



Full wwPDB EM Validation Report ⓘ

Mar 15, 2025 – 06:23 pm GMT

PDB ID : 9GHD
EMDB ID : EMD-51353
Title : Escherichia coli 70S ribosome in complex with Staphylococcus aureus FusB-EF-G (FusB-EF-G-70S*)
Authors : Gonzalez-Lopez, A.; Selmer, M.
Deposited on : 2024-08-15
Resolution : 2.41 Å (reported)
Based on initial models : 8P2H, 9GHE

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:

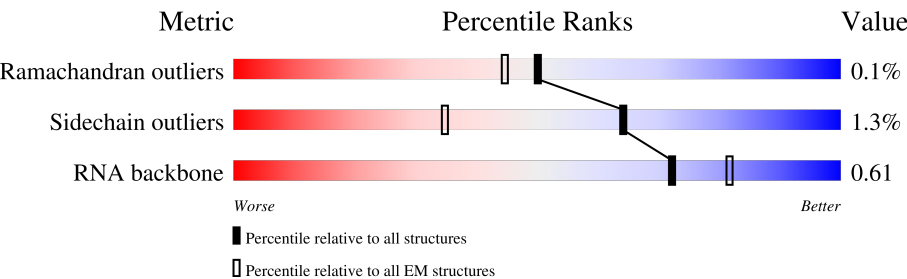
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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



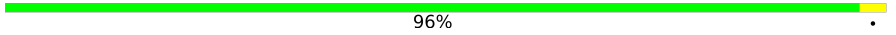



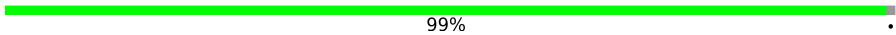
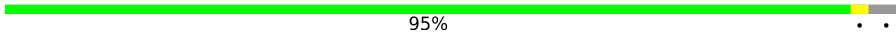


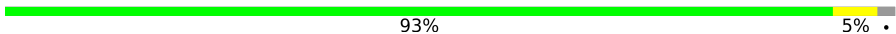
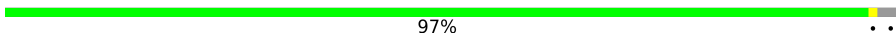
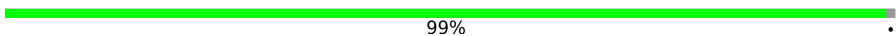

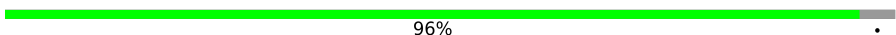
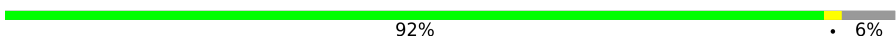


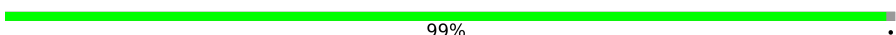

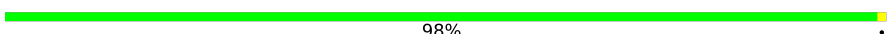



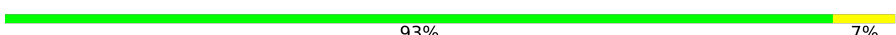
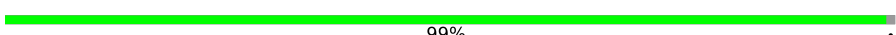
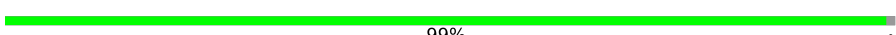
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	
2	1	46	
3	2	65	
4	3	38	
5	4	70	
6	9	24	
7	A	1554	
8	B	241	
9	C	233	


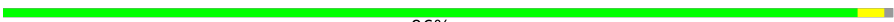












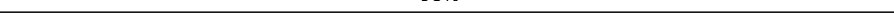
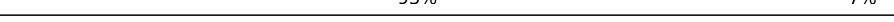

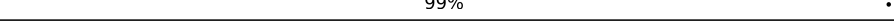

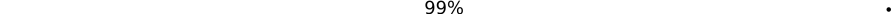
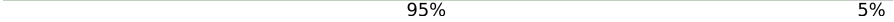
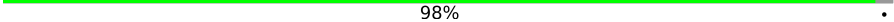
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Mol	Chain	Length	Quality of chain
10	D	206	
11	E	167	
12	F	135	
13	G	179	
14	H	130	
15	I	130	
16	J	103	
17	K	129	
18	L	124	
19	M	118	
20	N	101	
21	O	89	
22	P	82	
23	Q	84	
24	R	75	
25	S	92	
26	T	87	
27	U	71	
28	V	213	
29	W	693	
30	Z	77	
31	a	2930	
32	b	119	
33	c	273	
34	d	209	

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Mol	Chain	Length	Quality of chain
35	e	201	 100%
36	f	179	 96% ..
37	g	177	 94% • 5%
38	h	149	 26% • 72%
39	i	142	 99% •
40	j	123	 99% •
41	k	144	 99% •
42	l	136	 99% •
43	m	127	 93% 7%
44	n	117	 97% • •
45	o	115	 98% • •
46	p	118	 99% •
47	q	103	 99% •
48	r	110	 98% • •
49	s	100	 93% 7%
50	t	104	 89% 11%
51	u	94	 99% •
52	v	85	 88% 12%
53	w	78	 99% •
54	x	63	 95% 5%
55	y	59	 98% •
56	z	57	 95% 5%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 143666 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 Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	50	Total	C	N	O	0	0
			413	267	75	71		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	45	Total	C	N	O	S	0	0
			367	222	88	55	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 protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	7	Total	C	N	O	P	0	0
			154	69	32	46	7		

- Molecule 7 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1514	Total	C	N	O	P	0	0
			32500	14503	5963	10520	1514		

- Molecule 8 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	222	Total	C	N	O	S	0	0
			1737	1099	312	318	8		

- Molecule 9 is a protein called 30S ribosomal protein S3.

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

- Molecule 10 is a protein called 30S ribosomal protein S4.

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

- Molecule 11 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	154	Total	C	N	O	S	0	0
			1135	706	215	208	6		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	150	Total	C	N	O	S	0	0
			1176	732	226	214	4		

- Molecule 14 is a protein called 30S ribosomal protein S8.

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

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	125	Total	C	N	O	S	0	0
			1001	622	200	176	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	96	Total	C	N	O	S	0	0
			775	487	148	139	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 18 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 19 is a protein called 30S ribosomal protein S13.

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

- Molecule 20 is a protein called 30S ribosomal protein S14.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 23 is a protein called 30S ribosomal protein S17.

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

- Molecule 24 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	64	Total	C	N	O	S	0	0
			524	330	99	94	1		

- Molecule 25 is a protein called 30S ribosomal protein S19.

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

- Molecule 26 is a protein called 30S ribosomal protein S20.

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

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 28 is a protein called Far1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	212	Total	C	N	O	S	0	0
			1765	1139	290	328	8		

- Molecule 29 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	214	Total	C	N	O	S	0	0
			1647	1035	277	323	12		

- Molecule 30 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	2782	Total	C	N	O	P	0	0
			59756	26665	11017	19292	2782		

- Molecule 32 is a RNA chain called 5S rRNA.

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

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1552	972	286	291	3		

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	168	Total	C	N	O	S	0	0
			1255	791	228	234	2		

- Molecule 38 is a protein called 50S ribosomal protein L9.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	141	Total	C	N	O	S	0	0
			1121	709	211	198	3		

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	modified residue	UNP P0ADY7

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

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

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	93	Total	C	N	O	S	0	0
			717	452	135	130			

- Molecule 51 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 52 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 53 is a protein called 50S ribosomal protein L28.

