



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 08:12 pm GMT

PDB ID : 6XZ7  
EMDB ID : EMD-10655  
Title : E. coli 50S ribosomal subunit in complex with dirithromycin, fMet-Phe-tRNA(Phe) and deacylated tRNA(iMet).  
Authors : Pichkur, E.B.; Polikanov, Y.S.; Myasnikov, A.G.; Konevega, A.L.  
Deposited on : 2020-02-03  
Resolution : 2.10 Å(reported)  
Based on initial model : 4YBB

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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  
buster-report : 1.1.7 (2018)  
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

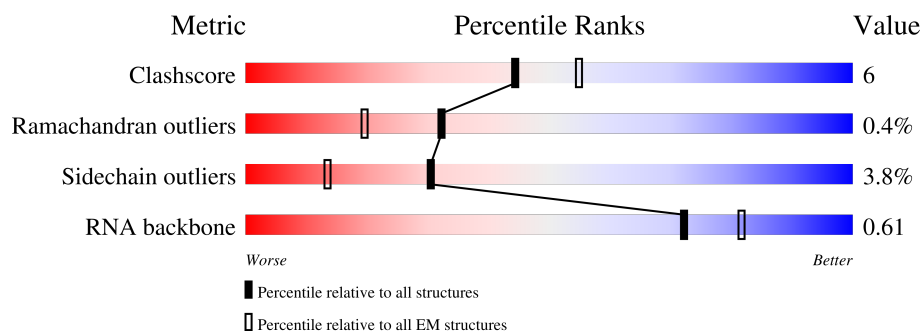
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.10 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)
Clashscore	210492	15764
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  $\geq 3$ , 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	A	2897	76% 21% .
2	B	120	80% 18% .
3	C	271	85% 15%
4	D	209	89% 11%
5	E	201	88% 11% .
6	F	177	54% 40% 6% .
7	G	176	70% 26% .

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Mol	Chain	Length	Quality of chain
8	H	135	<div><div></div><div>68%</div><div>29%</div><div></div></div> ..
9	I	134	<div><div></div><div>77%</div><div>21%</div><div></div></div> .
10	J	142	<div><div></div><div>87%</div><div>12%</div><div></div></div> .
11	K	123	<div><div></div><div>85%</div><div>15%</div><div></div></div>
12	L	144	<div><div></div><div>87%</div><div>13%</div><div></div></div>
13	M	136	<div><div></div><div>88%</div><div>11%</div><div></div></div> .
14	N	125	<div><div></div><div>93%</div><div>6%</div><div></div></div> .
15	O	117	<div><div></div><div>80%</div><div>19%</div><div></div></div> .
16	P	114	<div><div></div><div>84%</div><div>15%</div><div></div></div> .
17	Q	117	<div><div></div><div>97%</div><div></div><div></div></div> .
18	R	103	<div><div></div><div>90%</div><div>7%</div><div></div></div> ..
19	S	110	<div><div></div><div>92%</div><div>7%</div><div></div></div> .
20	T	93	<div><div></div><div>85%</div><div>14%</div><div></div></div> .
21	U	102	<div><div></div><div>86%</div><div>13%</div><div></div></div> .
22	V	94	<div><div></div><div>81%</div><div>18%</div><div></div></div> .
23	W	76	<div><div></div><div>87%</div><div>13%</div><div></div></div>
24	X	77	<div><div></div><div>88%</div><div>12%</div><div></div></div>
25	Y	62	<div><div></div><div>89%</div><div>11%</div><div></div></div>
26	Z	58	<div><div></div><div>90%</div><div>9%</div><div></div></div> .
27	a	56	<div><div></div><div>98%</div><div></div><div></div></div> .
28	b	51	<div><div></div><div>98%</div><div></div><div></div></div> .
29	c	46	<div><div></div><div>96%</div><div></div><div></div></div> .
30	d	64	<div><div></div><div>94%</div><div>6%</div><div></div></div>
31	e	38	<div><div></div><div>97%</div><div></div><div></div></div> .
32	f	76	<div><div></div><div>24%</div><div>55%</div><div>21%</div><div></div></div>



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Mol	Chain	Length	Quality of chain
33	g	76	 22% 47% 30%

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 94915 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2897	Total	C	N	O	P	3	0
			62252	27778	11454	20121	2899		

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	209	Total	C	N	O	S	1	0
			1566	980	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	135	Total	C	N	O	S	0	0
			1023	649	179	192	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	85	VAL	SER	conflict	UNP P0A7J3
H	86	THR	MET	conflict	UNP P0A7J3

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	136	Total	C	N	O	S	1	0
			1075	686	205	178	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	102	Total	C	N	O	S	0	0
			780	492	146	142			

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	76	Total	C	N	O	S	1	0
			580	359	117	103	1		

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

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

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

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

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

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

- Molecule 27 is a protein called 50S ribosomal protein L32.



