



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 06:01 pm GMT

PDB ID : 9GR1
EMDB ID : EMD-51517
Title : E. coli 70S-TEC complex in delivery state
Authors : Webster, M.W.; Weixlbaumer, A.
Deposited on : 2024-09-10
Resolution : 3.17 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 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 : **FAILED**
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

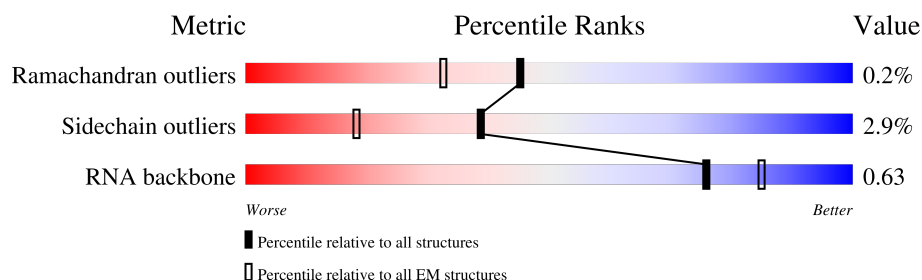
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 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	0	55	89% 7%
2	1	46	98% .
3	2	65	97% ..
4	3	38	97% .
5	A	1542	85% 13% .
6	B	241	88% 5% 7%
7	C	233	85% . 12%
8	D	206	99%
9	E	167	92% . 7%

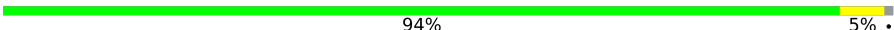
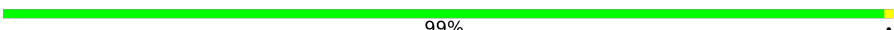
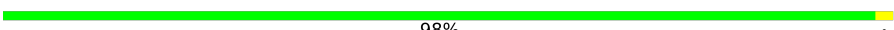
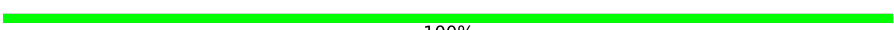








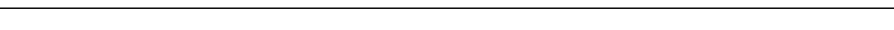
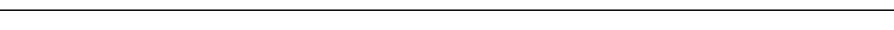
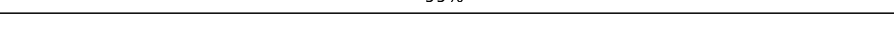

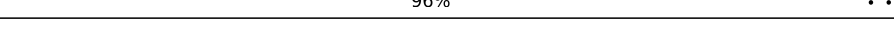
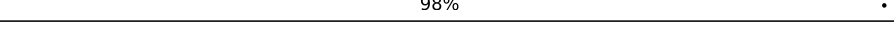
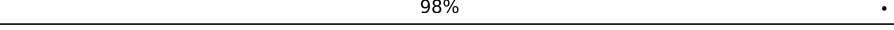
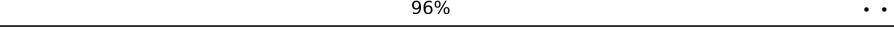

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Mol	Chain	Length	Quality of chain
10	F	135	
11	G	179	
12	H	130	
13	I	130	
14	J	103	
15	K	129	
16	L	124	
17	M	118	
18	N	101	
19	O	89	
20	P	82	
21	Q	84	
22	R	75	
23	S	92	
24	T	87	
25	U	71	
26	X	16	
27	Z	76	
28	a	2925	
29	b	119	
30	c	273	
31	d	209	
32	e	201	
33	f	179	
34	g	177	

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Mol	Chain	Length	Quality of chain
35	h	149	 94% 5% .
36	i	142	 99% .
37	j	123	 98% .
38	k	144	 100%
39	l	136	 99% .
40	m	127	 92% . 7%
41	n	117	 97% . .
42	o	115	 98% . .
43	p	118	 99% .
44	q	103	 99% .
45	r	110	 99% .
46	s	100	 89% . 7%
47	t	104	 94% . .
48	u	94	 99% .
49	v	85	 91% . 8%
50	w	78	 96% . .
51	x	63	 98% .
52	y	59	 98% .
53	z	57	 96% . .
54	4	10	 50% 50%
55	Y	77	 79% 18% .

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 142297 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 L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

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

- Molecule 5 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1513	Total	C	N	O	P	0	0
			32478	14493	5961	10511	1513		

- Molecule 6 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 10 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	116	Total	C	N	O	S	0	0
			902	558	183	156	5		

- Molecule 17 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 20 is a protein called 30S ribosomal protein S16.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 22 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 23 is a protein called 30S ribosomal protein S19.

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

- Molecule 24 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 25 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 26 is a RNA chain called mRNA in ribosome channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	13	Total	C	N	O	P	0	0
			271	122	44	92	13		

- Molecule 27 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Z	76	Total	C	N	O	P	S	0	0
			1624	724	290	533	76	1		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2748	Total	C	N	O	P	0	0
			59025	26336	10876	19065	2748		

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 30 is a protein called 50S ribosomal protein L2.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

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

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	148	Total	C	N	O	S	0	0
			1101	694	196	210	1		

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	77	ILE	VAL	conflict	UNP A0A140N711

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

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

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

- Molecule 53 is a protein called 50S ribosomal protein L32.

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

- Molecule 54 is a RNA chain called mRNA in SD-aSD duplex.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	10	Total	C	N	O	P	0	0
			223	99	48	66	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
55	Y	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	A	48	Total	K	0
			48	48	
57	a	112	Total	K	0
			112	112	
57	b	1	Total	K	0
			1	1	
57	c	4	Total	K	0
			4	4	
57	d	1	Total	K	0
			1	1	
57	e	1	Total	K	0
			1	1	
57	f	1	Total	K	0
			1	1	

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

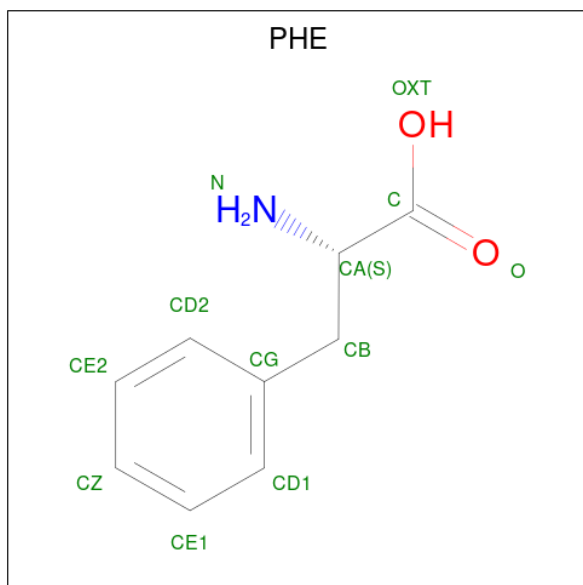
Mol	Chain	Residues	Atoms		AltConf
58	A	95	Total	Mg	0
			95	95	
58	N	1	Total	Mg	0
			1	1	
58	a	254	Total	Mg	0
			254	254	
58	b	5	Total	Mg	0
			5	5	
58	c	1	Total	Mg	0
			1	1	
58	d	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
58	k	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	
58	Y	1	Total	Mg	0
			1	1	

- Molecule 59 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
59	a	1	Total	C	N	O	0
			11	9	1	1	

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.

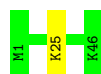
- Molecule 1: 50S ribosomal protein L33

Chain 0:  89% 7%



- Molecule 2: 50S ribosomal protein L34

Chain 1:  98%



- Molecule 3: 50S ribosomal protein L35

Chain 2:  97%



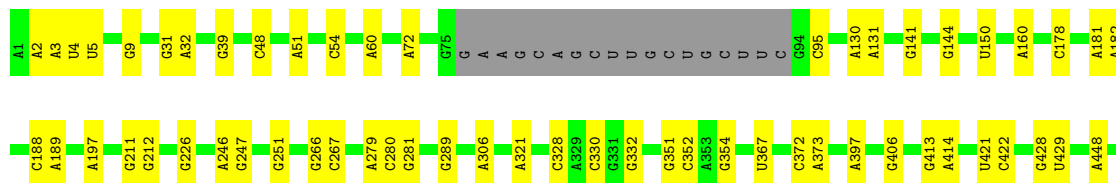
- Molecule 4: 50S ribosomal protein L36

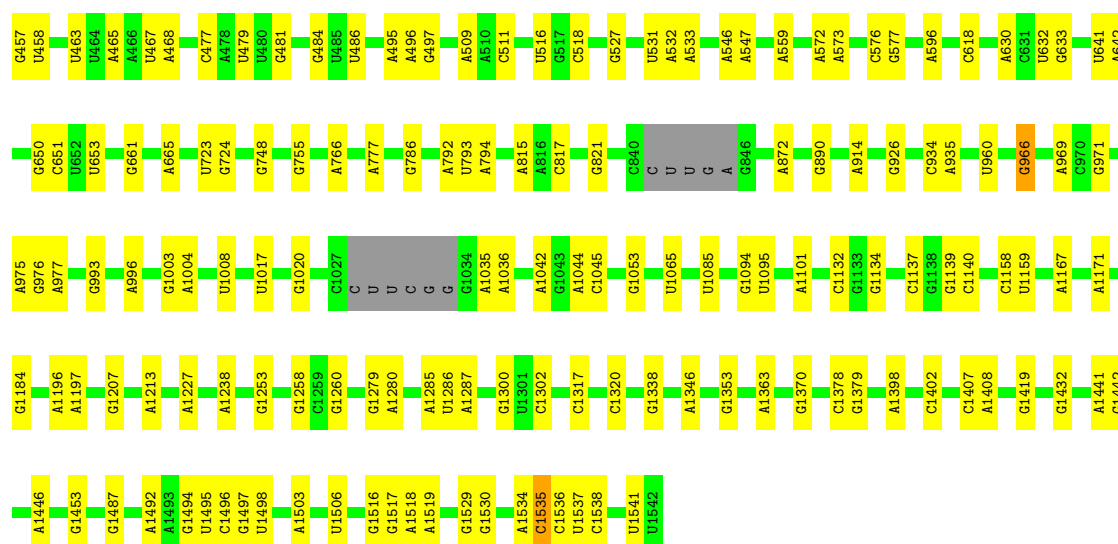
Chain 3:  97%



- Molecule 5: 16S ribosomal RNA

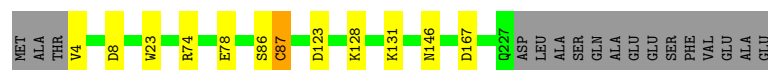
Chain A:  85% 13%





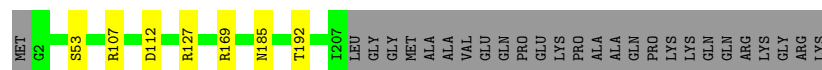
- Molecule 6: Small ribosomal subunit protein uS2