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

- Molecule 54 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 55 is a protein called 50S ribosomal protein L30.

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

- Molecule 56 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

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

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	A	31	Total	K	0
			31	31	
58	F	1	Total	K	0
			1	1	
58	M	1	Total	K	0
			1	1	
58	a	76	Total	K	0
			76	76	
58	c	2	Total	K	0
			2	2	
58	e	1	Total	K	0
			1	1	


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

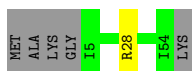
Mol	Chain	Residues	Atoms		AltConf
59	A	55	Total 55	Mg 55	0
59	a	240	Total 240	Mg 240	0
59	b	3	Total 3	Mg 3	0
59	c	2	Total 2	Mg 2	0
59	d	1	Total 1	Mg 1	0
59	p	1	Total 1	Mg 1	0
59	z	1	Total 1	Mg 1	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Large ribosomal subunit protein bL33

Chain 0:  89% 9%



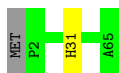
- Molecule 2: Large ribosomal subunit protein bL34

Chain 1:  98%



- Molecule 3: 50S ribosomal protein L35

Chain 2:  97%




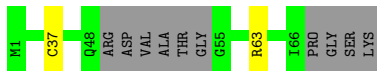
- Molecule 4: 50S ribosomal protein L36

Chain 3:  97%



- Molecule 5: 50S ribosomal protein L31

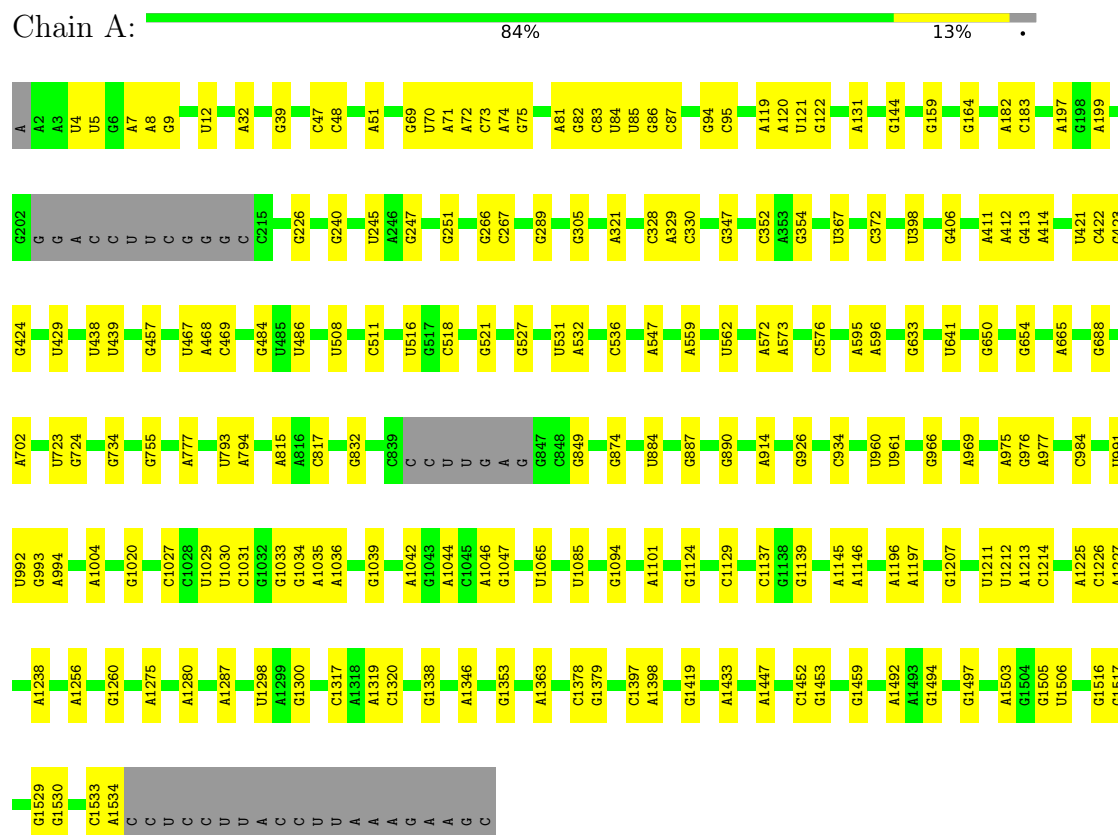
Chain 4:  83% 14%



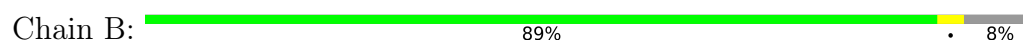
- Molecule 6: mRNA

Chain 9:  25% 71%

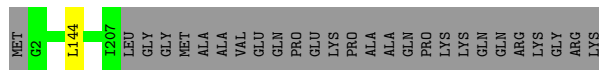
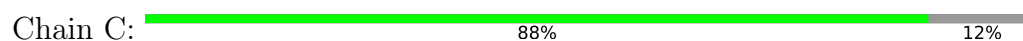
- Molecule 7: 16S rRNA



- Molecule 8: 30S ribosomal protein S2




- Molecule 9: 30S ribosomal protein S3

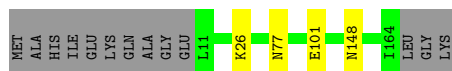


- Molecule 10: 30S ribosomal protein S4



- Molecule 11: 30S ribosomal protein S5

Chain E:  90% 8%




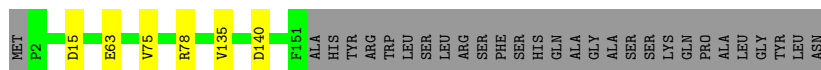
- Molecule 12: 30S ribosomal protein S6

Chain F:  75% 25%



- Molecule 13: 30S ribosomal protein S7

Chain G:  80% 16%



- Molecule 14: 30S ribosomal protein S8

Chain H:  99%




- Molecule 15: 30S ribosomal protein S9

Chain I:  95%




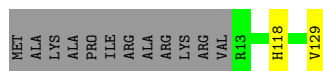
- Molecule 16: 30S ribosomal protein S10

Chain J:  89% 7%



- Molecule 17: Small ribosomal subunit protein uS11

Chain K:  89% 9%



- Molecule 18: 30S ribosomal protein S12

Chain L:  93% 5% .



- Molecule 19: 30S ribosomal protein S13

Chain M:  97% . .



- Molecule 20: 30S ribosomal protein S14

Chain N:  99% .



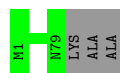
- Molecule 21: Small ribosomal subunit protein uS15

Chain O:  99% .



- Molecule 22: 30S ribosomal protein S16

Chain P:  96% .