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

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	51	Total	C	N	O		0	0
			414	266	76	72			

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

- Molecule 32 is a RNA chain called Deacylated tRNAi(Met).

Mol	Chain	Residues	Atoms						AltConf	Trace
32	f	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

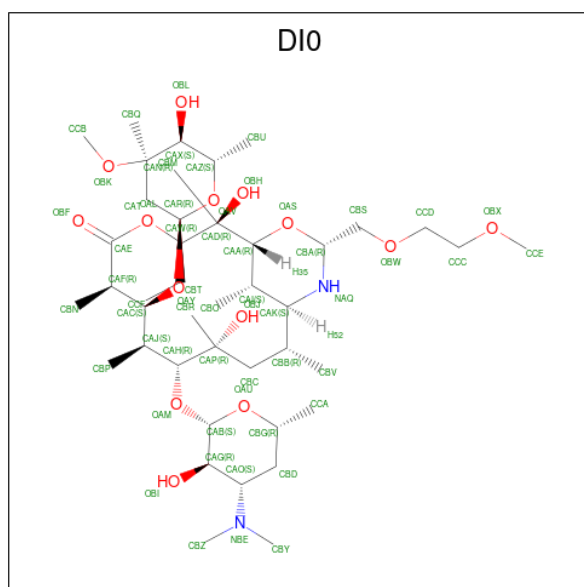
- Molecule 33 is a RNA chain called fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	g	76	Total	C	N	O	P	S	0	0
			1667	760	297	534	75	1		

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
34	A	174	Total Mg 174 174	0
34	B	3	Total Mg 3 3	0
34	U	1	Total Mg 1 1	0

- Molecule 35 is Dirithromycin (three-letter code: DI0) (formula:  $\text{C}_{42}\text{H}_{78}\text{N}_2\text{O}_{14}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			58	42	2	14	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	A	498	Total O 498 498	0
36	B	9	Total O 9 9	0
36	C	7	Total O 7 7	0
36	D	1	Total O 1 1	0
36	E	1	Total O 1 1	0

