40	1.43	1.34
26	1	745	1MG	C2-N3	5.40	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	1407	5MC	C4-N3	5.36	1.43	1.34
26	1	1939	5MU	C6-C5	5.35	1.43	1.34
29	5	20	H2U	C4-N3	5.34	1.46	1.37
29	5	32	4OC	C2-N3	5.27	1.47	1.36
26	1	2552	OMU	C6-C5	5.25	1.47	1.35
27	2	1498	UR3	C6-C5	5.24	1.47	1.35
27	2	966	2MG	C2-N2	5.21	1.45	1.33
26	1	1962	5MC	C2-N3	5.17	1.46	1.36
27	2	1407	5MC	C2-N3	5.15	1.46	1.36
27	2	1402	4OC	C2-N3	5.08	1.46	1.36
26	1	1915	3TD	C6-N1	5.06	1.44	1.36
26	1	2503	2MA	C6-N1	5.06	1.43	1.33
26	1	2498	OMC	C2-N3	5.05	1.46	1.36
27	2	1207	2MG	C2-N2	5.00	1.44	1.33
29	5	8	4SU	C4-S4	-4.99	1.58	1.68
27	2	527	7MG	C2-N3	4.86	1.44	1.33
26	1	1618	6MZ	C6-N6	4.83	1.43	1.35
27	2	527	7MG	C4-N3	4.81	1.45	1.34
27	2	966	2MG	C4-N3	4.62	1.48	1.37
26	1	2445	2MG	C2-N2	4.57	1.43	1.33
26	1	2498	OMC	C4-N3	4.54	1.43	1.34
26	1	2251	OMG	C2-N3	4.49	1.44	1.33
27	2	1516	2MG	C2-N2	4.47	1.43	1.33
26	1	2498	OMC	C4-N4	4.45	1.44	1.33
26	1	1835	2MG	C2-N2	4.45	1.43	1.33
26	1	2445	2MG	C4-N3	4.44	1.48	1.37
27	2	1207	2MG	C4-N3	4.42	1.48	1.37
29	5	32	4OC	C4-N4	4.41	1.45	1.35
26	1	2069	G7M	C4-N3	4.32	1.47	1.37
26	1	1939	5MU	O2-C2	-4.31	1.15	1.23
26	1	2251	OMG	C2-N2	4.31	1.44	1.34
26	1	2030	6MZ	C6-N6	4.29	1.42	1.35
27	2	1207	2MG	C2-N1	4.28	1.43	1.36
27	2	527	7MG	C2-N2	4.23	1.44	1.34
27	2	1402	4OC	C4-N4	4.23	1.44	1.35
27	2	967	5MC	C6-N1	4.23	1.45	1.38
26	1	745	1MG	C4-N3	4.20	1.47	1.37
27	2	1498	UR3	C2-N3	4.17	1.47	1.39
26	1	2251	OMG	C4-N3	4.15	1.47	1.37
26	1	1962	5MC	C6-N1	4.13	1.45	1.38
26	1	2498	OMC	C2-N1	4.13	1.48	1.40
26	1	1835	2MG	C4-N3	4.10	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	967	5MC	C4-N4	4.06	1.44	1.34
27	2	1407	5MC	C6-N1	4.04	1.45	1.38
29	5	8	4SU	C5-C4	3.99	1.47	1.42
27	2	1516	2MG	C4-N3	3.93	1.46	1.37
27	2	1516	2MG	C2-N1	3.83	1.42	1.36
27	2	966	2MG	C2-N1	3.80	1.42	1.36
27	2	1407	5MC	C4-N4	3.77	1.43	1.34
27	2	527	7MG	C4-N9	3.74	1.42	1.37
26	1	1962	5MC	C4-N4	3.73	1.43	1.34
27	2	967	5MC	C2-N1	3.73	1.48	1.40
27	2	1519	MA6	C5-C4	-3.66	1.31	1.40
26	1	2251	OMG	C5-C4	-3.63	1.33	1.43
27	2	1407	5MC	C2-N1	3.56	1.47	1.40
27	2	1402	4OC	C5-C4	3.54	1.48	1.40