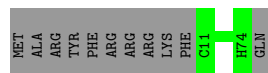
- Molecule 23: 30S ribosomal protein S17

Chain Q:  92% . 6%



- Molecule 24: 30S ribosomal protein S18

Chain R:  85% 15%



- Molecule 25: 30S ribosomal protein S19

MET
P2
A85
ASP
LYS
LYS
ALA
LYS
LYS
LYS

- Chain T: 99%

MET A2 A87

- Chain U: 76% 23%

MET
P2
R34
H56
ALA
LYS
LYS
LEU
ALA
ARG
GLU
ASN
ALA
ARG
ARG
THR
ARG
LEU
TYR

- Chain V: 98%

- Chain W:  30% 69%

MET	ARG	ARG	GLU	PHE	SER	LEU	GLU	LYS	THR	ARG	ASN	ILE	GLY	ILE	MET	ALA	HIS	ILE	ASP	GLY	LYS	THR	THR	THR	GLU	ARG	ILE	LEU	TYR	TYR	THR	THR	GLY	GLY	THR	GLY	GLU	THR	HIS	LYS	ILE	ILE	GLY	GLU	SER	GLN	MET	ASP	TRP	MET	GLU	GLN	GLU	GLN	ASP	ARG
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ILE	THR	THR	THR	SER	ALA	ALA	THR	THR	ALA	ALA	TRP	GLY	GLU	GLY	HIS	ARG	ASN	ILE	ILE	ASP	THR	THR	PRO	GLY	HIS	ASP	VAL	ASP	PHE	THR	THR	VAL	GLU	GLU	VAL	VAL	GLU	ARG	SER	SER	LEU	ARG	VAL	VAL	LEU	LEU	VAL	VAL	ASP	GLY	ALA	ALA	VAL	THR	THR	VAL	VAL	LEU	LEU	ASP	ASP	ALA	GLN	SER	THR	THR	GLU	THR	THR	GLU	THR	VAL
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ARG	GLN	ALA	THR	TYR	GLY	VAL	PRO	ARG	ILE	VAL	PHE	VAL	ASN	LYS	MET	ASP	LYS	LEU	GLY	ALA	ASN	PHE	GLU	TYR	SER	SER	THR	LEU	HIS	ASP	ARG	LEU	GLN	ALA	ASN	ALA	ALA	ALA	PRO	ILE	GLN	LEU	PRO	PHE	GLU	ALA	ILE	LEU	ASP	LEU	VAL
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NET	LYS	CYS	PHE	LYS	THR	ASN	ASP	LEU	GLY	THR	GLU	THR	ILE	GLU	GLY	ILE	GLU	GLY	ASP	HIS	LEU	ASP	ARG	ALA	ALA	GLU	GLY	ALA	ALA	VAL	SER	THR	SER	ASP	GLU	LEU	MET	GLY	LYS	TYR	LEU	GLY	ASP	GLU	GLU	ILE	VAL	SER	SER	SER	GLY
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LYS	GLU	ALA	ALA	ILE	ARG	GLN	ALA	THR	THR	ASN	VAL	GLU	PHE	TYR	PRO	VAL	LEU	CYS	GLY	THR	GLY	ASP	ASN	LYS	LYS	GLY	VAL	VAL	GLN	LEU	MET	LEU	ASP	ASP	TYR	LEU	PRO	PRO	SER	PRO	LEU	ASP	VAL	LYS	PRO	ILE	ILE	GLY	HIS	ARG	ALA	SER	ASN	PRO	GLU	GLU	GLU	VAL	VAL
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ALA	LYS	ALA	ASP	ASP	SER	GLU	PHE	ALA	ALA	LEU	ALA	ALA	PHE	LYS	VAL	MET	THR	PRO	TYR	VAL	GLY	LYS	LEU	THR	PHE	PHE	ARG	VAL	TYR	SER	SER	GLY	THR	MET	THR	SER	SER	ASN	LYS	VAL	TYR	GLY	LYS	GLY	THR	LYS	ARG	GLU	VAL	ARG	GLN	MET	HIS
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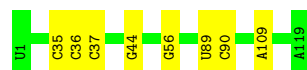
ASN	SER	ARG	GLN	GLU	ILE	ASP	THR	TYR	SER	GLY	ASP	ILE	ALA	ALA	ALA	VAL	GLY	LEU	LYS	ASP	THR	GLY	THR	GLY	ASP	LEU	THR	LEU	CYS	GLY	GLU	LYS	ASN	ASP	ILE	ILE	LEU	GLU	SER	MET	GLU	PHE	PRO	GLU	PRO	VAL	ILE	HIS	LEU	SER	SER	LYS	ALA	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP
LYS
MET
THR
GLN
ALA
LEU
VAL
LYS
LEU
GLN
GLU
ASP
PRO
THR
PHE
HIS
ALA
HIS
THR
GLU
GLU
GLY
GLN
VAL
ILE
ILE
GLY
GLY
MET
GLY
GLU
LEU
HIS
LEU
ASP
ASP
ILE
LEU
VAL
ASP
ARG
MET
LYS
LYS
GLU
CYS
ASN
VAL
GLY
ALA
PRO





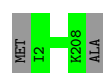
• Molecule 32: 5S rRNA



• Molecule 33: 50S ribosomal protein L2



• Molecule 34: 50S ribosomal protein L3



• Molecule 35: 50S ribosomal protein L4

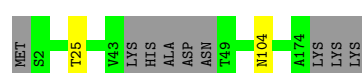


There are no outlier residues recorded for this chain.

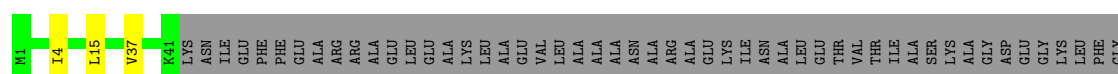
• Molecule 36: 50S ribosomal protein L5



• Molecule 37: 50S ribosomal protein L6



• Molecule 38: 50S ribosomal protein L9



SER
ILE
GLY
THR
ARG
ASP
TLE
ALA
ASP
ALA
VAL
THR
ALA
ALA
GLY
VAL
VAL
GLU
VAL
ALA
LYS
SER
GLU
VAL
ARG
LEU
PRO
ASN
GLY
VAL
LEU
ARG
THR
THR
GLY
GLU
HIS
GLU
VAL
SER
PHE
GLN
VAL
HIS
SER
GLU
PHE
ALA
LYS
VAL
TLE
VAL
ASN
VAL
VAL
ALA
GLU

- Molecule 39: 50S ribosomal protein L13

Chain i:  99% .

MET
K2
I142

- Molecule 40: 50S ribosomal protein L14

Chain j:  99% .

M1
L58
L123

- Molecule 41: 50S ribosomal protein L15

Chain k:  99% .

M1
K29
E144

- Molecule 42: Large ribosomal subunit protein uL16

Chain l:  99% .

M1
R6
M136

- Molecule 43: 50S ribosomal protein L17

Chain m:  93% 7%

M1
R118
SER
GLU
LYS
ALA
GLU
ALA
ALA
ALA
GLU

- Molecule 44: 50S ribosomal protein L18

Chain n:  97% ..

MET
D2
V49
K56
F117

- Molecule 45: 50S ribosomal protein L19

Chain o:  98% ..



- Molecule 46: 50S ribosomal protein L20

Chain p: 99%



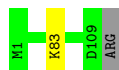
- Molecule 47: 50S ribosomal protein L21

Chain q: 99%



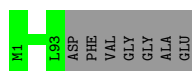
- Molecule 48: 50S ribosomal protein L22

Chain r: 98%



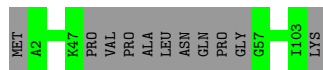
- Molecule 49: 50S ribosomal protein L23

Chain s: 93% 7%



- Molecule 50: 50S ribosomal protein L24

Chain t: 89% 11%



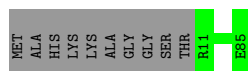
- Molecule 51: 50S ribosomal protein L25

Chain u: 99%



- Molecule 52: Large ribosomal subunit protein bL27

Chain v: 88% 12%



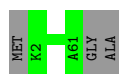
- Molecule 53: 50S ribosomal protein L28

Chain w: 99% .