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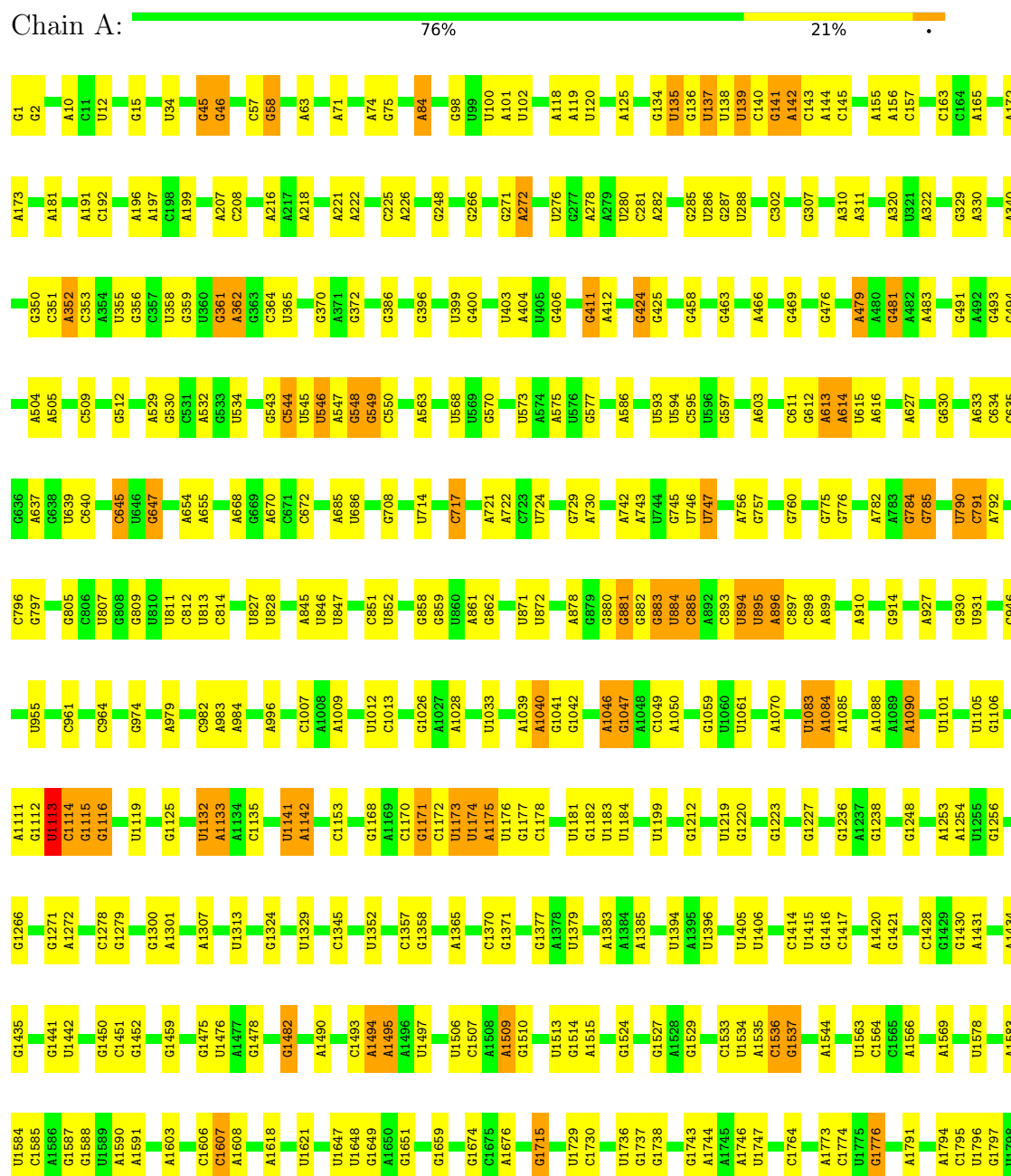
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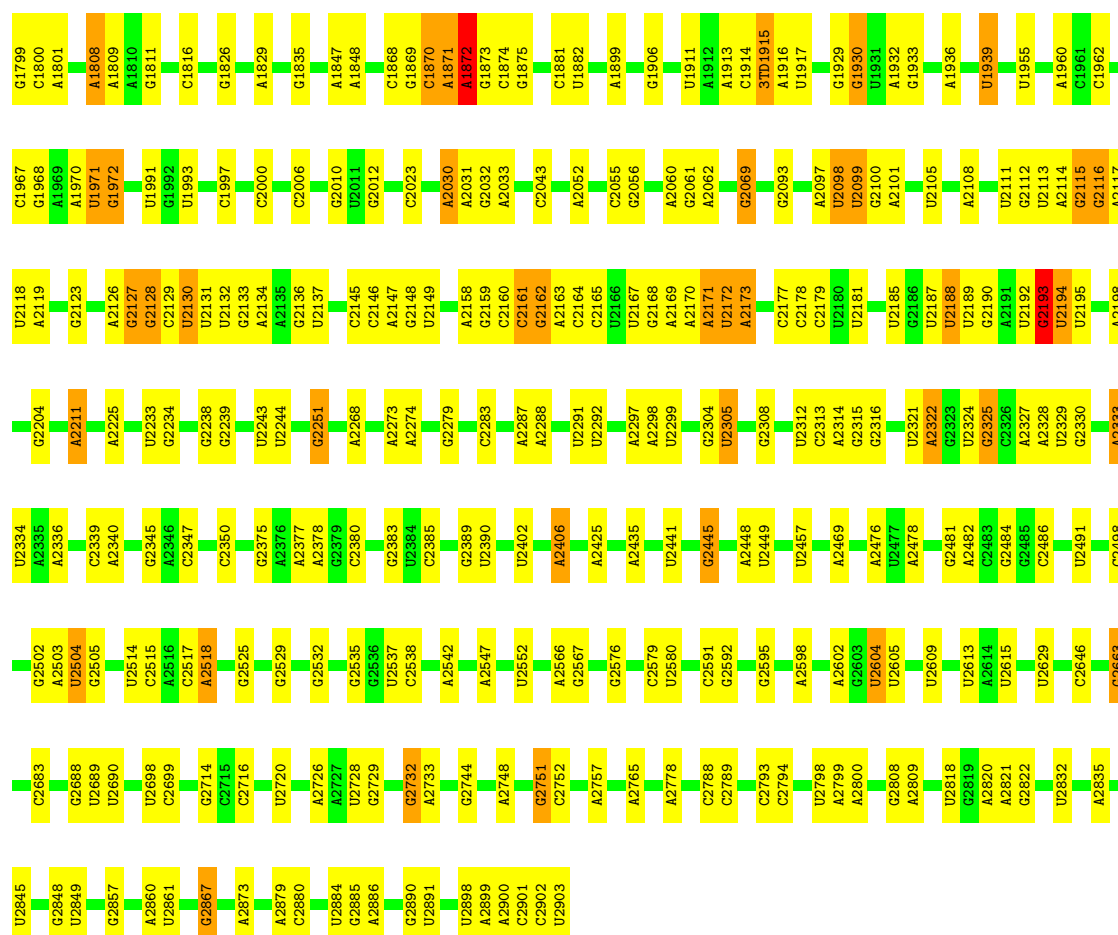
Mol	Chain	Residues	Atoms		AltConf
36	L	6	Total 6	O 6	0
36	N	1	Total 1	O 1	0
36	T	1	Total 1	O 1	0
36	d	4	Total 4	O 4	0