Chain B: 88% 5% 7%



- Molecule 7: Small ribosomal subunit protein uS3

Chain C: 85% 12%



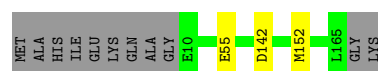
- Molecule 8: Small ribosomal subunit protein uS4

Chain D: 99%



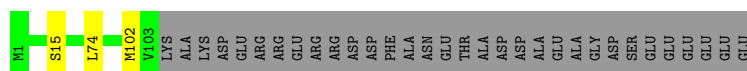
- Molecule 9: Small ribosomal subunit protein uS5

Chain E: 92% 7%



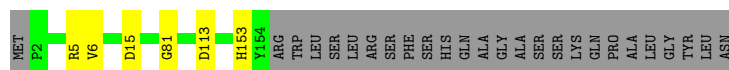
- Molecule 10: Small ribosomal subunit protein bS6, fully modified isoform

Chain F: 74% 24%



- Molecule 11: Small ribosomal subunit protein uS7

Chain G: 82% 15%



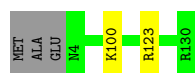
- Molecule 12: Small ribosomal subunit protein uS8

Chain H: 96%



- Molecule 13: Small ribosomal subunit protein uS9

Chain I: 96%



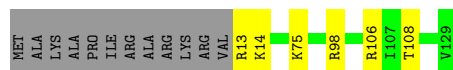
- Molecule 14: Small ribosomal subunit protein uS10

Chain J: 88% 7% 5%



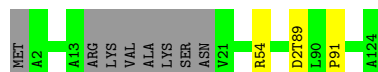
- Molecule 15: Small ribosomal subunit protein uS11

Chain K: 86% 5% 9%



- Molecule 16: Small ribosomal subunit protein uS12

Chain L: 91% 6%



- Molecule 17: Small ribosomal subunit protein uS13

Chain M: 95%



- Molecule 18: Small ribosomal subunit protein uS14

Chain N: 97% ..



- Molecule 19: Small ribosomal subunit protein uS15

Chain O: 98% ..



- Molecule 20: 30S ribosomal protein S16

Chain P: 99% .



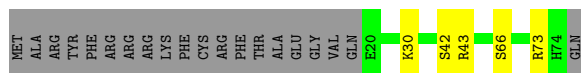
- Molecule 21: Small ribosomal subunit protein uS17

Chain Q: 89% 5% 6%



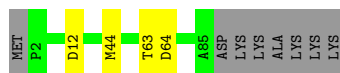
- Molecule 22: Small ribosomal subunit protein bS18

Chain R: 67% 7% 27%



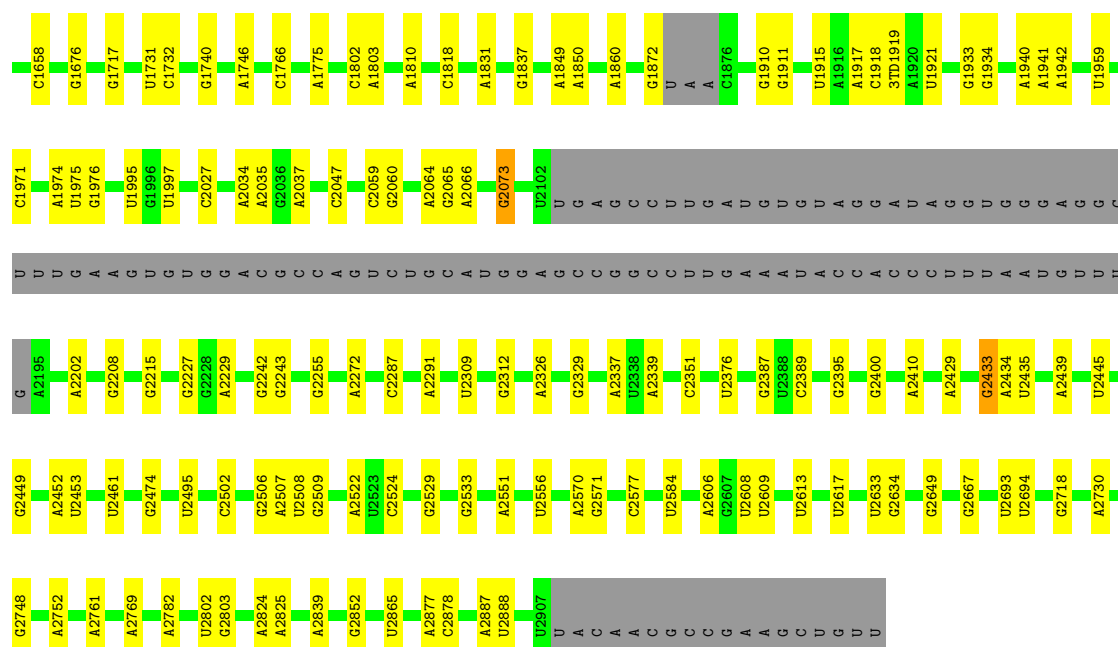
- Molecule 23: 30S ribosomal protein S19

Chain S: 87% . 9%



- Molecule 24: Small ribosomal subunit protein bS20

Chain T: 97% ..



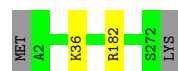
• Molecule 29: 5S ribosomal RNA

Chain b: 92% 8%



• Molecule 30: 50S ribosomal protein L2

Chain c: 99% ..



• Molecule 31: Large ribosomal subunit protein uL3

Chain d: 99% .



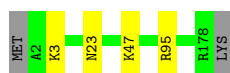
• Molecule 32: 50S ribosomal protein L4

Chain e: 98% .



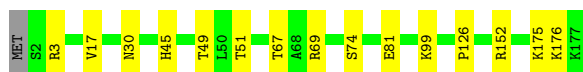
• Molecule 33: 50S ribosomal protein L5

Chain f: 97% ..



- Molecule 34: 50S ribosomal protein L6

Chain g: 91% 8% .



- Molecule 35: 50S ribosomal protein L9

Chain h: 94% 5% .



- Molecule 36: 50S ribosomal protein L13

Chain i: 99% .



- Molecule 37: 50S ribosomal protein L14

Chain j: 98% .



- Molecule 38: 50S ribosomal protein L15

Chain k: 100%

There are no outlier residues recorded for this chain.

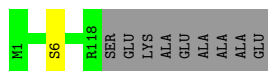
- Molecule 39: 50S ribosomal protein L16

Chain l: 99% .



- Molecule 40: 50S ribosomal protein L17

Chain m: 92% 7% .



- Molecule 41: 50S ribosomal protein L18

Chain n: 97% ..



- Molecule 42: 50S ribosomal protein L19

Chain o: 98% ..



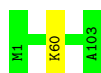
- Molecule 43: 50S ribosomal protein L20

Chain p: 99% .



- Molecule 44: 50S ribosomal protein L21

Chain q: 99% .



- Molecule 45: 50S ribosomal protein L22

Chain r: 99% .



- Molecule 46: 50S ribosomal protein L23

Chain s: 89% . 7%



- Molecule 47: 50S ribosomal protein L24

Chain t: 94% ..



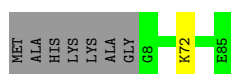
- Molecule 48: 50S ribosomal protein L25

Chain u: 99% .



- Molecule 49: 50S ribosomal protein L27

Chain v: 91% . 8%



- Molecule 50: 50S ribosomal protein L28

Chain w: 96% . .



- Molecule 51: 50S ribosomal protein L29

Chain x: 98% .



- Molecule 52: 50S ribosomal protein L30

Chain y: 98% .



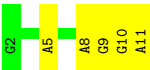
- Molecule 53: 50S ribosomal protein L32

Chain z: 96% . .

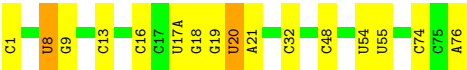
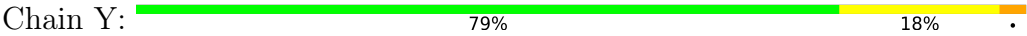


- Molecule 54: mRNA in SD-aSD duplex

Chain 4: 50% 50%



- Molecule 55: tRNA(fmet) P-site



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (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: OMG, 4SU, MA6, 1MG, 7MG, 3TD, 3AU, MG, 5MU, 4D4, G7M, OMC, 5MC, OMU, 4OC, MIA, UR3, PSU, ZN, K, 2MA, MEQ, D2T, H2U, 2MG, 6MZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.37	0/424	0.55	0/565
2	1	0.37	0/380	0.70	0/498
3	2	0.37	0/513	0.57	0/676
4	3	0.37	0/303	0.60	0/397
5	A	0.58	1/36083 (0.0%)	0.80	16/56274 (0.0%)
6	B	0.30	0/1784	0.51	0/2403
7	C	0.32	0/1651	0.53	0/2225
8	D	0.28	0/1665	0.55	0/2227
9	E	0.35	0/1165	0.54	0/1568
10	F	0.35	0/858	0.54	0/1160
11	G	0.29	0/1219	0.53	0/1635
12	H	0.34	0/989	0.50	0/1326
13	I	0.31	0/1034	0.59	0/1375
14	J	0.31	0/796	0.57	0/1077
15	K	0.34	0/893	0.58	0/1205
16	L	0.36	0/904	0.62	0/1211
17	M	0.28	0/900	0.56	0/1204
18	N	0.30	0/817	0.57	0/1088
19	O	0.30	0/722	0.53	0/964
20	P	0.29	0/653	0.64	0/877
21	Q	0.36	0/650	0.55	0/871
22	R	0.37	0/462	0.60	0/621
23	S	0.30	0/685	0.53	0/922
24	T	0.28	0/676	0.50	0/895
25	U	0.30	0/597	0.58	0/792
26	X	0.39	0/301	1.22	5/465 (1.1%)
27	Z	0.35	1/1584 (0.1%)	0.72	0/2463
28	a	0.98	0/65531	0.91	26/102222 (0.0%)
29	b	0.80	0/2850	0.77	0/4444
30	c	0.41	0/2121	0.61	0/2852
31	d	0.39	0/1576	0.56	0/2119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.37	0/1571	0.54	0/2113
33	f	0.33	0/1434	0.52	0/1926
34	g	0.36	0/1343	0.53	0/1816
35	h	0.33	0/1112	0.53	0/1503
36	i	0.40	0/1152	0.54	0/1551
37	j	0.39	0/955	0.62	0/1279
38	k	0.36	0/1062	0.62	0/1413
39	l	0.38	0/1081	0.58	0/1443
40	m	0.37	0/958	0.60	0/1281
41	n	0.36	0/902	0.57	0/1209
42	o	0.40	0/929	0.56	0/1242
43	p	0.39	0/960	0.57	0/1278
44	q	0.41	0/829	0.57	0/1107
45	r	0.35	0/864	0.55	0/1156
46	s	0.38	0/744	0.54	0/994
47	t	0.36	0/787	0.54	0/1051
48	u	0.39	0/766	0.52	0/1025
49	v	0.38	0/593	0.55	0/785
50	w	0.37	0/635	0.60	0/848
51	x	0.30	0/502	0.50	0/667
52	y	0.33	0/453	0.59	0/605
53	z	0.40	0/450	0.65	0/599
54	4	0.29	0/251	0.85	0/391
55	Y	0.38	1/1725 (0.1%)	0.80	0/2687
All	All	0.73	3/152844 (0.0%)	0.80	47/228590 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1407	5MC	O3'-P	20.37	1.85	1.61
55	Y	1	C	OP3-P	-10.62	1.48	1.61
27	Z	1	G	OP3-P	-10.60	1.48	1.61