27	2	1518	MA6	C5-C4	-3.51	1.31	1.40
29	5	76	8AN	C5-C4	-3.50	1.31	1.40
29	5	32	4OC	C2-N1	3.50	1.47	1.40
27	2	1402	4OC	O2-C2	-3.48	1.17	1.23
26	1	1962	5MC	O2-C2	-3.47	1.17	1.23
27	2	1516	2MG	C5-C4	-3.47	1.34	1.43
29	5	32	4OC	C5-C4	3.44	1.48	1.40
26	1	747	5MU	O4-C4	-3.40	1.17	1.23
26	1	2251	OMG	O6-C6	-3.35	1.16	1.23
26	1	2445	2MG	C5-C4	-3.34	1.34	1.43
26	1	2445	2MG	O6-C6	-3.33	1.16	1.23
27	2	1402	4OC	C2-N1	3.28	1.47	1.40
26	1	745	1MG	C5-C4	-3.28	1.34	1.43
26	1	1835	2MG	C2-N1	3.27	1.42	1.36
27	2	527	7MG	O6-C6	-3.26	1.17	1.23
27	2	1407	5MC	O2-C2	-3.23	1.17	1.23
27	2	967	5MC	O2-C2	-3.22	1.17	1.23
27	2	1207	2MG	C5-C4	-3.21	1.34	1.43
29	5	8	4SU	C6-N1	3.19	1.45	1.38
26	1	2552	OMU	C4-N3	3.15	1.44	1.38
26	1	1939	5MU	O4-C4	-3.14	1.17	1.23
26	1	1962	5MC	C2-N1	3.13	1.46	1.40
26	1	2069	G7M	C2-N2	3.13	1.41	1.34
26	1	2030	6MZ	C5-C4	-3.13	1.32	1.40
26	1	1835	2MG	O6-C6	-3.11	1.17	1.23
26	1	2498	OMC	C6-N1	3.09	1.45	1.38
26	1	1618	6MZ	C5-C4	-3.08	1.32	1.40
27	2	527	7MG	C2-N1	3.08	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	1915	3TD	O2-C2	-3.07	1.17	1.23
27	2	527	7MG	C5-C6	3.07	1.51	1.43
26	1	1835	2MG	C5-C4	-3.06	1.35	1.43
29	5	76	8AN	C6-N6	3.06	1.45	1.34
26	1	746	PSU	C6-C5	3.06	1.38	1.35
29	5	32	4OC	O2-C2	-3.06	1.18	1.23
26	1	2552	OMU	O4-C4	-3.05	1.18	1.24
26	1	747	5MU	O2-C2	-3.05	1.17	1.23
29	5	55	PSU	C6-C5	3.04	1.38	1.35
27	2	1207	2MG	C6-N1	3.02	1.42	1.37
26	1	2445	2MG	C2-N1	3.01	1.41	1.36
27	2	1516	2MG	O6-C6	-3.01	1.17	1.23
27	2	1498	UR3	O2-C2	-2.97	1.17	1.22
27	2	1402	4OC	C6-N1	2.94	1.45	1.38
26	1	745	1MG	O6-C6	-2.93	1.16	1.22
27	2	1498	UR3	O4-C4	-2.92	1.17	1.23
29	5	8	4SU	O2-C2	-2.92	1.17	1.23
26	1	1911	PSU	C6-C5	2.89	1.38	1.35
27	2	966	2MG	C5-C4	-2.85	1.35	1.43
26	1	2503	2MA	C6-C5	2.83	1.53	1.43
27	2	1207	2MG	C5-C6	2.82	1.53	1.47
27	2	516	PSU	C6-C5	2.80	1.38	1.35
26	1	2498	OMC	O2-C2	-2.78	1.18	1.23
26	1	2445	2MG	C5-C6	2.76	1.53	1.47
29	5	76	8AN	C3'-N3'	-2.74	1.43	1.47
29	5	54	5MU	O4-C4	-2.73	1.18	1.23
27	2	966	2MG	C6-N1	2.70	1.41	1.37
26	1	2069	G7M	C5-C4	-2.67	1.33	1.39
27	2	1516	2MG	C6-N1	2.66	1.41	1.37
26	1	1917	PSU	C6-C5	2.66	1.38	1.35
26	1	2030	6MZ	C9-N6	-2.66	1.40	1.45