- Molecule 54: 50S ribosomal protein L29

Chain x: 95% 5% .



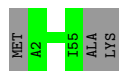
- Molecule 55: 50S ribosomal protein L30

Chain y: 98% .



- Molecule 56: 50S ribosomal protein L32

Chain z: 95% 5% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30847	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 ($e^-/\text{\AA}^2$)	45.47	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k 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: OMC, 1MG, OMG, MEQ, ZN, MS6, MG, UR3, IAS, H2U, K, G7M, PSU, D2T, 2MG, 5MU, 4OC, 2MA, 3TD, MA6, OMU, 4D4, 5MC, 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	0.31	0/420	0.54	0/560
2	1	0.30	0/370	0.58	0/487
3	2	0.33	0/513	0.54	0/676
4	3	0.30	0/303	0.58	0/397
5	4	0.32	0/488	0.56	0/649
6	9	0.47	0/173	0.83	0/268
7	A	0.42	0/36110	0.89	0/56322
8	B	0.29	0/1768	0.54	0/2381
9	C	0.28	0/1651	0.53	0/2225
10	D	0.29	0/1665	0.54	0/2227
11	E	0.29	0/1148	0.54	0/1545
12	F	0.28	0/843	0.50	0/1140
13	G	0.29	0/1190	0.52	0/1595
14	H	0.29	0/989	0.55	0/1326
15	I	0.29	0/1013	0.56	0/1350
16	J	0.28	0/784	0.60	0/1059
17	K	0.30	0/884	0.53	0/1191
18	L	0.29	0/945	0.61	0/1268
19	M	0.29	0/900	0.54	0/1204
20	N	0.30	0/817	0.53	0/1088
21	O	0.29	0/722	0.50	0/964
22	P	0.28	0/639	0.56	0/859
23	Q	0.28	0/650	0.56	0/871
24	R	0.28	0/532	0.55	0/715
25	S	0.32	0/685	0.54	0/922
26	T	0.28	0/676	0.48	0/895
27	U	0.32	0/467	0.60	0/620
28	V	0.29	0/1798	0.49	0/2415
29	W	0.30	0/1679	0.51	0/2261
30	Z	0.45	0/1813	0.89	0/2825
31	a	0.41	0/66355	0.89	4/103511 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.43	0/2850	0.90	0/4444
33	c	0.29	0/2121	0.57	0/2852
34	d	0.29	0/1562	0.52	0/2102
35	e	0.28	0/1571	0.51	0/2113
36	f	0.29	0/1434	0.54	0/1926
37	g	0.29	0/1273	0.54	0/1725
38	h	0.30	0/306	0.55	0/413
39	i	0.28	0/1144	0.52	0/1541
40	j	0.28	0/955	0.55	0/1279
41	k	0.31	0/1062	0.52	0/1413
42	l	0.29	0/1073	0.55	0/1433
43	m	0.28	0/958	0.53	0/1281
44	n	0.29	0/902	0.54	0/1209
45	o	0.29	0/929	0.54	0/1242
46	p	0.28	0/960	0.52	0/1278
47	q	0.30	0/829	0.54	0/1107
48	r	0.28	0/852	0.55	0/1142
49	s	0.27	0/744	0.54	0/994
50	t	0.30	0/721	0.56	0/956
51	u	0.29	0/758	0.54	0/1015
52	v	0.32	0/576	0.54	0/762
53	w	0.30	0/635	0.54	0/848
54	x	0.26	0/492	0.48	0/655
55	y	0.29	0/453	0.51	0/605
56	z	0.30	0/435	0.56	0/581
All	All	0.38	0/154585	0.81	4/230732 (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
4	3	0	1
10	D	0	1
16	J	0	1
17	K	0	1
27	U	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	512	G	O4'-C1'-N9	6.25	113.20	108.20
31	a	2447	G	C3'-C2'-C1'	-5.36	97.21	101.50
31	a	242	G	C3'-C2'-C1'	-5.03	97.47	101.50
31	a	512	G	C1'-O4'-C4'	-5.01	105.89	109.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	36	ARG	Sidechain
10	D	184	ARG	Sidechain
16	J	38	GLY	Peptide
17	K	118	HIS	Peptide
27	U	34	ARG	Sidechain

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	48/55 (87%)	48 (100%)	0	0	100	100
2	1	43/46 (94%)	43 (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
5	4	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
8	B	220/241 (91%)	214 (97%)	5 (2%)	1 (0%)	25	36
9	C	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
10	D	203/206 (98%)	202 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	E	152/167 (91%)	150 (99%)	2 (1%)	0	100	100
12	F	99/135 (73%)	98 (99%)	1 (1%)	0	100	100
13	G	148/179 (83%)	147 (99%)	1 (1%)	0	100	100
14	H	127/130 (98%)	127 (100%)	0	0	100	100
15	I	123/130 (95%)	120 (98%)	3 (2%)	0	100	100
16	J	92/103 (89%)	87 (95%)	4 (4%)	1 (1%)	12	17
17	K	113/129 (88%)	111 (98%)	2 (2%)	0	100	100
18	L	118/124 (95%)	114 (97%)	4 (3%)	0	100	100
19	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
20	N	98/101 (97%)	98 (100%)	0	0	100	100
21	O	86/89 (97%)	86 (100%)	0	0	100	100
22	P	77/82 (94%)	75 (97%)	2 (3%)	0	100	100
23	Q	77/84 (92%)	77 (100%)	0	0	100	100
24	R	62/75 (83%)	62 (100%)	0	0	100	100
25	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	53/71 (75%)	53 (100%)	0	0	100	100
28	V	210/213 (99%)	208 (99%)	2 (1%)	0	100	100
29	W	212/693 (31%)	209 (99%)	3 (1%)	0	100	100
33	c	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
34	d	204/209 (98%)	200 (98%)	4 (2%)	0	100	100
35	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
36	f	175/179 (98%)	174 (99%)	1 (1%)	0	100	100
37	g	164/177 (93%)	162 (99%)	2 (1%)	0	100	100
38	h	39/149 (26%)	38 (97%)	1 (3%)	0	100	100
39	i	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
40	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
41	k	142/144 (99%)	139 (98%)	2 (1%)	1 (1%)	19	27
42	l	132/136 (97%)	131 (99%)	1 (1%)	0	100	100
43	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
44	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
46	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
47	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
48	r	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
49	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
50	t	89/104 (86%)	89 (100%)	0	0	100	100
51	u	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
52	v	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
53	w	75/78 (96%)	75 (100%)	0	0	100	100
54	x	58/63 (92%)	58 (100%)	0	0	100	100
55	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
56	z	52/57 (91%)	52 (100%)	0	0	100	100
All	All	5832/6819 (86%)	5752 (99%)	77 (1%)	3 (0%)	50	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	J	57	VAL
41	k	29	LYS
8	B	165	ASP