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1495	U	P-O3'-C3'	15.04	137.74	119.70
5	A	1495	U	OP2-P-O3'	-14.46	73.40	105.20
5	A	1495	U	OP1-P-O3'	9.75	126.66	105.20
5	A	1407	5MC	O3'-P-O5'	8.46	120.08	104.00
28	a	2433	G	P-O3'-C3'	-8.18	109.88	119.70
28	a	12	U	N3-C2-O2	-8.06	116.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	X	21	C	O3'-P-O5'	-7.74	89.30	104.00
28	a	512	G	O4'-C1'-N9	7.38	114.11	108.20
5	A	1407	5MC	P-O3'-C3'	-7.20	111.06	119.70
5	A	1495	U	O3'-P-O5'	6.78	116.88	104.00
26	X	21	C	OP2-P-O3'	6.75	120.04	105.20
28	a	986	A	O4'-C1'-N9	6.71	113.57	108.20
28	a	12	U	C2-N1-C1'	6.64	125.67	117.70
5	A	1407	5MC	OP1-P-O3'	-6.47	90.96	105.20
28	a	1940	A	O4'-C1'-N9	6.46	113.36	108.20
28	a	12	U	N1-C2-O2	6.42	127.29	122.80
5	A	1158	C	C2-N1-C1'	6.38	125.82	118.80
26	X	23	C	C2-N1-C1'	6.35	125.79	118.80
28	a	2852	G	O4'-C1'-N9	6.18	113.15	108.20
5	A	178	C	N1-C2-O2	6.03	122.52	118.90
5	A	178	C	N3-C2-O2	-5.90	117.77	121.90
5	A	872	A	O4'-C1'-N9	5.83	112.86	108.20
28	a	395	U	O4'-C1'-N1	5.80	112.84	108.20
26	X	23	C	C3'-C2'-C1'	-5.79	96.87	101.50
28	a	576	A	O5'-P-OP1	-5.74	100.53	105.70
28	a	1326	G	O4'-C1'-N9	5.74	112.79	108.20
28	a	792	U	C5-C6-N1	-5.71	119.85	122.70
28	a	750	G	O4'-C1'-N9	5.70	112.76	108.20
28	a	554	U	N3-C2-O2	-5.66	118.24	122.20
28	a	2649	G	O4'-C1'-N9	5.52	112.62	108.20
28	a	1658	C	C6-N1-C2	-5.50	118.10	120.30
5	A	792	A	O4'-C1'-N9	5.47	112.58	108.20
28	a	205	G	O4'-C1'-N9	5.47	112.57	108.20
28	a	1313	G	O4'-C1'-N9	5.39	112.51	108.20
5	A	1158	C	N1-C2-O2	5.39	122.14	118.90
5	A	477	C	N3-C2-O2	-5.33	118.17	121.90
28	a	177	G	O4'-C1'-N9	5.32	112.46	108.20
28	a	2395	G	O4'-C1'-N9	5.32	112.45	108.20
28	a	329	G	O5'-P-OP2	-5.30	100.93	105.70
28	a	2433	G	OP2-P-O3'	5.25	116.76	105.20
28	a	786	G	P-O3'-C3'	5.25	126.00	119.70
28	a	512	G	C1'-O4'-C4'	-5.25	105.70	109.90
5	A	1535	C	OP2-P-O3'	5.13	116.49	105.20
28	a	370	G	O4'-C1'-N9	-5.11	104.11	108.20
26	X	21	C	P-O3'-C3'	5.05	125.76	119.70
28	a	12	U	C6-N1-C2	-5.04	117.97	121.00
5	A	1535	C	P-O3'-C3'	5.03	125.74	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
6	B	222/241 (92%)	210 (95%)	9 (4%)	3 (1%)	9	38
7	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
8	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
9	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
10	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
11	G	151/179 (84%)	136 (90%)	13 (9%)	2 (1%)	10	39
12	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
13	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
14	J	96/103 (93%)	88 (92%)	7 (7%)	1 (1%)	13	45
15	K	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
16	L	111/124 (90%)	107 (96%)	3 (3%)	1 (1%)	14	47
17	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
18	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
19	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
20	P	79/82 (96%)	73 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Q	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
22	R	53/75 (71%)	51 (96%)	1 (2%)	1 (2%)	6	31
23	S	82/92 (89%)	74 (90%)	8 (10%)	0	100	100
24	T	84/87 (97%)	84 (100%)	0	0	100	100
25	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
30	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
31	d	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
32	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
33	f	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
34	g	174/177 (98%)	160 (92%)	13 (8%)	1 (1%)	22	55
35	h	146/149 (98%)	134 (92%)	10 (7%)	2 (1%)	9	38
36	i	140/142 (99%)	140 (100%)	0	0	100	100
37	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
38	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
39	l	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
40	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
41	n	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
42	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
43	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
44	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
45	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
46	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
47	t	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	13	45
48	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
49	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
50	w	75/78 (96%)	75 (100%)	0	0	100	100
51	x	60/63 (95%)	60 (100%)	0	0	100	100
52	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
53	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5515/5843 (94%)	5313 (96%)	190 (3%)	12 (0%)	45	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	87	CYS
6	B	131	LYS
11	G	81	GLY
14	J	57	VAL
34	g	126	PRO
6	B	86	SER
35	h	42	LYS
35	h	76	GLU
11	G	153	HIS
22	R	73	ARG
47	t	39	ILE
16	L	91	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	0	46/49 (94%)	44 (96%)	2 (4%)	25	54
2	1	38/38 (100%)	37 (97%)	1 (3%)	41	68
3	2	51/52 (98%)	50 (98%)	1 (2%)	50	73
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	65
6	B	186/199 (94%)	176 (95%)	10 (5%)	18	48
7	C	170/190 (90%)	163 (96%)	7 (4%)	26	56
8	D	172/173 (99%)	171 (99%)	1 (1%)	84	92
9	E	119/126 (94%)	116 (98%)	3 (2%)	42	68
10	F	90/116 (78%)	87 (97%)	3 (3%)	33	62
11	G	126/147 (86%)	122 (97%)	4 (3%)	34	63
12	H	104/105 (99%)	100 (96%)	4 (4%)	28	58
13	I	105/107 (98%)	103 (98%)	2 (2%)	52	74
14	J	86/90 (96%)	80 (93%)	6 (7%)	12	39
15	K	90/99 (91%)	84 (93%)	6 (7%)	13	41
16	L	96/103 (93%)	95 (99%)	1 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	M	93/96 (97%)	90 (97%)	3 (3%)	34	63
18	N	83/84 (99%)	81 (98%)	2 (2%)	44	69
19	O	76/77 (99%)	75 (99%)	1 (1%)	65	82
20	P	65/65 (100%)	65 (100%)	0	100	100
21	Q	73/78 (94%)	69 (94%)	4 (6%)	18	47
22	R	48/65 (74%)	44 (92%)	4 (8%)	9	32
23	S	72/79 (91%)	68 (94%)	4 (6%)	17	47
24	T	65/66 (98%)	63 (97%)	2 (3%)	35	63
25	U	60/61 (98%)	57 (95%)	3 (5%)	20	50
30	c	216/218 (99%)	214 (99%)	2 (1%)	75	88
31	d	163/163 (100%)	160 (98%)	3 (2%)	54	75
32	e	165/165 (100%)	160 (97%)	5 (3%)	36	64
33	f	148/150 (99%)	144 (97%)	4 (3%)	40	67
34	g	137/138 (99%)	123 (90%)	14 (10%)	6	23
35	h	113/114 (99%)	107 (95%)	6 (5%)	19	48
36	i	116/116 (100%)	114 (98%)	2 (2%)	56	77
37	j	104/104 (100%)	102 (98%)	2 (2%)	52	74
38	k	103/103 (100%)	103 (100%)	0	100	100
39	l	108/108 (100%)	107 (99%)	1 (1%)	75	88
40	m	98/103 (95%)	97 (99%)	1 (1%)	73	86
41	n	86/87 (99%)	83 (96%)	3 (4%)	31	60
42	o	99/100 (99%)	98 (99%)	1 (1%)	73	86
43	p	89/90 (99%)	89 (100%)	0	100	100
44	q	84/84 (100%)	83 (99%)	1 (1%)	67	83
45	r	93/93 (100%)	92 (99%)	1 (1%)	70	84
46	s	80/84 (95%)	76 (95%)	4 (5%)	20	50
47	t	83/85 (98%)	80 (96%)	3 (4%)	30	59
48	u	78/78 (100%)	77 (99%)	1 (1%)	65	82
49	v	58/63 (92%)	57 (98%)	1 (2%)	56	77
50	w	67/68 (98%)	65 (97%)	2 (3%)	36	64
51	x	54/55 (98%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	y	48/49 (98%)	48 (100%)	0	100	100
53	z	47/48 (98%)	46 (98%)	1 (2%)	48	72
All	All	4585/4765 (96%)	4452 (97%)	133 (3%)	39	65