### 3 Residue-property plots

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

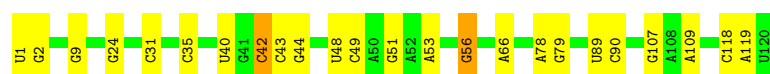
#### • Molecule 1: 23S rRNA





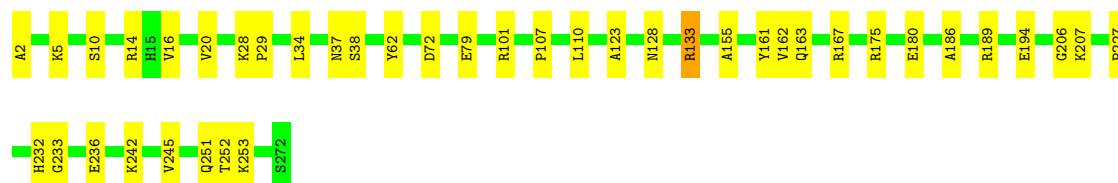
• Molecule 2: 5S rRNA

Chain B: 80% 18% .



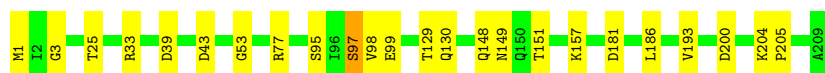
• Molecule 3: 50S ribosomal protein L2

Chain C: 85% 15%



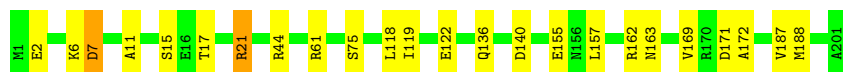
• Molecule 4: 50S ribosomal protein L3

Chain D: 89% 11%



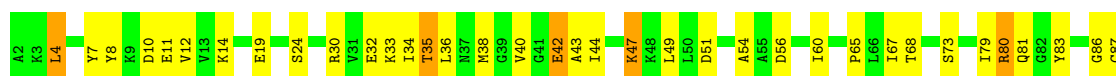
- Molecule 5: 50S ribosomal protein L4

Chain E: 88% 11% .



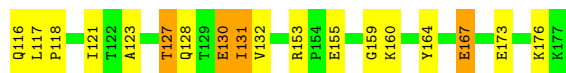
- Molecule 6: 50S ribosomal protein L5

Chain F: 54% 40% 6% .



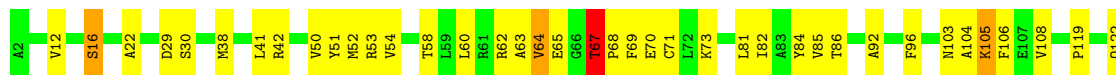
- Molecule 7: 50S ribosomal protein L6

Chain G: 70% 26% .