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%)	45 (98%)	1 (2%)	47	65
2	1	37/38 (97%)	37 (100%)	0	100	100
3	2	51/52 (98%)	50 (98%)	1 (2%)	50	68
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	53 (96%)	2 (4%)	30	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	B	184/199 (92%)	178 (97%)	6 (3%)	33	51
9	C	170/190 (90%)	169 (99%)	1 (1%)	84	92
10	D	172/173 (99%)	166 (96%)	6 (4%)	31	49
11	E	117/126 (93%)	113 (97%)	4 (3%)	32	50
12	F	88/116 (76%)	88 (100%)	0	100	100
13	G	124/147 (84%)	118 (95%)	6 (5%)	21	35
14	H	104/105 (99%)	104 (100%)	0	100	100
15	I	103/107 (96%)	101 (98%)	2 (2%)	52	70
16	J	85/90 (94%)	83 (98%)	2 (2%)	44	63
17	K	89/98 (91%)	88 (99%)	1 (1%)	70	84
18	L	101/103 (98%)	96 (95%)	5 (5%)	20	34
19	M	93/96 (97%)	92 (99%)	1 (1%)	70	84
20	N	83/84 (99%)	83 (100%)	0	100	100
21	O	76/77 (99%)	76 (100%)	0	100	100
22	P	64/65 (98%)	64 (100%)	0	100	100
23	Q	73/78 (94%)	71 (97%)	2 (3%)	40	58
24	R	55/65 (85%)	55 (100%)	0	100	100
25	S	72/79 (91%)	72 (100%)	0	100	100
26	T	65/66 (98%)	65 (100%)	0	100	100
27	U	48/61 (79%)	48 (100%)	0	100	100
28	V	203/204 (100%)	200 (98%)	3 (2%)	60	77
29	W	174/579 (30%)	171 (98%)	3 (2%)	56	73
33	c	216/218 (99%)	215 (100%)	1 (0%)	86	94
34	d	162/163 (99%)	162 (100%)	0	100	100
35	e	165/165 (100%)	165 (100%)	0	100	100
36	f	148/150 (99%)	143 (97%)	5 (3%)	32	50
37	g	130/138 (94%)	128 (98%)	2 (2%)	60	77
38	h	32/114 (28%)	29 (91%)	3 (9%)	7	10
39	i	115/116 (99%)	115 (100%)	0	100	100
40	j	104/104 (100%)	103 (99%)	1 (1%)	73	85
41	k	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	l	107/107 (100%)	106 (99%)	1 (1%)	75	87
43	m	98/103 (95%)	98 (100%)	0	100	100
44	n	86/87 (99%)	83 (96%)	3 (4%)	31	49
45	o	99/100 (99%)	98 (99%)	1 (1%)	73	85
46	p	89/90 (99%)	89 (100%)	0	100	100
47	q	84/84 (100%)	83 (99%)	1 (1%)	67	82
48	r	92/93 (99%)	91 (99%)	1 (1%)	70	84
49	s	80/84 (95%)	80 (100%)	0	100	100
50	t	76/85 (89%)	76 (100%)	0	100	100
51	u	77/78 (99%)	77 (100%)	0	100	100
52	v	56/63 (89%)	56 (100%)	0	100	100
53	w	67/68 (98%)	67 (100%)	0	100	100
54	x	54/55 (98%)	54 (100%)	0	100	100
55	y	48/49 (98%)	48 (100%)	0	100	100
56	z	46/48 (96%)	46 (100%)	0	100	100
All	All	4900/5608 (87%)	4835 (99%)	65 (1%)	64	80

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	ARG
3	2	31	HIS
5	4	37	CYS
5	4	63	ARG
8	B	23	TRP
8	B	78	GLU
8	B	95	ARG
8	B	103	ASN
8	B	161	LEU
8	B	204	ASP
9	C	144	LEU
10	D	35	GLU
10	D	44	ARG
10	D	45	LYS
10	D	99	ASP
10	D	128	ARG
10	D	147	GLU

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Mol	Chain	Res	Type
11	E	26	LYS
11	E	77	ASN
11	E	101	GLU
11	E	148	ASN
13	G	15	ASP
13	G	63	GLU
13	G	75	VAL
13	G	78	ARG
13	G	135	VAL
13	G	140	ASP
15	I	42	GLU
15	I	123	ARG
16	J	36	VAL
16	J	75	ASP
17	K	129	VAL
18	L	4	VAL
18	L	14	ARG
18	L	15	LYS
18	L	52	VAL
18	L	55	VAL
19	M	14	HIS
23	Q	28	PHE
23	Q	42	THR
28	V	102	LYS
28	V	106	ILE
28	V	142	LYS
29	W	480	VAL
29	W	510	HIS
29	W	532	VAL
33	c	43	ARG
36	f	30	ARG
36	f	47	LYS
36	f	69	LYS
36	f	89	VAL
36	f	152	LEU
37	g	25	THR
37	g	104	ASN
38	h	4	ILE
38	h	15	LEU
38	h	37	VAL
40	j	58	LEU
42	l	6	ARG

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Mol	Chain	Res	Type
44	n	2	ASP
44	n	49	VAL
44	n	56	LYS
45	o	37	LYS
47	q	18	GLN
48	r	83	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	61	ASN
5	4	65	ASN
8	B	18	HIS
8	B	39	HIS
8	B	42	ASN
8	B	58	ASN
8	B	103	ASN
9	C	100	GLN
9	C	139	GLN
9	C	140	ASN
10	D	152	GLN
11	E	70	ASN
11	E	77	ASN
11	E	82	GLN
11	E	146	ASN
11	E	148	ASN
12	F	3	HIS
14	H	18	GLN
17	K	118	HIS
18	L	112	GLN
20	N	66	GLN
21	O	35	GLN
25	S	14	HIS
26	T	48	GLN
26	T	84	ASN
28	V	77	ASN
29	W	510	HIS
29	W	526	ASN
29	W	551	ASN
33	c	37	ASN
35	e	115	GLN
44	n	116	GLN

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Mol	Chain	Res	Type
46	p	44	GLN
46	p	72	ASN
47	q	12	HIS
47	q	43	ASN
51	u	12	GLN
51	u	49	ASN
54	x	45	GLN
55	y	20	HIS
56	z	6	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	Z	75/77 (97%)	17 (22%)	3 (4%)
31	a	2774/2930 (94%)	310 (11%)	0
32	b	118/119 (99%)	8 (6%)	0
6	9	6/24 (25%)	1 (16%)	0
7	A	1508/1554 (97%)	177 (11%)	37 (2%)
All	All	4481/4704 (95%)	513 (11%)	40 (0%)

All (513) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	9	19	G
7	A	4	U
7	A	5	U
7	A	8	A
7	A	9	G
7	A	32	A
7	A	39	G
7	A	47	C
7	A	48	C
7	A	51	A
7	A	69	G
7	A	71	A
7	A	72	A
7	A	73	C
7	A	74	A
7	A	75	G
7	A	81	A
7	A	82	G

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Mol	Chain	Res	Type
7	A	83	C
7	A	84	U
7	A	85	U
7	A	86	G
7	A	87	C
7	A	94	G
7	A	95	C
7	A	120	A
7	A	122	G
7	A	131	A
7	A	144	G
7	A	159	G
7	A	164	G
7	A	182	A
7	A	183	C
7	A	197	A
7	A	226	G
7	A	240	G
7	A	245	U
7	A	247	G
7	A	251	G
7	A	266	G
7	A	267	C
7	A	289	G
7	A	321	A
7	A	328	C
7	A	329	A
7	A	330	C
7	A	347	G
7	A	352	C
7	A	354	G
7	A	367	U
7	A	372	C
7	A	398	U
7	A	406	G
7	A	411	A
7	A	412	A
7	A	413	G
7	A	414	A
7	A	421	U
7	A	422	C
7	A	423	G