26	1	2580	PSU	O4'-C1'	-2.65	1.40	1.43
29	5	32	4OC	C6-N1	2.62	1.44	1.38
26	1	2504	PSU	C6-C5	2.58	1.38	1.35
26	1	1915	3TD	O4-C4	-2.58	1.17	1.23
27	2	966	2MG	O6-C6	-2.58	1.18	1.23
27	2	1498	UR3	C6-N1	2.55	1.44	1.38
26	1	1915	3TD	C4-N3	2.52	1.45	1.40
27	2	1207	2MG	O6-C6	-2.50	1.18	1.23
26	1	2457	PSU	C6-C5	2.47	1.38	1.35
29	5	54	5MU	O2-C2	-2.47	1.18	1.23
27	2	1516	2MG	C5-C6	2.43	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	2251	OMG	C5-C6	2.43	1.52	1.47
26	1	1618	6MZ	C6-N1	-2.43	1.30	1.34
26	1	2069	G7M	C2-N3	2.42	1.39	1.33
26	1	2030	6MZ	C5-N7	-2.42	1.31	1.39
26	1	2251	OMG	C2-N1	2.42	1.43	1.37
26	1	2580	PSU	C6-C5	2.41	1.38	1.35
26	1	2605	PSU	C6-C5	2.39	1.38	1.35
29	5	76	8AN	C2-N3	2.39	1.35	1.32
27	2	527	7MG	C6-N1	2.27	1.43	1.38
26	1	2552	OMU	O2-C2	-2.27	1.18	1.23
26	1	2580	PSU	C4-C5	-2.27	1.37	1.44
29	5	76	8AN	O2'-C2'	2.26	1.48	1.43
27	2	1518	MA6	C2-N3	2.25	1.35	1.32
26	1	1618	6MZ	C9-N6	-2.25	1.41	1.45
27	2	966	2MG	C5-C6	2.24	1.51	1.47
26	1	2069	G7M	C6-N1	2.22	1.41	1.37
26	1	2030	6MZ	C4-N3	-2.17	1.32	1.35
26	1	2503	2MA	C5-C4	-2.17	1.35	1.40
27	2	1519	MA6	C2-N3	2.17	1.35	1.32
26	1	2503	2MA	C6-N6	-2.16	1.26	1.34
26	1	2552	OMU	C6-N1	2.16	1.43	1.38
26	1	2498	OMC	C5-C4	2.16	1.47	1.42
26	1	1618	6MZ	C5-N7	-2.15	1.31	1.39
26	1	2605	PSU	C4-C5	-2.11	1.38	1.44
26	1	1835	2MG	C5-C6	2.11	1.51	1.47
26	1	2251	OMG	C6-N1	2.07	1.41	1.37
26	1	1835	2MG	C6-N1	2.04	1.40	1.37
26	1	1917	PSU	C4-C5	-2.04	1.38	1.44
26	1	955	PSU	O4'-C1'	-2.00	1.41	1.43

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	1519	MA6	N1-C6-N6	-13.54	102.81	117.06
27	2	1518	MA6	N1-C6-N6	-12.74	103.65	117.06
29	5	54	5MU	C5-C4-N3	12.27	125.79	115.31
26	1	747	5MU	C5-C4-N3	11.28	124.94	115.31
26	1	1939	5MU	C5-C4-N3	11.27	124.93	115.31
26	1	1939	5MU	C5-C6-N1	-10.71	112.32	123.34
29	5	54	5MU	C5-C6-N1	-9.98	113.08	123.34
26	1	747	5MU	C5-C6-N1	-8.71	114.38	123.34
29	5	76	8AN	C5-C6-N6	7.56	131.84	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	2503	2MA	C2-N3-C4	7.33	121.48	115.52
29	5	8	4SU	C4-N3-C2	-7.07	120.47	127.34
26	1	2030	6MZ	N3-C2-N1	-7.05	117.65	128.68
29	5	20	H2U	C4-N3-C2	-7.03	119.96	125.79