- Molecule 8: 50S ribosomal protein L10

Chain H: 68% 29% ..




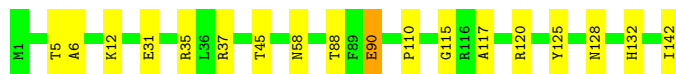
- Molecule 9: 50S ribosomal protein L11

Chain I: 77% 21% .




- Molecule 10: 50S ribosomal protein L13

Chain J:  87% 12%



- Molecule 11: 50S ribosomal protein L14

Chain K:  85% 15%



- Molecule 12: 50S ribosomal protein L15

Chain L:  87% 13%



- Molecule 13: 50S ribosomal protein L16

Chain M:  88% 11%




- Molecule 14: 50S ribosomal protein L17

Chain N:  93% 6%




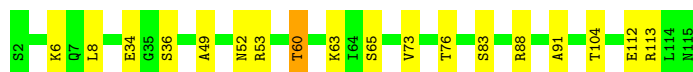
- Molecule 15: 50S ribosomal protein L18

Chain O:  80% 19%



- Molecule 16: 50S ribosomal protein L19

Chain P:  84% 15%




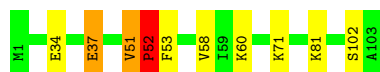
- Molecule 17: 50S ribosomal protein L20

Chain Q:  97% .




- Molecule 18: 50S ribosomal protein L21

Chain R:  90% 7% ..




- Molecule 19: 50S ribosomal protein L22

Chain S:  92% 7% .




- Molecule 20: 50S ribosomal protein L23

Chain T:  85% 14% .




- Molecule 21: 50S ribosomal protein L24

Chain U:  86% 13% .



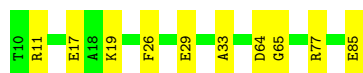
- Molecule 22: 50S ribosomal protein L25

Chain V:  81% 18% .




- Molecule 23: 50S ribosomal protein L27

Chain W:  87% 13%




- Molecule 24: 50S ribosomal protein L28



Chain X:  88% 12%




- Molecule 25: 50S ribosomal protein L29

Chain Y:  89% 11%



- Molecule 26: 50S ribosomal protein L30

Chain Z:  90% 9% .



- Molecule 27: 50S ribosomal protein L32

Chain a:  98% .



- Molecule 28: 50S ribosomal protein L33

Chain b:  98% .



- Molecule 29: 50S ribosomal protein L34

Chain c:  96% .



- Molecule 30: 50S ribosomal protein L35

Chain d:  94% 6%



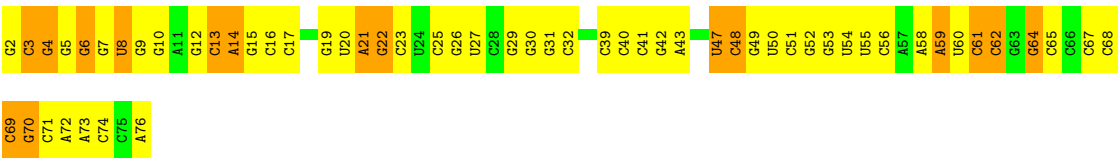
- Molecule 31: 50S ribosomal protein L36

Chain e:  97% .

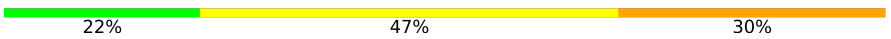


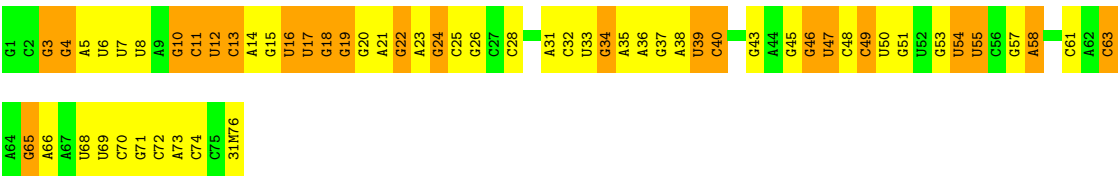
● Molecule 32: Deacylated tRNAi(Met)

Chain f:  24% 55% 21%



● Molecule 33: fMet-Phe-tRNA(Phe)