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	ARG
1	0	33	LYS
2	1	25	LYS
3	2	31	HIS
4	3	36	ARG
6	B	4	VAL
6	B	8	ASP
6	B	23	TRP
6	B	74	ARG
6	B	78	GLU
6	B	87	CYS
6	B	123	ASP
6	B	128	LYS
6	B	146	ASN
6	B	167	ASP
7	C	53	SER
7	C	107	ARG
7	C	112	ASP
7	C	127	ARG
7	C	169	ARG
7	C	185	ASN
7	C	192	THR
8	D	151	LYS
9	E	55	GLU
9	E	142	ASP
9	E	152	MET
10	F	15	SER
10	F	74	LEU
10	F	102	MET
11	G	5	ARG
11	G	6	VAL
11	G	15	ASP
11	G	113	ASP
12	H	54	ASP

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Mol	Chain	Res	Type
12	H	89	LYS
12	H	90	ASP
12	H	117	ARG
13	I	100	LYS
13	I	123	ARG
14	J	30	LYS
14	J	40	ILE
14	J	48	ARG
14	J	66	GLU
14	J	75	ASP
14	J	89	ARG
15	K	13	ARG
15	K	14	LYS
15	K	75	LYS
15	K	98	ARG
15	K	106	ARG
15	K	108	THR
16	L	54	ARG
17	M	31	LYS
17	M	83	LEU
17	M	90	ARG
18	N	49	GLN
18	N	55	SER
19	O	83	GLU
21	Q	40	ARG
21	Q	42	THR
21	Q	60	GLU
21	Q	77	ARG
22	R	30	LYS
22	R	42	SER
22	R	43	ARG
22	R	66	SER
23	S	12	ASP
23	S	44	MET
23	S	63	THR
23	S	64	ASP
24	T	23	SER
24	T	24	ARG
25	U	7	ARG
25	U	29	LEU
25	U	66	ARG
30	c	36	LYS

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Mol	Chain	Res	Type
30	c	182	ARG
31	d	1	MET
31	d	32	ASN
31	d	208	LYS
32	e	55	SER
32	e	107	SER
32	e	165	HIS
32	e	198	GLU
32	e	199	MET
33	f	3	LYS
33	f	23	ASN
33	f	47	LYS
33	f	95	ARG
34	g	3	ARG
34	g	17	VAL
34	g	30	ASN
34	g	45	HIS
34	g	49	THR
34	g	51	THR
34	g	67	THR
34	g	69	ARG
34	g	74	SER
34	g	81	GLU
34	g	99	LYS
34	g	152	ARG
34	g	175	LYS
34	g	176	LYS
35	h	43	ASN
35	h	57	LYS
35	h	83	LYS
35	h	116	ARG
35	h	134	VAL
35	h	142	VAL
36	i	11	VAL
36	i	96	ARG
37	j	105	ARG
37	j	113	MET
39	l	6	ARG
40	m	6	SER
41	n	13	ARG
41	n	68	LYS
41	n	88	LYS

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Mol	Chain	Res	Type
42	o	53	ARG
44	q	60	LYS
45	r	109	ASP
46	s	3	ARG
46	s	24	MET
46	s	25	GLU
46	s	27	SER
47	t	15	THR
47	t	52	LEU
47	t	100	SER
48	u	1	MET
49	v	72	LYS
50	w	42	SER
50	w	45	ARG
53	z	57	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
8	D	59	GLN
8	D	120	HIS
9	E	89	HIS
20	P	18	GLN
23	S	14	HIS
24	T	70	ASN
24	T	82	GLN
30	c	153	GLN
30	c	226	ASN
33	f	37	ASN
34	g	38	ASN
35	h	66	ASN
36	i	76	HIS
38	k	104	GLN
46	s	59	ASN
47	t	45	HIS
47	t	54	GLN
50	w	36	HIS
52	y	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	X	12/16 (75%)	5 (41%)	0
27	Z	73/76 (96%)	12 (16%)	1 (1%)
28	a	2738/2925 (93%)	257 (9%)	0
29	b	118/119 (99%)	10 (8%)	0
5	A	1505/1542 (97%)	191 (12%)	5 (0%)
54	4	9/10 (90%)	5 (55%)	0
55	Y	76/77 (98%)	12 (15%)	0
All	All	4531/4765 (95%)	492 (10%)	6 (0%)

All (492) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	2	A
5	A	3	A
5	A	4	U
5	A	5	U
5	A	9	G
5	A	31	G
5	A	32	A
5	A	39	G
5	A	48	C
5	A	51	A
5	A	54	C
5	A	60	A
5	A	72	A
5	A	95	C
5	A	130	A
5	A	131	A
5	A	141	G
5	A	144	G
5	A	150	U
5	A	160	A
5	A	181	A
5	A	182	A
5	A	188	C
5	A	189	A
5	A	197	A
5	A	211	G
5	A	212	G
5	A	226	G
5	A	246	A
5	A	247	G
5	A	251	G

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Mol	Chain	Res	Type
5	A	266	G
5	A	267	C
5	A	279	A
5	A	280	C
5	A	281	G
5	A	289	G
5	A	306	A
5	A	321	A
5	A	328	C
5	A	330	C
5	A	332	G
5	A	351	G
5	A	352	C
5	A	354	G
5	A	367	U
5	A	372	C
5	A	373	A
5	A	397	A
5	A	406	G
5	A	413	G
5	A	414	A
5	A	421	U
5	A	422	C
5	A	428	G
5	A	429	U
5	A	448	A
5	A	457	G
5	A	458	U
5	A	463	U
5	A	465	A
5	A	467	U
5	A	468	A
5	A	479	U
5	A	481	G
5	A	484	G
5	A	486	U
5	A	495	A
5	A	496	A
5	A	497	G
5	A	509	A
5	A	511	C
5	A	518	C

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Mol	Chain	Res	Type
5	A	531	U
5	A	532	A
5	A	533	A
5	A	546	A
5	A	547	A
5	A	559	A
5	A	572	A
5	A	573	A
5	A	576	C
5	A	577	G
5	A	596	A
5	A	618	C
5	A	630	A
5	A	632	U
5	A	633	G
5	A	642	A
5	A	650	G
5	A	651	C
5	A	653	U
5	A	661	G
5	A	665	A
5	A	723	U
5	A	724	G
5	A	748	G
5	A	755	G
5	A	777	A
5	A	793	U
5	A	794	A
5	A	815	A
5	A	817	C
5	A	821	G
5	A	890	G
5	A	914	A
5	A	926	G
5	A	934	C
5	A	935	A
5	A	960	U
5	A	966	2MG
5	A	969	A
5	A	971	G
5	A	975	A
5	A	976	G

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Mol	Chain	Res	Type
5	A	977	A
5	A	993	G
5	A	996	A
5	A	1003	G
5	A	1004	A
5	A	1008	U
5	A	1017	U
5	A	1020	G
5	A	1035	A
5	A	1036	A
5	A	1042	A
5	A	1044	A
5	A	1045	C
5	A	1053	G
5	A	1065	U
5	A	1085	U
5	A	1094	G
5	A	1095	U
5	A	1101	A
5	A	1132	C
5	A	1134	G
5	A	1137	C
5	A	1139	G
5	A	1140	C
5	A	1159	U
5	A	1167	A
5	A	1171	A
5	A	1184	G
5	A	1196	A
5	A	1197	A
5	A	1213	A
5	A	1227	A
5	A	1238	A
5	A	1253	G
5	A	1258	G
5	A	1260	G
5	A	1279	G
5	A	1280	A
5	A	1285	A
5	A	1286	U
5	A	1287	A
5	A	1300	G

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Mol	Chain	Res	Type
5	A	1302	C
5	A	1317	C
5	A	1320	C
5	A	1338	G
5	A	1346	A
5	A	1353	G
5	A	1363	A
5	A	1370	G
5	A	1378	C
5	A	1379	G
5	A	1398	A
5	A	1408	A
5	A	1419	G
5	A	1432	G
5	A	1441	A
5	A	1442	G
5	A	1446	A
5	A	1453	G
5	A	1487	G
5	A	1492	A
5	A	1494	G
5	A	1496	C
5	A	1497	G
5	A	1503	A
5	A	1506	U
5	A	1517	G
5	A	1529	G
5	A	1530	G
5	A	1534	A
5	A	1535	C
5	A	1536	C
5	A	1537	U
5	A	1538	C
5	A	1541	U
26	X	13	U
26	X	16	A
26	X	22	A
26	X	23	C
26	X	24	A
27	Z	8	4SU
27	Z	9	A
27	Z	16	H2U

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Mol	Chain	Res	Type
27	Z	17	C
27	Z	19	G
27	Z	20	H2U
27	Z	22	G
27	Z	44	G
27	Z	46	7MG
27	Z	48	C
27	Z	70	G
27	Z	74	C
28	a	10	A
28	a	15	G
28	a	34	U
28	a	42	A
28	a	71	A
28	a	74	A
28	a	75	G
28	a	101	A
28	a	102	U
28	a	118	A
28	a	119	A
28	a	120	U
28	a	125	A
28	a	136	G
28	a	139	U
28	a	140	C
28	a	142	A
28	a	163	C
28	a	165	A
28	a	181	A
28	a	196	A
28	a	215	G
28	a	216	A
28	a	221	A
28	a	222	A
28	a	248	G
28	a	272	A
28	a	276	U
28	a	277	G
28	a	278	A
28	a	279	A
28	a	281	C
28	a	287	G

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Mol	Chain	Res	Type
28	a	311	A
28	a	329	G
28	a	330	A
28	a	345	A
28	a	361	G
28	a	367	G
28	a	386	G
28	a	405	U
28	a	411	G
28	a	412	A
28	a	481	G
28	a	491	G
28	a	505	A
28	a	509	C
28	a	530	G
28	a	531	C
28	a	532	A
28	a	565	A
28	a	575	U
28	a	577	A
28	a	605	A
28	a	617	U
28	a	629	A
28	a	639	A
28	a	647	C
28	a	648	U
28	a	649	G
28	a	655	U
28	a	656	A
28	a	657	A
28	a	688	U
28	a	719	C
28	a	732	A
28	a	749	5MU
28	a	766	A
28	a	777	G
28	a	778	G
28	a	784	A
28	a	786	G
28	a	787	G
28	a	807	G
28	a	814	C