26	1	2552	OMU	C4-N3-C2	-6.41	118.13	126.58
26	1	2030	6MZ	C2-N1-C6	6.24	121.94	116.59
26	1	747	5MU	O4-C4-C5	-6.18	117.73	124.90
26	1	1939	5MU	N3-C2-N1	6.11	123.00	114.89
29	5	76	8AN	N3-C2-N1	-6.07	119.19	128.68
27	2	1518	MA6	N3-C2-N1	-5.96	119.37	128.68
26	1	2457	PSU	N1-C2-N3	5.83	121.74	115.13
26	1	2030	6MZ	C1'-N9-C4	-5.79	116.48	126.64
27	2	1498	UR3	C4-N3-C2	-5.69	119.21	124.56
26	1	1939	5MU	C4-N3-C2	-5.66	120.03	127.35
26	1	1618	6MZ	N3-C2-N1	-5.63	119.87	128.68
27	2	1519	MA6	N3-C2-N1	-5.46	120.15	128.68
26	1	2504	PSU	C4-N3-C2	-5.44	118.51	126.34
26	1	1915	3TD	N1-C2-N3	5.42	120.42	116.14
26	1	2457	PSU	C4-N3-C2	-5.41	118.54	126.34
26	1	955	PSU	C4-N3-C2	-5.40	118.56	126.34
26	1	955	PSU	N1-C2-N3	5.32	121.16	115.13
29	5	8	4SU	C5-C4-N3	5.29	119.59	114.69
29	5	54	5MU	O4-C4-C5	-5.19	118.89	124.90
26	1	747	5MU	N3-C2-N1	5.09	121.64	114.89
27	2	527	7MG	C5-C6-N1	5.01	119.81	110.99
26	1	2580	PSU	N1-C2-N3	4.95	120.74	115.13
26	1	1939	5MU	C5M-C5-C6	-4.94	116.25	122.85
26	1	2552	OMU	C5-C4-N3	4.83	122.06	114.84
27	2	516	PSU	C4-N3-C2	-4.81	119.40	126.34
26	1	2580	PSU	C4-N3-C2	-4.66	119.62	126.34
26	1	2605	PSU	C4-N3-C2	-4.60	119.71	126.34
29	5	54	5MU	C4-N3-C2	-4.57	121.43	127.35
26	1	746	PSU	C4-N3-C2	-4.57	119.76	126.34
29	5	76	8AN	N6-C6-N1	-4.56	109.12	118.57
29	5	55	PSU	N1-C2-N3	4.51	120.25	115.13
26	1	2504	PSU	N1-C2-N3	4.47	120.20	115.13
29	5	55	PSU	C4-N3-C2	-4.45	119.92	126.34
26	1	746	PSU	N1-C2-N3	4.39	120.11	115.13
26	1	1911	PSU	N1-C2-N3	4.39	120.10	115.13
46	q	89	0TD	OD2-CG-CB	4.36	122.56	113.15
26	1	747	5MU	C4-N3-C2	-4.34	121.73	127.35
26	1	1917	PSU	C4-N3-C2	-4.32	120.11	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	54	5MU	C5M-C5-C4	4.29	123.49	118.77
27	2	516	PSU	N1-C2-N3	4.29	119.98	115.13
26	1	1911	PSU	C4-N3-C2	-4.25	120.22	126.34
26	1	745	1MG	C5-C6-N1	4.23	120.27	113.90
27	2	527	7MG	C2-N3-C4	4.22	119.81	112.30
29	5	54	5MU	C5M-C5-C6	-4.15	117.31	122.85
26	1	1917	PSU	N1-C2-N3	4.12	119.80	115.13
27	2	1407	5MC	C5-C6-N1	-4.12	119.10	123.34
26	1	1915	3TD	C4-N3-C2	-3.97	120.30	124.61
26	1	2605	PSU	N1-C2-N3	3.95	119.60	115.13