Chain g:  22% 47% 30%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	401905	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 2MA, OMC, 6MZ, DI0, 4D4, PSU, MG, M2G, OMU, 1MG, 2MG, 4SU, OMG, MEQ, 1MA, 5MU, H2U, YYG, 5MC, 3TD, 31M, 7MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.72	1/69172 (0.0%)	0.74	7/107908 (0.0%)
2	B	0.56	0/2872	0.71	0/4478
3	C	0.37	0/2122	0.46	0/2852
4	D	0.36	0/1576	0.46	0/2119
5	E	0.34	0/1571	0.44	0/2113
6	F	0.29	0/1435	0.45	0/1926
7	G	0.30	0/1343	0.46	0/1816
8	H	0.42	0/1037	0.56	0/1402
9	I	0.47	0/993	0.64	0/1341
10	J	0.37	0/1152	0.43	0/1551
11	K	0.36	0/955	0.47	0/1279
12	L	0.34	0/1062	0.47	0/1413
13	M	0.36	0/1081	0.45	0/1443
14	N	0.35	0/1006	0.44	0/1345
15	O	0.31	0/910	0.44	0/1219
16	P	0.36	0/929	0.45	0/1242
17	Q	0.40	0/960	0.38	0/1278
18	R	0.41	0/829	0.54	1/1107 (0.1%)
19	S	0.36	0/864	0.45	0/1156
20	T	0.32	0/745	0.42	0/994
21	U	0.33	0/788	0.48	1/1051 (0.1%)
22	V	0.33	0/766	0.42	0/1025
23	W	0.37	0/587	0.44	0/776
24	X	0.37	0/635	0.46	0/848
25	Y	0.27	0/502	0.37	0/667
26	Z	0.31	0/453	0.44	0/605
27	a	0.35	0/450	0.45	0/599
28	b	0.32	0/421	0.44	0/561
29	c	0.34	0/380	0.43	0/498
30	d	0.38	0/513	0.46	0/676
31	e	0.35	0/303	0.44	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	f	0.80	4/1725 (0.2%)	1.72	77/2689 (2.9%)
33	g	0.68	1/1458 (0.1%)	1.38	33/2272 (1.5%)
All	All	0.64	6/101595 (0.0%)	0.73	119/152646 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	59	A	O3'-P	-6.50	1.53	1.61
32	f	39	C	O3'-P	-6.25	1.53	1.61
32	f	12	G	O3'-P	-6.06	1.53	1.61
32	f	25	C	O3'-P	-6.00	1.53	1.61
1	A	1774	C	O3'-P	-5.19	1.54	1.61

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	62	C	N1-C1'-C2'	-11.72	98.76	114.00
32	f	30	G	N9-C1'-C2'	-10.75	100.03	114.00
33	g	13	C	C4'-C3'-O3'	9.83	132.66	113.00
33	g	13	C	N1-C1'-C2'	-9.76	101.27	112.00
33	g	24	G	N9-C1'-C2'	-9.75	101.28	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	R	51	VAL	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62252	0	31324	392	0
2	B	2569	0	1301	13	0
3	C	2083	0	2154	22	0
4	D	1566	0	1617	14	0
5	E	1552	0	1619	13	0
6	F	1411	0	1444	95	0
7	G	1323	0	1371	31	0
8	H	1023	0	1052	36	0
9	I	979	0	1028	30	0
10	J	1129	0	1162	10	0
11	K	946	0	1023	10	0
12	L	1053	0	1129	12	0
13	M	1075	0	1155	10	0
14	N	993	0	1034	6	0
15	O	900	0	935	18	0
16	P	917	0	962	10	0
17	Q	947	0	1019	3	0
18	R	816	0	839	7	0
19	S	857	0	922	5	0
20	T	739	0	807	14	0
21	U	780	0	830	7	0
22	V	753	0	780	11	0
23	W	580	0	593	5	0
24	X	625	0	652	4	0
25	Y	501	0	531	3	0
26	Z	449	0	487	3	0
27	a	444	0	458	0	0
28	b	414	0	442	0	0
29	c	377	0	418	0	0
30	d	504	0	572	0	0
31	e	302	0	343	0	0
32	f	1625	0	829	0	0
33	g	1667	0	880	0	0
34	A	174	0	0	0	0
34	B	3	0	0	0	0
34	U	1	0	0	0	0
35	A	58	0	0	1	0
36	A	498	0	0	13	0
36	B	9	0	0	0	0
36	C	7	0	0	1	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	L	6	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	d	4	0	0	0	0
All	All	94915	0	61712	730	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 730 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:G:N2	1:A:894:U:O2	1.56	1.37
1:A:1:G:N2	1:A:2902:C:O2	1.64	1.30
9:I:98:VAL:O	9:I:138:LEU:HD23	1.22	1.25
1:A:1:G:N1	1:A:2902:C:N3	1.92	1.17
1:A:1050:A:N3	1:A:2751:G:C2	2.13	1.17

There are no symmetry-related clashes.