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Mol	Chain	Res	Type
28	a	829	U
28	a	830	U
28	a	848	U
28	a	861	G
28	a	884	G
28	a	886	U
28	a	887	C
28	a	890	C
28	a	892	C
28	a	893	G
28	a	897	U
28	a	898	A
28	a	899	C
28	a	901	A
28	a	912	A
28	a	916	G
28	a	933	U
28	a	948	C
28	a	963	C
28	a	976	G
28	a	985	A
28	a	998	A
28	a	1014	U
28	a	1015	C
28	a	1024	G
28	a	1035	U
28	a	1042	A
28	a	1049	G
28	a	1110	U
28	a	1112	G
28	a	1113	A
28	a	1114	G
28	a	1118	G
28	a	1124	G
28	a	1134	U
28	a	1137	C
28	a	1144	A
28	a	1173	G
28	a	1255	A
28	a	1258	G
28	a	1273	G
28	a	1274	A

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Mol	Chain	Res	Type
28	a	1302	G
28	a	1303	A
28	a	1354	U
28	a	1367	A
28	a	1381	U
28	a	1385	A
28	a	1413	U
28	a	1418	G
28	a	1430	C
28	a	1436	A
28	a	1454	G
28	a	1455	A
28	a	1484	G
28	a	1495	C
28	a	1510	A
28	a	1511	A
28	a	1512	G
28	a	1517	A
28	a	1531	G
28	a	1536	U
28	a	1537	A
28	a	1538	C
28	a	1539	G
28	a	1568	A
28	a	1571	A
28	a	1580	U
28	a	1585	A
28	a	1587	C
28	a	1610	A
28	a	1649	U
28	a	1650	U
28	a	1651	G
28	a	1676	G
28	a	1717	G
28	a	1731	U
28	a	1732	C
28	a	1740	G
28	a	1746	A
28	a	1766	C
28	a	1775	A
28	a	1802	C
28	a	1803	A

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Mol	Chain	Res	Type
28	a	1810	A
28	a	1818	C
28	a	1831	A
28	a	1849	A
28	a	1850	A
28	a	1860	A
28	a	1872	G
28	a	1910	G
28	a	1911	G
28	a	1917	A
28	a	1918	C
28	a	1933	G
28	a	1934	G
28	a	1941	A
28	a	1942	A
28	a	1959	U
28	a	1971	C
28	a	1974	A
28	a	1975	U
28	a	1976	G
28	a	1995	U
28	a	1997	U
28	a	2027	C
28	a	2035	A
28	a	2037	A
28	a	2047	C
28	a	2059	C
28	a	2060	G
28	a	2064	A
28	a	2065	G
28	a	2066	A
28	a	2073	G7M
28	a	2202	A
28	a	2208	G
28	a	2215	G
28	a	2227	G
28	a	2229	A
28	a	2242	G
28	a	2243	G
28	a	2272	A
28	a	2287	C
28	a	2291	A

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Mol	Chain	Res	Type
28	a	2309	U
28	a	2312	G
28	a	2326	A
28	a	2329	G
28	a	2337	A
28	a	2339	A
28	a	2351	C
28	a	2376	U
28	a	2387	G
28	a	2389	C
28	a	2400	G
28	a	2410	A
28	a	2429	A
28	a	2433	G
28	a	2434	A
28	a	2435	U
28	a	2439	A
28	a	2445	U
28	a	2452	A
28	a	2474	G
28	a	2495	U
28	a	2506	G
28	a	2509	G
28	a	2522	A
28	a	2524	C
28	a	2529	G
28	a	2533	G
28	a	2551	A
28	a	2570	A
28	a	2571	G
28	a	2577	C
28	a	2606	A
28	a	2613	U
28	a	2617	U
28	a	2633	U
28	a	2634	G
28	a	2667	G
28	a	2693	U
28	a	2694	U
28	a	2718	G
28	a	2730	A
28	a	2748	G

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Mol	Chain	Res	Type
28	a	2752	A
28	a	2761	A
28	a	2769	A
28	a	2782	A
28	a	2802	U
28	a	2803	G
28	a	2824	A
28	a	2825	A
28	a	2839	A
28	a	2865	U
28	a	2877	A
28	a	2878	C
28	a	2887	A
28	a	2888	U
29	b	35	C
29	b	36	C
29	b	45	A
29	b	56	G
29	b	57	A
29	b	67	G
29	b	89	U
29	b	90	C
29	b	99	A
29	b	109	A
54	4	5	A
54	4	8	A
54	4	9	G
54	4	10	G
54	4	11	A
55	Y	8	4SU
55	Y	9	G
55	Y	13	C
55	Y	16	C
55	Y	17(A)	U
55	Y	18	G
55	Y	19	G
55	Y	20	H2U
55	Y	21	A
55	Y	48	C
55	Y	74	C
55	Y	76	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	641	U
5	A	766	A
5	A	786	G
5	A	1035	A
5	A	1535	C
27	Z	19	G

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

53 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
28	PSU	a	957	28	18,21,22	1.07	1 (5%)	22,30,33	1.79	2 (9%)
27	3AU	Z	47	27	18,21,29	3.38	8 (44%)	26,30,43	1.64	5 (19%)
27	PSU	Z	55	27	18,21,22	1.10	1 (5%)	22,30,33	1.81	5 (22%)
55	H2U	Y	20	55	18,21,22	3.11	5 (27%)	21,30,33	1.96	5 (23%)
5	UR3	A	1498	5	19,22,23	2.57	6 (31%)	26,32,35	1.38	3 (11%)
28	1MG	a	747	28	18,26,27	2.52	5 (27%)	19,39,42	1.16	2 (10%)
55	PSU	Y	55	55	18,21,22	1.12	1 (5%)	22,30,33	1.76	4 (18%)
28	PSU	a	2461	28	18,21,22	1.09	1 (5%)	22,30,33	1.84	4 (18%)
28	6MZ	a	1620	28	18,25,26	2.12	3 (16%)	16,36,39	2.21	4 (25%)
28	PSU	a	1915	28	18,21,22	1.01	1 (5%)	22,30,33	1.78	3 (13%)
28	5MC	a	1966	28,57	18,22,23	0.81	0	26,32,35	0.53	0
28	6MZ	a	2034	28	18,25,26	2.08	5 (27%)	16,36,39	2.18	4 (25%)
28	OMC	a	2502	28,58	19,22,23	0.81	1 (5%)	26,31,34	0.66	0
28	2MA	a	2507	28,58,57	19,25,26	3.17	8 (42%)	21,37,40	2.64	4 (19%)
5	MA6	A	1518	5	18,26,27	1.01	1 (5%)	19,38,41	2.66	3 (15%)
55	5MU	Y	54	55	19,22,23	1.39	5 (26%)	28,32,35	2.07	6 (21%)
28	H2U	a	2453	28	18,21,22	0.64	0	21,30,33	1.07	3 (14%)
16	D2T	L	89	16	7,9,10	1.36	1 (14%)	6,11,13	1.79	2 (33%)
28	2MG	a	1837	28	18,26,27	1.36	3 (16%)	16,38,41	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PSU	a	2508	28,57	18,21,22	1.03	1 (5%)	22,30,33	1.87	4 (18%)
5	2MG	A	1207	5,57	18,26,27	1.20	3 (16%)	16,38,41	0.92	1 (6%)
5	PSU	A	516	5	18,21,22	0.99	1 (5%)	22,30,33	1.71	5 (22%)
27	MIA	Z	37	27	18,24,32	1.53	3 (16%)	18,35,47	1.54	3 (16%)
27	4SU	Z	8	27	18,21,22	4.19	8 (44%)	26,30,33	2.25	4 (15%)
28	OMG	a	2255	28,55,57	18,26,27	1.31	3 (16%)	19,38,41	0.80	1 (5%)
5	2MG	A	1516	5	18,26,27	1.33	3 (16%)	16,38,41	0.90	1 (6%)
5	5MC	A	1407	5	18,22,23	0.83	1 (5%)	26,32,35	0.58	0
5	G7M	A	527	5	20,26,27	2.42	7 (35%)	17,39,42	1.14	1 (5%)
5	2MG	A	966	5	18,26,27	1.26	3 (16%)	16,38,41	0.84	0
28	PSU	a	748	28,58	18,21,22	1.10	2 (11%)	22,30,33	1.60	3 (13%)
28	PSU	a	2584	28	18,21,22	1.07	2 (11%)	22,30,33	1.77	3 (13%)
27	H2U	Z	16	27	18,21,22	3.06	5 (27%)	21,30,33	2.09	5 (23%)
28	3TD	a	1919	28	18,22,23	4.02	7 (38%)	22,32,35	1.79	3 (13%)
27	PSU	Z	32	27	18,21,22	1.06	1 (5%)	22,30,33	1.77	5 (22%)
28	PSU	a	2608	28	18,21,22	1.06	1 (5%)	22,30,33	1.85	3 (13%)
28	PSU	a	2609	28	18,21,22	1.08	1 (5%)	22,30,33	1.89	4 (18%)
39	4D4	l	81	39	9,11,12	0.54	0	8,13,15	1.03	1 (12%)
27	PSU	Z	39	27	18,21,22	1.05	1 (5%)	22,30,33	1.80	5 (22%)
55	4SU	Y	8	55	18,21,22	4.19	8 (44%)	26,30,33	2.26	5 (19%)
5	MA6	A	1519	5	18,26,27	1.04	1 (5%)	19,38,41	2.77	3 (15%)
28	OMU	a	2556	28,58,57	19,22,23	3.07	7 (36%)	26,31,34	1.66	4 (15%)
28	PSU	a	1921	28	18,21,22	1.04	1 (5%)	22,30,33	1.84	4 (18%)
5	4OC	A	1402	5	20,23,24	2.98	8 (40%)	26,32,35	0.94	1 (3%)
28	G7M	a	2073	28,57	20,26,27	2.45	7 (35%)	17,39,42	1.12	2 (11%)
27	7MG	Z	46	27	20,25,27	3.36	10 (50%)	27,37,42	2.11	8 (29%)
27	5MU	Z	54	27	19,22,23	1.38	5 (26%)	28,32,35	2.09	6 (21%)
28	2MG	a	2449	28	18,26,27	1.46	3 (16%)	16,38,41	0.66	0
28	5MU	a	749	28	19,22,23	0.72	0	28,32,35	0.56	0
28	5MU	a	1943	28,57	19,22,23	0.81	0	28,32,35	0.46	0
27	H2U	Z	20	27	18,21,22	3.13	5 (27%)	21,30,33	1.99	5 (23%)
5	5MC	A	967	5	18,22,23	0.76	0	26,32,35	0.61	0
55	OMC	Y	32	55	19,22,23	3.01	8 (42%)	26,31,34	0.90	2 (7%)
31	MEQ	d	150	31	8,9,10	0.82	0	5,10,12	0.76	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
28	PSU	a	957	28	-	0/7/25/26	0/2/2/2
27	3AU	Z	47	27	-	2/7/25/35	0/2/2/2
27	PSU	Z	55	27	-	0/7/25/26	0/2/2/2
55	H2U	Y	20	55	-	7/7/38/39	0/2/2/2
5	UR3	A	1498	5	-	0/7/25/26	0/2/2/2
28	1MG	a	747	28	-	0/3/25/26	0/3/3/3
55	PSU	Y	55	55	-	0/7/25/26	0/2/2/2
28	PSU	a	2461	28	-	0/7/25/26	0/2/2/2
28	6MZ	a	1620	28	-	0/5/27/28	0/3/3/3
28	PSU	a	1915	28	-	0/7/25/26	0/2/2/2
28	5MC	a	1966	28,57	-	0/7/25/26	0/2/2/2
28	6MZ	a	2034	28	-	2/5/27/28	0/3/3/3
28	OMC	a	2502	28,58	-	0/9/27/28	0/2/2/2
28	2MA	a	2507	28,58,57	-	2/3/25/26	0/3/3/3
5	MA6	A	1518	5	-	0/7/29/30	0/3/3/3
55	5MU	Y	54	55	-	0/7/25/26	0/2/2/2
28	H2U	a	2453	28	-	0/7/38/39	0/2/2/2
16	D2T	L	89	16	-	3/7/12/14	-
28	2MG	a	1837	28	-	0/5/27/28	0/3/3/3
28	PSU	a	2508	28,57	-	0/7/25/26	0/2/2/2
5	2MG	A	1207	5,57	-	0/5/27/28	0/3/3/3
5	PSU	A	516	5	-	0/7/25/26	0/2/2/2
27	MIA	Z	37	27	-	0/3/25/34	0/3/3/3
27	4SU	Z	8	27	-	2/7/25/26	0/2/2/2
28	OMG	a	2255	28,55,57	-	1/5/27/28	0/3/3/3
5	2MG	A	1516	5	-	0/5/27/28	0/3/3/3
5	5MC	A	1407	5	-	0/7/25/26	0/2/2/2
5	G7M	A	527	5	-	0/3/25/26	0/3/3/3
5	2MG	A	966	5	-	0/5/27/28	0/3/3/3
28	PSU	a	748	28,58	-	1/7/25/26	0/2/2/2
28	PSU	a	2584	28	-	0/7/25/26	0/2/2/2
27	H2U	Z	16	27	-	0/7/38/39	0/2/2/2
28	3TD	a	1919	28	-	2/7/25/26	0/2/2/2
27	PSU	Z	32	27	-	0/7/25/26	0/2/2/2
28	PSU	a	2608	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2609	28	-	0/7/25/26	0/2/2/2
39	4D4	l	81	39	-	6/11/12/14	-
27	PSU	Z	39	27	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	4SU	Y	8	55	-	2/7/25/26	0/2/2/2
5	MA6	A	1519	5	-	3/7/29/30	0/3/3/3
28	OMU	a	2556	28,58,57	-	0/9/27/28	0/2/2/2
28	PSU	a	1921	28	-	0/7/25/26	0/2/2/2
5	4OC	A	1402	5	-	0/9/29/30	0/2/2/2
28	G7M	a	2073	28,57	-	2/3/25/26	0/3/3/3
27	7MG	Z	46	27	-	2/7/34/38	0/3/3/3
27	5MU	Z	54	27	-	0/7/25/26	0/2/2/2
28	2MG	a	2449	28	-	0/5/27/28	0/3/3/3
28	5MU	a	749	28	-	0/7/25/26	0/2/2/2
28	5MU	a	1943	28,57	-	0/7/25/26	0/2/2/2
27	H2U	Z	20	27	-	2/7/38/39	0/2/2/2
5	5MC	A	967	5	-	0/7/25/26	0/2/2/2
55	OMC	Y	32	55	-	3/9/27/28	0/2/2/2
31	MEQ	d	150	31	-	2/8/9/11	-