29	5	54	5MU	N3-C2-N1	3.93	120.11	114.89
27	2	1516	2MG	C5-C6-N1	3.86	120.77	113.95
26	1	1939	5MU	C5M-C5-C4	3.83	122.98	118.77
26	1	2445	2MG	C5-C6-N1	3.75	120.58	113.95
26	1	2552	OMU	N3-C2-N1	3.75	119.87	114.89
26	1	1939	5MU	O4-C4-C5	-3.75	120.56	124.90
27	2	967	5MC	C5-C6-N1	-3.69	119.54	123.34
26	1	1962	5MC	C5-C6-N1	-3.65	119.58	123.34
29	5	8	4SU	N3-C2-N1	3.64	119.72	114.89
27	2	966	2MG	C5-C6-N1	3.63	120.36	113.95
26	1	1835	2MG	C5-C6-N1	3.62	120.35	113.95
27	2	1207	2MG	C5-C6-N1	3.54	120.20	113.95
27	2	527	7MG	C5-C4-N3	-3.48	121.51	128.13
29	5	8	4SU	C1'-N1-C2	3.46	123.83	117.57
27	2	527	7MG	C5-C4-N9	3.38	110.73	106.35
26	1	747	5MU	C6-N1-C2	-3.38	117.88	121.30
26	1	1618	6MZ	C2-N1-C6	3.34	119.45	116.59
26	1	1939	5MU	O2-C2-N1	-3.34	118.35	122.79
27	2	1516	2MG	CM2-N2-C2	-3.32	116.53	123.86
29	5	8	4SU	C5-C4-S4	-3.32	120.19	124.47
26	1	955	PSU	O2-C2-N1	-3.29	119.17	122.79
26	1	1939	5MU	C6-C5-C4	3.27	120.76	118.03
26	1	747	5MU	O2-C2-N1	-3.25	118.46	122.79
26	1	745	1MG	O6-C6-C5	-3.18	118.56	124.19
26	1	2503	2MA	N3-C2-N1	-3.17	119.95	125.73
26	1	2552	OMU	O4-C4-C5	-3.12	119.67	125.16
29	5	20	H2U	N3-C2-N1	3.08	119.91	116.65
26	1	2251	OMG	C5-C6-N1	3.07	119.37	113.95
26	1	745	1MG	C8-N7-C5	3.04	108.78	102.99
26	1	2457	PSU	O2-C2-N1	-3.04	119.44	122.79
29	5	20	H2U	C5-C4-N3	2.93	119.94	116.65
26	1	1939	5MU	O4-C4-N3	-2.93	114.50	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	1939	5MU	C1'-N1-C2	2.85	122.73	117.57
27	2	527	7MG	C4-C5-N7	2.81	109.43	105.53
26	1	2069	G7M	C2-N1-C6	-2.78	119.98	125.10
26	1	2552	OMU	O2-C2-N1	-2.78	119.10	122.79
26	1	745	1MG	C2-N1-C6	-2.77	118.69	120.95
26	1	2251	OMG	C8-N7-C5	2.76	108.26	102.99
26	1	2457	PSU	C6-N1-C2	-2.76	119.86	122.68
26	1	2552	OMU	C2'-C1'-N1	-2.75	108.88	114.22
27	2	1207	2MG	C8-N7-C5	2.75	108.22	102.99
26	1	2498	OMC	O2-C2-N3	-2.74	117.87	122.33
26	1	1962	5MC	CM5-C5-C6	-2.65	119.31	122.85
27	2	527	7MG	O6-C6-C5	-2.64	121.06	127.54
26	1	1917	PSU	O2-C2-N1	-2.63	119.89	122.79
29	5	55	PSU	O2-C2-N1	-2.62	119.90	122.79
26	1	2504	PSU	O2-C2-N1	-2.62	119.91	122.79
26	1	2030	6MZ	C4-C5-N7	-2.61	106.68	109.40
26	1	2069	G7M	N2-C2-N1	2.61	122.27	116.71