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Mol	Chain	Res	Type
7	A	424	G
7	A	429	U
7	A	438	U
7	A	439	U
7	A	457	G
7	A	467	U
7	A	468	A
7	A	469	C
7	A	484	G
7	A	486	U
7	A	508	U
7	A	511	C
7	A	518	C
7	A	521	G
7	A	531	U
7	A	532	A
7	A	536	C
7	A	547	A
7	A	559	A
7	A	562	U
7	A	572	A
7	A	573	A
7	A	576	C
7	A	596	A
7	A	633	G
7	A	650	G
7	A	654	G
7	A	665	A
7	A	688	G
7	A	723	U
7	A	724	G
7	A	734	G
7	A	755	G
7	A	777	A
7	A	793	U
7	A	794	A
7	A	815	A
7	A	817	C
7	A	832	G
7	A	849	G
7	A	874	G
7	A	887	G

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Mol	Chain	Res	Type
7	A	890	G
7	A	914	A
7	A	926	G
7	A	934	C
7	A	960	U
7	A	961	U
7	A	969	A
7	A	975	A
7	A	976	G
7	A	977	A
7	A	984	C
7	A	992	U
7	A	993	G
7	A	994	A
7	A	1004	A
7	A	1020	G
7	A	1027	C
7	A	1029	U
7	A	1030	U
7	A	1031	C
7	A	1033	G
7	A	1034	G
7	A	1035	A
7	A	1036	A
7	A	1039	G
7	A	1042	A
7	A	1044	A
7	A	1046	A
7	A	1065	U
7	A	1085	U
7	A	1094	G
7	A	1101	A
7	A	1137	C
7	A	1139	G
7	A	1145	A
7	A	1146	A
7	A	1196	A
7	A	1197	A
7	A	1212	U
7	A	1213	A
7	A	1214	C
7	A	1225	A

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Mol	Chain	Res	Type
7	A	1226	C
7	A	1227	A
7	A	1238	A
7	A	1256	A
7	A	1260	G
7	A	1275	A
7	A	1280	A
7	A	1287	A
7	A	1300	G
7	A	1317	C
7	A	1319	A
7	A	1320	C
7	A	1338	G
7	A	1346	A
7	A	1353	G
7	A	1363	A
7	A	1378	C
7	A	1379	G
7	A	1398	A
7	A	1419	G
7	A	1433	A
7	A	1447	A
7	A	1453	G
7	A	1492	A
7	A	1494	G
7	A	1497	G
7	A	1503	A
7	A	1505	G
7	A	1506	U
7	A	1517	G
7	A	1529	G
7	A	1530	G
7	A	1533	C
7	A	1534	A
30	Z	6	G
30	Z	9	G
30	Z	14	A
30	Z	17(A)	U
30	Z	18	G
30	Z	19	G
30	Z	21	A
30	Z	46	G

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Mol	Chain	Res	Type
30	Z	48	C
30	Z	50	U
30	Z	51	C
30	Z	58	A
30	Z	64	G
30	Z	65	C
30	Z	68	C
30	Z	75	C
30	Z	76	A
31	a	10	A
31	a	12	U
31	a	15	G
31	a	34	U
31	a	63	A
31	a	71	A
31	a	74	A
31	a	75	G
31	a	101	A
31	a	103	A
31	a	118	A
31	a	119	A
31	a	120	U
31	a	131	A
31	a	135	U
31	a	139	U
31	a	142	A
31	a	162	U
31	a	181	A
31	a	196	A
31	a	199	A
31	a	215	G
31	a	216	A
31	a	221	A
31	a	222	A
31	a	228	C
31	a	248	G
31	a	272	A
31	a	276	U
31	a	277	G
31	a	278	A
31	a	279	A
31	a	281	C

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Mol	Chain	Res	Type
31	a	285	G
31	a	289	G
31	a	311	A
31	a	330	A
31	a	346	A
31	a	353	C
31	a	354	A
31	a	361	G
31	a	362	A
31	a	386	G
31	a	411	G
31	a	412	A
31	a	451	U
31	a	481	G
31	a	491	G
31	a	503	A
31	a	504	A
31	a	505	A
31	a	509	C
31	a	513	A
31	a	531	C
31	a	532	A
31	a	533	G
31	a	544	C
31	a	545	U
31	a	547	A
31	a	548	G
31	a	549	G
31	a	555	G
31	a	556	A
31	a	563	A
31	a	573	U
31	a	574	A
31	a	575	A
31	a	586	A
31	a	603	A
31	a	613	A
31	a	614	A
31	a	615	U
31	a	627	A
31	a	637	A
31	a	645	C

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Mol	Chain	Res	Type
31	a	646	U
31	a	647	G
31	a	653	U
31	a	654	A
31	a	655	A
31	a	686	U
31	a	716	A
31	a	717	C
31	a	730	A
31	a	747	5MU
31	a	764	A
31	a	765	C
31	a	775	G
31	a	776	G
31	a	782	A
31	a	784	G
31	a	785	G
31	a	805	G
31	a	812	C
31	a	827	U
31	a	828	U
31	a	845	A
31	a	846	U
31	a	858	G
31	a	859	G
31	a	910	A
31	a	914	G
31	a	915	C
31	a	931	U
31	a	934	U
31	a	946	C
31	a	961	C
31	a	974	G
31	a	983	A
31	a	996	A
31	a	1012	U
31	a	1013	C
31	a	1022	G
31	a	1026	G
31	a	1033	U
31	a	1041	G
31	a	1047	G

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Mol	Chain	Res	Type
31	a	1054	A
31	a	1059	G
31	a	1060	U
31	a	1061	U
31	a	1069	A
31	a	1070	A
31	a	1077	A
31	a	1080	A
31	a	1083	U
31	a	1087	G
31	a	1088	A
31	a	1091	G
31	a	1101	U
31	a	1112	G
31	a	1116	G
31	a	1130	U
31	a	1132	U
31	a	1133	A
31	a	1134	A
31	a	1135	C
31	a	1142	A
31	a	1169	A
31	a	1170	C
31	a	1179	G
31	a	1253	A
31	a	1256	G
31	a	1271	G
31	a	1272	A
31	a	1273	U
31	a	1300	G
31	a	1301	A
31	a	1302	A
31	a	1303	G
31	a	1321	A
31	a	1352	U
31	a	1365	A
31	a	1379	U
31	a	1383	A
31	a	1409	U
31	a	1411	U
31	a	1416	G
31	a	1419	A

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Mol	Chain	Res	Type
31	a	1428	C
31	a	1452	G
31	a	1453	A
31	a	1455	G
31	a	1458	U
31	a	1460	U
31	a	1482	G
31	a	1490	A
31	a	1493	C
31	a	1494	A
31	a	1508	A
31	a	1509	A
31	a	1510	G
31	a	1515	A
31	a	1534	U
31	a	1535	A
31	a	1536	C
31	a	1537	G
31	a	1538	G
31	a	1569	A
31	a	1578	U
31	a	1585	C
31	a	1608	A
31	a	1647	U
31	a	1648	U
31	a	1649	G
31	a	1674	G
31	a	1715	G
31	a	1729	U
31	a	1730	C
31	a	1734	G
31	a	1737	G
31	a	1738	G
31	a	1744	A
31	a	1764	C
31	a	1773	A
31	a	1782	U
31	a	1791	A
31	a	1800	C
31	a	1801	A
31	a	1808	A
31	a	1809	A