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1919	3TD	C6-C5	12.08	1.49	1.35
27	Z	20	H2U	C2-N1	9.70	1.49	1.35
55	Y	20	H2U	C2-N1	9.65	1.49	1.35
55	Y	8	4SU	C4-N3	9.58	1.47	1.37
27	Z	8	4SU	C4-N3	9.41	1.47	1.37
27	Z	16	H2U	C2-N1	9.37	1.49	1.35
28	a	1919	3TD	C2-N1	8.61	1.48	1.37
27	Z	8	4SU	C2-N1	7.99	1.51	1.38
55	Y	8	4SU	C2-N1	7.73	1.50	1.38
28	a	2507	2MA	C4-N3	7.57	1.47	1.35
27	Z	47	3AU	C2-N1	7.32	1.50	1.38
28	a	1620	6MZ	C6-N6	7.20	1.46	1.35
27	Z	47	3AU	C6-C5	6.98	1.51	1.35
28	a	2034	6MZ	C6-N6	6.88	1.46	1.35
27	Z	8	4SU	C2-N3	6.66	1.49	1.38
55	Y	8	4SU	C2-N3	6.58	1.49	1.38
27	Z	20	H2U	C2-N3	6.52	1.49	1.38
55	Y	20	H2U	C2-N3	6.50	1.49	1.38
27	Z	47	3AU	C2-N3	6.50	1.49	1.38
27	Z	16	H2U	C2-N3	6.48	1.49	1.38
55	Y	32	OMC	C2-N3	6.43	1.49	1.36
5	A	1402	4OC	C4-N3	6.31	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1498	UR3	C2-N1	6.29	1.47	1.38
28	a	2507	2MA	C2-N3	6.27	1.45	1.34
28	a	2556	OMU	C2-N3	6.26	1.49	1.38
28	a	747	1MG	C2-N3	6.16	1.45	1.34
27	Z	8	4SU	C6-C5	6.05	1.49	1.35
55	Y	8	4SU	C6-C5	6.05	1.49	1.35
27	Z	46	7MG	C2-N3	6.05	1.47	1.33
5	A	1402	4OC	C6-C5	6.04	1.49	1.35
27	Z	46	7MG	C4-N3	5.97	1.48	1.34
28	a	2073	G7M	C2-N2	5.94	1.48	1.34
55	Y	32	OMC	C6-C5	5.91	1.48	1.35
28	a	2556	OMU	C2-N1	5.90	1.47	1.38
28	a	747	1MG	C2-N2	5.88	1.44	1.34
28	a	2507	2MA	C2-N1	5.84	1.44	1.34
5	A	1498	UR3	C6-C5	5.75	1.48	1.35
55	Y	8	4SU	C5-C4	5.71	1.49	1.42
27	Z	8	4SU	C5-C4	5.68	1.49	1.42
27	Z	46	7MG	C4-N9	5.66	1.44	1.37
5	A	1402	4OC	C2-N3	5.66	1.47	1.36
28	a	2507	2MA	C6-N1	5.65	1.44	1.33
28	a	1919	3TD	C6-N1	5.44	1.45	1.36
55	Y	8	4SU	C4-S4	-5.41	1.58	1.68
5	A	527	G7M	C2-N3	5.39	1.46	1.33
27	Z	8	4SU	C4-S4	-5.33	1.58	1.68
55	Y	32	OMC	C4-N3	5.25	1.45	1.34
28	a	2556	OMU	C6-C5	5.24	1.47	1.35
27	Z	47	3AU	C4-N3	5.19	1.47	1.38
28	a	2556	OMU	O4-C4	-5.18	1.14	1.24
27	Z	20	H2U	C4-N3	5.03	1.46	1.37
27	Z	16	H2U	C4-N3	4.95	1.46	1.37
5	A	527	G7M	C4-N3	4.92	1.49	1.37
55	Y	20	H2U	C4-N3	4.91	1.46	1.37
27	Z	46	7MG	C2-N2	4.89	1.45	1.34
27	Z	46	7MG	C5-C4	4.88	1.44	1.37
55	Y	32	OMC	C4-N4	4.87	1.45	1.33
28	a	2073	G7M	C2-N3	4.79	1.44	1.33
5	A	527	G7M	C2-N2	4.76	1.45	1.34
5	A	1402	4OC	C4-N4	4.68	1.45	1.35
28	a	747	1MG	C4-N3	4.62	1.48	1.37
5	A	1498	UR3	C2-N3	4.53	1.47	1.39
55	Y	32	OMC	C2-N1	4.53	1.49	1.40
28	a	2556	OMU	O2-C2	-4.46	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Z	46	7MG	C2-N1	4.39	1.48	1.37
27	Z	46	7MG	C5-C6	4.34	1.53	1.42
28	a	2073	G7M	C4-N3	4.17	1.47	1.37
27	Z	37	MIA	C6-N6	4.13	1.49	1.34
28	a	1919	3TD	C2-N3	3.93	1.47	1.38
28	a	1837	2MG	C8-N7	-3.76	1.28	1.35
28	a	2449	2MG	C8-N7	-3.75	1.28	1.35
28	a	2556	OMU	C4-N3	3.70	1.45	1.38
5	A	1402	4OC	C5-C4	3.65	1.48	1.40
27	Z	46	7MG	C6-N1	3.60	1.45	1.38
5	A	527	G7M	C6-N1	3.59	1.43	1.37
55	Y	55	PSU	C6-C5	3.58	1.39	1.35
5	A	1402	4OC	C2-N1	3.49	1.47	1.40
27	Z	55	PSU	C6-C5	3.46	1.39	1.35
27	Z	46	7MG	O6-C6	-3.45	1.17	1.23
5	A	1402	4OC	O2-C2	-3.44	1.17	1.23
5	A	1516	2MG	C8-N7	-3.42	1.29	1.35
27	Z	39	PSU	C6-C5	3.36	1.39	1.35
5	A	966	2MG	C8-N7	-3.36	1.29	1.35
27	Z	32	PSU	C6-C5	3.36	1.39	1.35
27	Z	47	3AU	C6-N1	3.33	1.46	1.38
28	a	2556	OMU	C6-N1	3.30	1.45	1.38
28	a	2073	G7M	C6-N1	3.29	1.42	1.37
27	Z	8	4SU	C6-N1	3.28	1.45	1.38
28	a	2255	OMG	C8-N7	-3.24	1.29	1.35
55	Y	8	4SU	C6-N1	3.24	1.45	1.38
55	Y	8	4SU	O2-C2	-3.20	1.17	1.23
27	Z	46	7MG	C5-N7	3.14	1.44	1.35
5	A	1518	MA6	C5-C4	-3.14	1.32	1.40
55	Y	32	OMC	C6-N1	3.13	1.45	1.38
5	A	527	G7M	C5-C6	3.09	1.53	1.45
28	a	1921	PSU	C6-C5	3.07	1.38	1.35
28	a	2073	G7M	O6-C6	-3.05	1.17	1.23
5	A	1519	MA6	C5-C4	-3.03	1.32	1.40
5	A	1207	2MG	C8-N7	-2.99	1.29	1.35
28	a	748	PSU	C6-C5	2.99	1.38	1.35
27	Z	8	4SU	O2-C2	-2.98	1.17	1.23
5	A	516	PSU	C6-C5	2.96	1.38	1.35
28	a	2508	PSU	C6-C5	2.95	1.38	1.35
28	a	2507	2MA	C6-C5	2.92	1.54	1.43
28	a	2461	PSU	C6-C5	2.91	1.38	1.35
28	a	957	PSU	C6-C5	2.90	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2449	2MG	C5-C6	-2.89	1.41	1.47
28	a	1915	PSU	C6-C5	2.87	1.38	1.35
27	Z	37	MIA	C2-N3	2.87	1.36	1.32
5	A	1402	4OC	C6-N1	2.85	1.44	1.38
27	Z	47	3AU	O4-C4	-2.83	1.19	1.24
28	a	2073	G7M	C5-C6	2.83	1.52	1.45
5	A	1516	2MG	C5-C6	-2.79	1.41	1.47
5	A	1498	UR3	O2-C2	-2.77	1.17	1.22
27	Z	47	3AU	C5-C4	2.75	1.49	1.43
5	A	966	2MG	C5-C6	-2.73	1.41	1.47
5	A	527	G7M	C2-N1	2.71	1.44	1.37
28	a	1837	2MG	C5-C6	-2.69	1.41	1.47
5	A	1498	UR3	O4-C4	-2.69	1.17	1.23
28	a	2255	OMG	C5-C6	-2.69	1.42	1.47
27	Z	54	5MU	C6-C5	2.67	1.39	1.34
55	Y	32	OMC	O2-C2	-2.67	1.18	1.23
5	A	1498	UR3	C6-N1	2.64	1.44	1.38
55	Y	54	5MU	C4-N3	-2.61	1.34	1.38
55	Y	54	5MU	C6-C5	2.60	1.38	1.34
28	a	2609	PSU	C6-C5	2.60	1.38	1.35
27	Z	54	5MU	C4-N3	-2.59	1.34	1.38
28	a	2034	6MZ	C5-C4	-2.58	1.34	1.40
28	a	2608	PSU	C6-C5	2.58	1.38	1.35
28	a	1620	6MZ	C5-C4	-2.57	1.34	1.40
27	Z	47	3AU	O2-C2	-2.55	1.18	1.23
28	a	747	1MG	O6-C6	-2.52	1.17	1.22
28	a	2584	PSU	C6-C5	2.51	1.38	1.35
28	a	1919	3TD	O4-C4	-2.50	1.17	1.23
28	a	747	1MG	C5-C4	-2.49	1.36	1.43
5	A	1207	2MG	C5-C6	-2.46	1.42	1.47
28	a	2073	G7M	C2-N1	2.37	1.43	1.37
55	Y	54	5MU	C6-N1	-2.36	1.34	1.38
27	Z	16	H2U	O2-C2	-2.36	1.18	1.23
28	a	1919	3TD	C1'-C5	2.36	1.55	1.50
5	A	527	G7M	O6-C6	-2.35	1.18	1.23
55	Y	32	OMC	C5-C4	2.35	1.48	1.42
55	Y	20	H2U	O2-C2	-2.34	1.18	1.23
27	Z	20	H2U	O2-C2	-2.31	1.18	1.23
28	a	2034	6MZ	C2-N1	2.30	1.38	1.33
27	Z	54	5MU	C6-N1	-2.28	1.34	1.38
28	a	2507	2MA	C5-C4	-2.27	1.34	1.40
28	a	2449	2MG	C5-C4	-2.26	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1837	2MG	C5-C4	-2.26	1.37	1.43
55	Y	54	5MU	C2-N1	2.26	1.42	1.38
28	a	2584	PSU	O4'-C1'	-2.25	1.40	1.43
28	a	2034	6MZ	C2-N3	2.23	1.35	1.32
27	Z	37	MIA	C5-C4	-2.23	1.35	1.40
55	Y	20	H2U	O4-C4	-2.23	1.18	1.23
28	a	2507	2MA	C5-N7	-2.21	1.31	1.39
28	a	1919	3TD	C4-N3	2.20	1.45	1.40
27	Z	20	H2U	O4-C4	-2.18	1.18	1.23
5	A	1516	2MG	C5-C4	-2.18	1.37	1.43
27	Z	54	5MU	C4-C5	2.15	1.48	1.44
55	Y	54	5MU	C4-C5	2.14	1.48	1.44
27	Z	16	H2U	O4-C4	-2.14	1.18	1.23
28	a	2034	6MZ	C5-N7	-2.11	1.32	1.39
28	a	1620	6MZ	C2-N3	2.11	1.35	1.32
27	Z	54	5MU	C2-N1	2.10	1.41	1.38
28	a	2255	OMG	C5-C4	-2.10	1.37	1.43
5	A	1207	2MG	C5-C4	-2.10	1.37	1.43
28	a	2502	OMC	C4-N3	-2.09	1.30	1.34
5	A	1407	5MC	C4-N3	-2.06	1.30	1.34
28	a	2507	2MA	C8-N7	2.05	1.38	1.34
5	A	966	2MG	C5-C4	-2.04	1.37	1.43
28	a	748	PSU	O4'-C1'	-2.01	1.41	1.43
16	L	89	D2T	CB1-SB	-2.01	1.75	1.79