29	5	20	H2U	C5-C6-N1	2.59	120.16	111.61
27	2	527	7MG	C2-N1-C6	-2.59	120.38	125.10
27	2	1207	2MG	CM2-N2-C2	-2.58	118.16	123.86
27	2	1402	4OC	CM4-N4-C4	-2.58	117.41	122.45
29	5	32	4OC	CM4-N4-C4	-2.55	117.46	122.45
26	1	2030	6MZ	C9-N6-C6	-2.55	120.67	122.87
29	5	54	5MU	O4-C4-N3	-2.50	115.32	120.12
27	2	1516	2MG	O6-C6-C5	-2.46	119.56	124.37
27	2	966	2MG	O6-C6-C5	-2.42	119.64	124.37
29	5	55	PSU	C6-N1-C2	-2.42	120.21	122.68
26	1	2580	PSU	O4'-C1'-C2'	2.42	108.55	105.14
26	1	2503	2MA	CM2-C2-N1	2.41	120.92	117.15
26	1	2552	OMU	CM2-O2'-C2'	-2.41	108.21	114.52
26	1	2445	2MG	CM2-N2-C2	-2.36	118.64	123.86
26	1	1835	2MG	C8-N7-C5	2.35	107.47	102.99
26	1	2445	2MG	C8-N7-C5	2.33	107.43	102.99
26	1	2580	PSU	C6-N1-C2	-2.33	120.30	122.68
26	1	1939	5MU	C6-N1-C2	-2.33	118.94	121.30
26	1	746	PSU	O2-C2-N1	-2.32	120.24	122.79
27	2	967	5MC	CM5-C5-C6	-2.31	119.76	122.85
29	5	20	H2U	O2-C2-N1	-2.31	120.21	123.11
27	2	966	2MG	C8-N7-C5	2.31	107.38	102.99
27	2	1498	UR3	C3U-N3-C4	2.30	121.18	117.89
27	2	1516	2MG	C8-N7-C5	2.30	107.37	102.99
26	1	1835	2MG	O6-C6-C5	-2.30	119.88	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	55	PSU	C6-C5-C4	2.30	119.80	118.20
26	1	2251	OMG	C2-N1-C6	-2.29	120.89	125.10
46	q	89	0TD	OD1-CG-CB	-2.28	117.67	122.44
29	5	32	4OC	C6-C5-C4	2.25	119.72	116.96
26	1	2605	PSU	O2-C2-N3	-2.23	117.61	121.82
26	1	2504	PSU	C5-C4-N3	2.22	121.61	116.58
26	1	2457	PSU	C6-C5-C4	2.22	119.75	118.20
26	1	747	5MU	C5M-C5-C6	-2.21	119.90	122.85
29	5	54	5MU	C1'-N1-C2	2.21	121.56	117.57
26	1	746	PSU	C6-N1-C2	-2.20	120.43	122.68
26	1	2445	2MG	O6-C6-C5	-2.19	120.10	124.37
26	1	1911	PSU	C6-N1-C2	-2.19	120.45	122.68
26	1	1618	6MZ	C9-N6-C6	-2.16	121.01	122.87
26	1	1915	3TD	C6-C5-C4	2.16	119.71	118.22
26	1	1917	PSU	C6-N1-C2	-2.15	120.49	122.68
27	2	1207	2MG	O6-C6-C5	-2.12	120.24	124.37
26	1	1911	PSU	O2-C2-N1	-2.10	120.48	122.79
26	1	1835	2MG	CM2-N2-C2	-2.09	119.24	123.86
26	1	955	PSU	C6-N1-C2	-2.07	120.56	122.68
27	2	516	PSU	C5-C4-N3	2.05	121.23	116.58
26	1	2069	G7M	CN7-N7-C8	-2.05	115.56	125.43
27	2	527	7MG	C6-C5-C4	-2.04	118.41	122.62
26	1	2605	PSU	C5-C4-N3	2.00	121.11	116.58