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Mol	Chain	Res	Type
31	a	1816	C
31	a	1847	A
31	a	1848	A
31	a	1858	A
31	a	1870	C
31	a	1871	A
31	a	1872	A
31	a	1873	G
31	a	1906	G
31	a	1907	G
31	a	1913	A
31	a	1914	C
31	a	1929	G
31	a	1930	G
31	a	1931	U
31	a	1937	A
31	a	1938	A
31	a	1955	U
31	a	1967	C
31	a	1970	A
31	a	1971	U
31	a	1972	G
31	a	1991	U
31	a	1993	U
31	a	2020	A
31	a	2023	C
31	a	2031	A
31	a	2033	A
31	a	2043	C
31	a	2055	C
31	a	2056	G
31	a	2060	A
31	a	2061	G
31	a	2062	A
31	a	2069	G7M
31	a	2093	G
31	a	2096	C
31	a	2193	G
31	a	2198	A
31	a	2204	G
31	a	2211	A
31	a	2225	A

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Mol	Chain	Res	Type
31	a	2238	G
31	a	2268	A
31	a	2278	A
31	a	2283	C
31	a	2287	A
31	a	2288	A
31	a	2305	U
31	a	2308	G
31	a	2312	U
31	a	2322	A
31	a	2324	U
31	a	2325	G
31	a	2333	A
31	a	2335	A
31	a	2347	C
31	a	2350	C
31	a	2366	A
31	a	2383	G
31	a	2385	C
31	a	2402	U
31	a	2406	A
31	a	2425	A
31	a	2428	G
31	a	2429	G
31	a	2430	A
31	a	2431	U
31	a	2435	A
31	a	2441	U
31	a	2448	A
31	a	2469	A
31	a	2476	A
31	a	2478	A
31	a	2491	U
31	a	2502	G
31	a	2505	G
31	a	2518	A
31	a	2529	G
31	a	2547	A
31	a	2566	A
31	a	2567	G
31	a	2573	C
31	a	2602	A

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Mol	Chain	Res	Type
31	a	2609	U
31	a	2613	U
31	a	2629	U
31	a	2663	G
31	a	2689	U
31	a	2690	U
31	a	2714	G
31	a	2716	C
31	a	2726	A
31	a	2744	G
31	a	2748	A
31	a	2750	A
31	a	2757	A
31	a	2765	A
31	a	2778	A
31	a	2791	G
31	a	2798	U
31	a	2799	A
31	a	2803	G
31	a	2809	A
31	a	2820	A
31	a	2821	A
31	a	2874	C
31	a	2883	A
31	a	2884	U
32	b	35	C
32	b	36	C
32	b	37	C
32	b	44	G
32	b	56	G
32	b	89	U
32	b	90	C
32	b	109	A

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	7	A
7	A	12	U
7	A	70	U
7	A	73	C
7	A	119	A

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Mol	Chain	Res	Type
7	A	121	U
7	A	199	A
7	A	305	G
7	A	412	A
7	A	438	U
7	A	531	U
7	A	595	A
7	A	641	U
7	A	702	A
7	A	884	U
7	A	991	U
7	A	992	U
7	A	993	G
7	A	1034	G
7	A	1035	A
7	A	1042	A
7	A	1047	G
7	A	1094	G
7	A	1124	G
7	A	1129	C
7	A	1145	A
7	A	1196	A
7	A	1211	U
7	A	1225	A
7	A	1298	U
7	A	1319	A
7	A	1320	C
7	A	1397	C
7	A	1447	A
7	A	1452	C
7	A	1459	G
7	A	1505	G
30	Z	7	G
30	Z	17(A)	U
30	Z	18	G