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1519	MA6	N1-C6-N6	-9.71	106.84	117.06
28	a	2507	2MA	C1'-N9-C4	9.39	143.13	126.64
5	A	1518	MA6	N1-C6-N6	-9.21	107.36	117.06
55	Y	8	4SU	C4-N3-C2	-7.98	119.59	127.34
27	Z	8	4SU	C4-N3-C2	-7.85	119.72	127.34
27	Z	16	H2U	C4-N3-C2	-7.28	119.75	125.79
27	Z	46	7MG	C5-C4-N3	-7.12	120.45	127.80
27	Z	20	H2U	C4-N3-C2	-6.89	120.07	125.79
55	Y	20	H2U	C4-N3-C2	-6.77	120.18	125.79
5	A	1519	MA6	N3-C2-N1	-6.02	119.28	128.68
28	a	1919	3TD	N1-C2-N3	5.90	120.79	116.14
5	A	1518	MA6	N3-C2-N1	-5.86	119.52	128.68
27	Z	8	4SU	C5-C4-N3	5.76	120.03	114.69
55	Y	8	4SU	C5-C4-N3	5.66	119.94	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	37	MIA	N3-C2-N1	-5.36	120.30	128.68
28	a	1620	6MZ	N3-C2-N1	-5.32	120.36	128.68
27	Z	54	5MU	C4-N3-C2	-5.19	120.63	127.35
28	a	2461	PSU	N1-C2-N3	5.09	120.90	115.13
55	Y	54	5MU	C4-N3-C2	-5.07	120.79	127.35
28	a	2556	OMU	C4-N3-C2	-5.04	119.93	126.58
28	a	2609	PSU	N1-C2-N3	5.01	120.80	115.13
28	a	1620	6MZ	C9-N6-C6	5.00	127.18	122.87
28	a	2034	6MZ	N3-C2-N1	-4.96	120.92	128.68
28	a	2508	PSU	N1-C2-N3	4.94	120.73	115.13
28	a	2034	6MZ	C9-N6-C6	4.93	127.12	122.87
28	a	957	PSU	C4-N3-C2	-4.93	119.23	126.34
27	Z	47	3AU	C4-N3-C2	-4.89	120.13	126.58
5	A	1498	UR3	C4-N3-C2	-4.85	119.99	124.56
28	a	1921	PSU	C4-N3-C2	-4.83	119.38	126.34
28	a	2608	PSU	C4-N3-C2	-4.82	119.40	126.34
28	a	1915	PSU	C4-N3-C2	-4.80	119.42	126.34
28	a	2609	PSU	C4-N3-C2	-4.77	119.46	126.34
27	Z	54	5MU	N3-C2-N1	4.74	121.18	114.89
28	a	2608	PSU	N1-C2-N3	4.71	120.47	115.13
28	a	2584	PSU	C4-N3-C2	-4.71	119.56	126.34
28	a	1921	PSU	N1-C2-N3	4.69	120.45	115.13
27	Z	54	5MU	C5-C4-N3	4.69	119.31	115.31
28	a	2508	PSU	C4-N3-C2	-4.68	119.60	126.34
28	a	957	PSU	N1-C2-N3	4.66	120.41	115.13
55	Y	54	5MU	C5-C4-N3	4.64	119.28	115.31
55	Y	54	5MU	N3-C2-N1	4.62	121.03	114.89
55	Y	55	PSU	C4-N3-C2	-4.59	119.72	126.34
27	Z	55	PSU	C4-N3-C2	-4.58	119.75	126.34
27	Z	39	PSU	C4-N3-C2	-4.57	119.76	126.34
27	Z	39	PSU	N1-C2-N3	4.53	120.26	115.13
28	a	2461	PSU	C4-N3-C2	-4.48	119.88	126.34
27	Z	32	PSU	C4-N3-C2	-4.47	119.90	126.34
28	a	748	PSU	C4-N3-C2	-4.46	119.91	126.34
28	a	1915	PSU	N1-C2-N3	4.46	120.18	115.13
27	Z	55	PSU	N1-C2-N3	4.44	120.16	115.13
28	a	2584	PSU	N1-C2-N3	4.44	120.16	115.13
27	Z	32	PSU	N1-C2-N3	4.40	120.11	115.13
27	Z	54	5MU	O4-C4-C5	-4.35	119.86	124.90
27	Z	46	7MG	C2-N3-C4	4.33	120.01	112.30
55	Y	55	PSU	N1-C2-N3	4.28	119.98	115.13
5	A	516	PSU	C4-N3-C2	-4.26	120.19	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	Y	54	5MU	O4-C4-C5	-4.25	119.97	124.90
5	A	516	PSU	N1-C2-N3	4.22	119.91	115.13
28	a	2556	OMU	N3-C2-N1	4.16	120.42	114.89
28	a	748	PSU	N1-C2-N3	4.14	119.82	115.13
27	Z	47	3AU	N3-C2-N1	3.99	120.19	114.89
28	a	2507	2MA	C2-N3-C4	3.96	118.74	115.52
28	a	1919	3TD	C4-N3-C2	-3.91	120.37	124.61
55	Y	8	4SU	N3-C2-N1	3.85	119.99	114.89
28	a	2507	2MA	CM2-C2-N1	3.83	123.12	117.15
28	a	2034	6MZ	C1'-N9-C4	-3.69	120.15	126.64
27	Z	8	4SU	N3-C2-N1	3.68	119.77	114.89
27	Z	54	5MU	C5-C6-N1	-3.64	119.59	123.34
28	a	2507	2MA	N3-C2-N1	-3.63	119.11	125.73
28	a	747	1MG	C5-C6-N1	3.60	119.32	113.90
28	a	1620	6MZ	C2-N1-C6	3.48	119.58	116.59
27	Z	8	4SU	C5-C4-S4	-3.47	119.99	124.47
55	Y	54	5MU	C5-C6-N1	-3.37	119.87	123.34
55	Y	8	4SU	C5-C4-S4	-3.34	120.16	124.47
27	Z	16	H2U	N3-C2-N1	3.32	120.17	116.65
55	Y	20	H2U	N3-C2-N1	3.26	120.11	116.65
27	Z	47	3AU	C5-C4-N3	3.24	119.69	114.84
28	a	2508	PSU	O2-C2-N1	-3.22	119.25	122.79
27	Z	20	H2U	N3-C2-N1	3.09	119.92	116.65
27	Z	46	7MG	O6-C6-C5	-3.06	120.22	127.24
28	a	2556	OMU	C5-C4-N3	3.00	119.32	114.84
27	Z	16	H2U	C5-C4-N3	2.96	119.97	116.65
5	A	516	PSU	O2-C2-N1	-2.95	119.54	122.79
28	a	2461	PSU	C6-N1-C2	-2.93	119.69	122.68
5	A	1518	MA6	C1'-N9-C4	2.91	131.76	126.64
28	a	2034	6MZ	C2-N1-C6	2.89	119.06	116.59
5	A	527	G7M	C2-N1-C6	-2.87	119.81	125.10
27	Z	46	7MG	C2-N1-C6	-2.83	119.95	125.10
27	Z	47	3AU	O4-C4-C5	-2.82	120.20	125.16
28	a	2073	G7M	C2-N1-C6	-2.80	119.94	125.10
27	Z	20	H2U	C5-C6-N1	2.78	120.78	111.61
27	Z	20	H2U	C5-C4-N3	2.77	119.76	116.65
55	Y	20	H2U	C5-C6-N1	2.75	120.67	111.61
28	a	1620	6MZ	C1'-N9-C4	-2.74	121.82	126.64
27	Z	32	PSU	O2-C2-N1	-2.69	119.83	122.79
5	A	1498	UR3	C6-N1-C2	-2.66	119.41	121.79
27	Z	55	PSU	O2-C2-N1	-2.66	119.86	122.79
27	Z	46	7MG	N9-C4-N3	2.63	129.40	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	16	H2U	C5-C6-N1	2.62	120.26	111.61
55	Y	55	PSU	O2-C2-N1	-2.60	119.92	122.79
5	A	1402	4OC	C6-C5-C4	2.59	120.13	116.96
27	Z	16	H2U	O2-C2-N1	-2.59	119.86	123.11
55	Y	20	H2U	C5-C4-N3	2.58	119.55	116.65
28	a	2508	PSU	C6-N1-C2	-2.57	120.05	122.68
28	a	1921	PSU	O2-C2-N1	-2.56	119.97	122.79
28	a	2609	PSU	C6-N1-C2	-2.54	120.08	122.68
27	Z	54	5MU	O2-C2-N1	-2.51	119.46	122.79
27	Z	46	7MG	C5-C4-N9	2.49	110.15	106.68
5	A	1519	MA6	C1'-N9-C4	2.49	131.01	126.64
28	a	1919	3TD	C6-C5-C4	2.47	119.93	118.22
27	Z	39	PSU	O2-C2-N1	-2.47	120.07	122.79
27	Z	46	7MG	C5-C6-N1	2.45	119.61	112.31
5	A	516	PSU	C6-N1-C2	-2.42	120.20	122.68
28	a	2556	OMU	O4-C4-C5	-2.42	120.90	125.16
27	Z	32	PSU	C6-N1-C2	-2.41	120.22	122.68
5	A	1207	2MG	O6-C6-C5	2.40	129.07	124.37
16	L	89	D2T	OD2-CG-CB	2.40	118.34	113.15
28	a	747	1MG	C8-N7-C5	2.40	107.55	102.99
28	a	1915	PSU	O2-C2-N1	-2.37	120.18	122.79
27	Z	55	PSU	C6-C5-C4	2.34	119.84	118.20
28	a	2584	PSU	O4'-C1'-C2'	2.32	108.42	105.14
16	L	89	D2T	O-C-CA	-2.29	118.78	124.78
28	a	2453	H2U	C5-C4-N3	-2.28	114.09	116.65
28	a	2453	H2U	C4-N3-C2	2.27	127.67	125.79
28	a	2608	PSU	C6-C5-C4	2.27	119.78	118.20
55	Y	8	4SU	O2-C2-N1	-2.26	119.78	122.79
5	A	516	PSU	O4'-C1'-C2'	2.26	108.33	105.14
27	Z	47	3AU	O2-C2-N1	-2.25	119.80	122.79
39	l	81	4D4	O-C-CA	-2.24	118.90	124.78
27	Z	39	PSU	C6-C5-C4	2.23	119.75	118.20
5	A	1498	UR3	C1'-N1-C2	2.21	120.72	116.99
28	a	2461	PSU	O2-C2-N3	-2.21	117.66	121.82
27	Z	39	PSU	C6-N1-C2	-2.20	120.43	122.68
28	a	2073	G7M	N2-C2-N1	2.19	121.38	116.71
28	a	748	PSU	C6-N1-C2	-2.19	120.44	122.68
28	a	2255	OMG	O6-C6-C5	2.16	128.60	124.37
28	a	2609	PSU	O2-C2-N1	-2.15	120.43	122.79
27	Z	20	H2U	O2-C2-N1	-2.12	120.45	123.11
5	A	1516	2MG	O6-C6-C5	2.11	128.50	124.37
28	a	2453	H2U	O2-C2-N3	-2.11	117.56	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	55	PSU	C6-N1-C2	-2.10	120.54	122.68
55	Y	55	PSU	C6-N1-C2	-2.09	120.54	122.68
55	Y	20	H2U	O2-C2-N1	-2.08	120.50	123.11
55	Y	32	OMC	O2-C2-N3	-2.06	118.98	122.33
55	Y	32	OMC	C1'-N1-C2	2.05	122.99	118.42
28	a	1837	2MG	O6-C6-C5	2.04	128.35	124.37
55	Y	54	5MU	C1'-N1-C2	2.03	121.25	117.57
27	Z	46	7MG	C4-C5-N7	2.03	110.08	106.13
27	Z	37	MIA	C1'-N9-C4	2.03	130.20	126.64
27	Z	37	MIA	C5-C6-N6	2.02	123.42	120.35
27	Z	32	PSU	C6-C5-C4	2.01	119.60	118.20
28	a	1921	PSU	C6-C5-C4	2.00	119.60	118.20