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	2	516	PSU	O4'-C1'-C5-C4
27	2	516	PSU	O4'-C1'-C5-C6
29	5	20	H2U	O4'-C1'-N1-C6
46	q	89	0TD	CG-CB-SB-CSB
26	1	746	PSU	C2'-C1'-C5-C4
26	1	1915	3TD	O4'-C1'-C5-C4
26	1	1915	3TD	C2'-C1'-C5-C6
26	1	1915	3TD	O4'-C1'-C5-C6
26	1	1915	3TD	C3'-C4'-C5'-O5'
26	1	1915	3TD	O4'-C4'-C5'-O5'
26	1	2251	OMG	C1'-C2'-O2'-CM2
26	1	2445	2MG	C3'-C4'-C5'-O5'
26	1	2030	6MZ	O4'-C4'-C5'-O5'
26	1	2030	6MZ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
29	5	76	8AN	C3'-C4'-C5'-O5'
29	5	54	5MU	C3'-C4'-C5'-O5'
29	5	54	5MU	O4'-C4'-C5'-O5'
26	1	1618	6MZ	O4'-C4'-C5'-O5'
26	1	1618	6MZ	C3'-C4'-C5'-O5'
29	5	76	8AN	C4'-C5'-O5'-P
29	5	20	H2U	O4'-C4'-C5'-O5'
29	5	20	H2U	C3'-C4'-C5'-O5'
26	1	2445	2MG	O4'-C4'-C5'-O5'
27	2	966	2MG	C3'-C4'-C5'-O5'
27	2	1402	4OC	O4'-C4'-C5'-O5'
29	5	76	8AN	O4'-C4'-C5'-O5'
26	1	2552	OMU	C3'-C2'-O2'-CM2
27	2	966	2MG	O4'-C4'-C5'-O5'
29	5	8	4SU	C2'-C1'-N1-C6
29	5	8	4SU	O4'-C1'-N1-C6
29	5	20	H2U	O4'-C1'-N1-C2
27	2	527	7MG	C3'-C4'-C5'-O5'
27	2	1402	4OC	C3'-C4'-C5'-O5'
27	2	527	7MG	C4'-C5'-O5'-P
26	1	746	PSU	O4'-C1'-C5-C6
29	5	8	4SU	C2'-C1'-N1-C2
26	1	2503	2MA	C4'-C5'-O5'-P
29	5	8	4SU	O4'-C1'-N1-C2
26	1	2069	G7M	O4'-C4'-C5'-O5'
29	5	20	H2U	C2'-C1'-N1-C2
26	1	2503	2MA	O4'-C4'-C5'-O5'
26	1	2498	OMC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 440 ligands modelled in this entry, 439 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	FME	5	104	29	8,9,10	0.88	0	7,9,11	1.82	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	5	104	29	-	4/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	5	104	FME	CA-N-CN	4.05	129.05	122.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	5	104	FME	CB-CA-N-CN
59	5	104	FME	N-CA-CB-CG
59	5	104	FME	CB-CG-SD-CE
59	5	104	FME	CA-CB-CG-SD

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	147:G	O3'	148:G	P	3.01
1	2	1276:G	O3'	1277:C	P	2.98

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12635. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

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 ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.