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

39 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
7	PSU	A	516	59,7	18,21,22	0.90	1 (5%)	22,30,33	0.64	0
31	5MC	a	1962	31	18,22,23	0.33	0	26,32,35	0.48	0
7	5MC	A	1407	7	18,22,23	0.33	0	26,32,35	0.58	0
31	OMC	a	2498	31,59	19,22,23	0.27	0	26,31,34	0.48	0
31	G7M	a	2069	31	20,26,27	1.15	3 (15%)	17,39,42	0.48	0
7	5MC	A	967	7	18,22,23	0.32	0	26,32,35	0.49	0
7	4OC	A	1402	7	20,23,24	0.37	0	26,32,35	0.49	0
7	2MG	A	1207	58,7	18,26,27	1.02	2 (11%)	16,38,41	0.75	0
7	MA6	A	1519	7	18,26,27	0.74	0	19,38,41	0.56	0
34	MEQ	d	150	34	8,9,10	0.42	0	5,10,12	0.54	0
31	2MG	a	2445	31	18,26,27	1.03	2 (11%)	16,38,41	0.69	0
7	G7M	A	527	7	20,26,27	1.14	2 (10%)	17,39,42	0.50	0
7	UR3	A	1498	7	19,22,23	0.28	0	26,32,35	0.68	0
31	5MU	a	1939	31,58	19,22,23	0.28	0	28,32,35	0.35	0
31	OMU	a	2552	31	19,22,23	0.20	0	26,31,34	0.46	0
18	D2T	L	89	18	7,9,10	0.95	0	6,11,13	2.24	4 (66%)
42	4D4	l	81	42	9,11,12	0.50	0	8,13,15	0.60	0
31	2MG	a	1835	31	18,26,27	1.04	2 (11%)	16,38,41	0.67	0
17	IAS	K	119	17	6,7,8	0.92	0	6,8,10	1.01	0
31	PSU	a	2605	31	18,21,22	0.93	1 (5%)	22,30,33	0.74	0
31	3TD	a	1915	31	18,22,23	0.96	1 (5%)	22,32,35	0.63	0
31	PSU	a	2604	31	18,21,22	0.91	1 (5%)	22,30,33	0.69	0
31	6MZ	a	1618	31	18,25,26	0.67	0	16,36,39	0.70	1 (6%)
31	PSU	a	2504	31,58	18,21,22	0.89	1 (5%)	22,30,33	0.69	0
31	PSU	a	1917	31	18,21,22	0.90	1 (5%)	22,30,33	0.54	0
31	H2U	a	2449	31	18,21,22	0.61	0	21,30,33	0.85	2 (9%)
31	6MZ	a	2030	31	18,25,26	0.68	0	16,36,39	0.77	1 (6%)
31	OMG	a	2251	31,58,30	18,26,27	1.00	2 (11%)	19,38,41	0.69	0
31	2MA	a	2503	31,59,58	19,25,26	1.03	1 (5%)	21,37,40	1.81	5 (23%)
31	PSU	a	2580	31,58	18,21,22	0.94	1 (5%)	22,30,33	0.78	1 (4%)
31	5MU	a	747	31	19,22,23	0.27	0	28,32,35	0.37	0
31	PSU	a	955	31	18,21,22	0.92	1 (5%)	22,30,33	0.58	0
7	2MG	A	966	7	18,26,27	1.01	2 (11%)	16,38,41	0.81	0
31	PSU	a	2457	31	18,21,22	0.91	1 (5%)	22,30,33	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MA6	A	1518	7	18,26,27	0.75	0	19,38,41	0.46	0
31	PSU	a	1911	31	18,21,22	0.89	1 (5%)	22,30,33	0.65	0
7	2MG	A	1516	7	18,26,27	1.01	2 (11%)	16,38,41	0.79	0
31	PSU	a	746	31,59	18,21,22	0.91	1 (5%)	22,30,33	0.62	0
31	1MG	a	745	31	18,26,27	0.97	1 (5%)	19,39,42	0.53	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
7	PSU	A	516	59,7	-	0/7/25/26	0/2/2/2
31	5MC	a	1962	31	-	4/7/25/26	0/2/2/2
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
31	OMC	a	2498	31,59	-	0/9/27/28	0/2/2/2
31	G7M	a	2069	31	-	2/3/25/26	0/3/3/3
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
7	2MG	A	1207	58,7	-	0/5/27/28	0/3/3/3
7	MA6	A	1519	7	-	0/7/29/30	0/3/3/3
34	MEQ	d	150	34	-	2/8/9/11	-
31	2MG	a	2445	31	-	0/5/27/28	0/3/3/3
7	G7M	A	527	7	-	1/3/25/26	0/3/3/3
7	UR3	A	1498	7	-	0/7/25/26	0/2/2/2
31	5MU	a	1939	31,58	-	0/7/25/26	0/2/2/2
31	OMU	a	2552	31	-	0/9/27/28	0/2/2/2
18	D2T	L	89	18	-	2/7/12/14	-
42	4D4	l	81	42	-	1/11/12/14	-
31	2MG	a	1835	31	-	0/5/27/28	0/3/3/3
17	IAS	K	119	17	-	2/7/7/8	-
31	PSU	a	2605	31	-	0/7/25/26	0/2/2/2
31	3TD	a	1915	31	-	2/7/25/26	0/2/2/2
31	PSU	a	2604	31	-	0/7/25/26	0/2/2/2
31	6MZ	a	1618	31	-	0/5/27/28	0/3/3/3
31	PSU	a	2504	31,58	-	0/7/25/26	0/2/2/2
31	PSU	a	1917	31	-	0/7/25/26	0/2/2/2
31	H2U	a	2449	31	-	0/7/38/39	0/2/2/2
31	6MZ	a	2030	31	-	2/5/27/28	0/3/3/3
31	OMG	a	2251	31,58,30	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	2MA	a	2503	31,59,58	-	2/3/25/26	0/3/3/3
31	PSU	a	2580	31,58	-	0/7/25/26	0/2/2/2
31	5MU	a	747	31	-	0/7/25/26	0/2/2/2
31	PSU	a	955	31	-	0/7/25/26	0/2/2/2
7	2MG	A	966	7	-	0/5/27/28	0/3/3/3
31	PSU	a	2457	31	-	0/7/25/26	0/2/2/2
7	MA6	A	1518	7	-	0/7/29/30	0/3/3/3
31	PSU	a	1911	31	-	2/7/25/26	0/2/2/2
7	2MG	A	1516	7	-	0/5/27/28	0/3/3/3
31	PSU	a	746	31,59	-	3/7/25/26	0/2/2/2
31	1MG	a	745	31	-	0/3/25/26	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	2580	PSU	C6-C5	3.74	1.39	1.35
31	a	2605	PSU	C6-C5	3.66	1.39	1.35
31	a	1915	3TD	C6-C5	3.64	1.39	1.35
31	a	746	PSU	C6-C5	3.62	1.39	1.35
31	a	2457	PSU	C6-C5	3.59	1.39	1.35
31	a	955	PSU	C6-C5	3.58	1.39	1.35
7	A	516	PSU	C6-C5	3.55	1.39	1.35
31	a	1917	PSU	C6-C5	3.53	1.39	1.35
31	a	2504	PSU	C6-C5	3.53	1.39	1.35
31	a	2604	PSU	C6-C5	3.53	1.39	1.35
31	a	1911	PSU	C6-C5	3.51	1.39	1.35
7	A	527	G7M	C8-N9	3.46	1.39	1.33
31	a	2069	G7M	C8-N9	3.42	1.39	1.33
31	a	2069	G7M	C8-N7	2.66	1.38	1.33
31	a	2251	OMG	C5-C6	-2.61	1.42	1.47
31	a	1835	2MG	C5-C6	-2.53	1.42	1.47
7	A	527	G7M	C8-N7	2.53	1.37	1.33
7	A	1207	2MG	C5-C6	-2.49	1.42	1.47
31	a	2445	2MG	C5-C6	-2.48	1.42	1.47
7	A	966	2MG	C5-C6	-2.48	1.42	1.47
7	A	1516	2MG	C5-C6	-2.42	1.42	1.47
31	a	2503	2MA	C6-N1	2.22	1.37	1.33
31	a	745	1MG	C5-C4	-2.19	1.37	1.43
31	a	1835	2MG	C8-N7	-2.17	1.31	1.35
31	a	2251	OMG	C8-N7	-2.12	1.31	1.35
31	a	2069	G7M	C5-C6	-2.09	1.40	1.45
7	A	1516	2MG	C8-N7	-2.07	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	2445	2MG	C8-N7	-2.04	1.31	1.35
7	A	966	2MG	C8-N7	-2.02	1.31	1.35
7	A	1207	2MG	C8-N7	-2.02	1.31	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	2503	2MA	C5-C6-N1	-5.49	117.40	121.01
31	a	2503	2MA	C5-C6-N6	4.23	126.79	120.35
18	L	89	D2T	CB-CA-N	3.81	117.23	109.10
31	a	2503	2MA	CM2-C2-N1	2.85	121.61	117.15
18	L	89	D2T	OD1-CG-CB	-2.53	117.15	122.44
31	a	2449	H2U	O2-C2-N1	-2.31	120.20	123.11
31	a	2580	PSU	C3'-C2'-C1'	2.30	104.32	101.64
31	a	2449	H2U	N3-C2-N1	2.17	118.95	116.65
31	a	2030	6MZ	C2-N1-C6	2.17	118.45	116.59
31	a	2503	2MA	C2-N1-C6	2.17	121.46	118.08
18	L	89	D2T	OD2-CG-CB	2.16	117.83	113.15
31	a	2503	2MA	N3-C2-N1	-2.16	121.80	125.73
18	L	89	D2T	O-C-CA	-2.07	119.34	124.78
31	a	1618	6MZ	C2-N1-C6	2.01	118.31	116.59

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	a	746	PSU	C2'-C1'-C5-C4
31	a	1911	PSU	O4'-C1'-C5-C4
31	a	1911	PSU	O4'-C1'-C5-C6
31	a	1915	3TD	C3'-C4'-C5'-O5'
31	a	1915	3TD	O4'-C4'-C5'-O5'
31	a	2030	6MZ	O4'-C4'-C5'-O5'
31	a	2251	OMG	C1'-C2'-O2'-CM2
31	a	2030	6MZ	C3'-C4'-C5'-O5'
34	d	150	MEQ	NE2-CD-CG-CB
34	d	150	MEQ	OE1-CD-CG-CB
18	L	89	D2T	CG-CB-SB-CB1
31	a	2069	G7M	C4'-C5'-O5'-P
31	a	2503	2MA	C4'-C5'-O5'-P
31	a	746	PSU	O4'-C1'-C5-C4
31	a	1962	5MC	O4'-C1'-N1-C6
31	a	1962	5MC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
17	K	119	IAS	O-C-CA-N
18	L	89	D2T	SB-CB-CG-OD2
7	A	527	G7M	C3'-C4'-C5'-O5'
31	a	2503	2MA	O4'-C4'-C5'-O5'
31	a	746	PSU	O4'-C1'-C5-C6
17	K	119	IAS	CA-CB-CG-OD1
31	a	2069	G7M	O4'-C4'-C5'-O5'
31	a	1962	5MC	O4'-C1'-N1-C2
42	l	81	4D4	O-C-CA-CB
31	a	1962	5MC	C2'-C1'-N1-C2

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 417 ligands modelled in this entry, 417 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.