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	Z	46	7MG	O4'-C4'-C5'-O5'
39	l	81	4D4	NH1-CZ-NE-CD
55	Y	20	H2U	O4'-C1'-N1-C6
55	Y	32	OMC	C1'-C2'-O2'-CM2
28	a	2034	6MZ	O4'-C4'-C5'-O5'
28	a	2255	OMG	C1'-C2'-O2'-CM2
27	Z	46	7MG	C3'-C4'-C5'-O5'
27	Z	47	3AU	O4'-C4'-C5'-O5'
55	Y	20	H2U	O4'-C4'-C5'-O5'
28	a	2034	6MZ	C3'-C4'-C5'-O5'
31	d	150	MEQ	OE1-CD-CG-CB
31	d	150	MEQ	NE2-CD-CG-CB
27	Z	8	4SU	C3'-C4'-C5'-O5'
27	Z	8	4SU	O4'-C4'-C5'-O5'
27	Z	47	3AU	C3'-C4'-C5'-O5'
55	Y	8	4SU	C3'-C4'-C5'-O5'
55	Y	8	4SU	O4'-C4'-C5'-O5'
5	A	1519	MA6	O4'-C4'-C5'-O5'
5	A	1519	MA6	C3'-C4'-C5'-O5'
5	A	1519	MA6	C5-C6-N6-C10
28	a	1919	3TD	O4'-C4'-C5'-O5'
39	l	81	4D4	NH2-CZ-NE-CD
55	Y	20	H2U	C3'-C4'-C5'-O5'
28	a	2073	G7M	C4'-C5'-O5'-P
55	Y	20	H2U	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
39	l	81	4D4	OB-CB-CG-CD
39	l	81	4D4	CG-CD-NE-CZ
39	l	81	4D4	NE-CD-CG-CB
16	L	89	D2T	CA-CB-SB-CB1
28	a	2507	2MA	C4'-C5'-O5'-P
16	L	89	D2T	SB-CB-CG-OD2
55	Y	32	OMC	C2'-C1'-N1-C6
28	a	1919	3TD	C3'-C4'-C5'-O5'
16	L	89	D2T	CG-CB-SB-CB1
27	Z	20	H2U	C2'-C1'-N1-C2
28	a	748	PSU	O4'-C1'-C5-C6
55	Y	32	OMC	C2'-C1'-N1-C2
55	Y	20	H2U	C2'-C1'-N1-C6
55	Y	20	H2U	O4'-C1'-N1-C2
55	Y	20	H2U	C2'-C1'-N1-C2
27	Z	20	H2U	O4'-C4'-C5'-O5'
28	a	2073	G7M	O4'-C4'-C5'-O5'
28	a	2507	2MA	O4'-C4'-C5'-O5'
39	l	81	4D4	O-C-CA-CB

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 530 ligands modelled in this entry, 529 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	PHE	a	3001	-	10,11,12	0.43	0	10,13,15	0.30	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
59	PHE	a	3001	-	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1532:U	O3'	1533:C	P	3.52
1	A	1407:5MC	O3'	1408:A	P	1.85