## 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	
3	C	269/271 (99%)	265 (98%)	4 (2%)	0	100	100
4	D	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	25	23
5	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
6	F	175/177 (99%)	163 (93%)	11 (6%)	1 (1%)	22	19
7	G	174/176 (99%)	168 (97%)	5 (3%)	1 (1%)	22	19
8	H	133/135 (98%)	109 (82%)	18 (14%)	6 (4%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	3	1
10	J	140/142 (99%)	140 (100%)	0	0	100	100
11	K	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
12	L	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
13	M	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
14	N	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
15	O	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
16	P	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
17	Q	115/117 (98%)	115 (100%)	0	0	100	100
18	R	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	13	9
19	S	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
20	T	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
21	U	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
22	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	W	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
24	X	75/77 (97%)	75 (100%)	0	0	100	100
25	Y	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	Z	56/58 (97%)	56 (100%)	0	0	100	100
27	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
28	b	49/51 (96%)	49 (100%)	0	0	100	100
29	c	44/46 (96%)	44 (100%)	0	0	100	100
30	d	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	e	36/38 (95%)	36 (100%)	0	0	100	100
All	All	3291/3351 (98%)	3184 (97%)	93 (3%)	14 (0%)	32	29

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	104	ALA
8	H	106	PHE
9	I	15	ALA
9	I	19	ASN
18	R	52	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	
3	C	216/216 (100%)	213 (99%)	3 (1%)	62	70
4	D	163/163 (100%)	160 (98%)	3 (2%)	54	61
5	E	165/165 (100%)	158 (96%)	7 (4%)	25	26
6	F	148/148 (100%)	127 (86%)	21 (14%)	2	1
7	G	137/137 (100%)	125 (91%)	12 (9%)	8	5
8	H	103/103 (100%)	97 (94%)	6 (6%)	17	15
9	I	104/104 (100%)	102 (98%)	2 (2%)	52	59
10	J	116/116 (100%)	112 (97%)	4 (3%)	32	35
11	K	104/104 (100%)	102 (98%)	2 (2%)	52	59
12	L	103/103 (100%)	101 (98%)	2 (2%)	52	59
13	M	108/108 (100%)	104 (96%)	4 (4%)	29	31
14	N	102/102 (100%)	101 (99%)	1 (1%)	73	79
15	O	87/87 (100%)	85 (98%)	2 (2%)	45	51
16	P	99/99 (100%)	93 (94%)	6 (6%)	15	13
17	Q	89/89 (100%)	89 (100%)	0	100	100
18	R	84/84 (100%)	82 (98%)	2 (2%)	44	49
19	S	93/93 (100%)	91 (98%)	2 (2%)	47	53
20	T	80/80 (100%)	77 (96%)	3 (4%)	28	30
21	U	83/83 (100%)	79 (95%)	4 (5%)	21	21
22	V	78/78 (100%)	76 (97%)	2 (3%)	41	46
23	W	57/58 (98%)	56 (98%)	1 (2%)	54	61
24	X	67/67 (100%)	65 (97%)	2 (3%)	36	40
25	Y	54/54 (100%)	52 (96%)	2 (4%)	29	31
26	Z	48/48 (100%)	46 (96%)	2 (4%)	25	26
27	a	47/47 (100%)	46 (98%)	1 (2%)	48	55
28	b	45/46 (98%)	44 (98%)	1 (2%)	47	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	c	38/38 (100%)	36 (95%)	2 (5%)	19	18
30	d	51/51 (100%)	47 (92%)	4 (8%)	10	8
31	e	34/34 (100%)	33 (97%)	1 (3%)	37	41
All	All	2703/2705 (100%)	2599 (96%)	104 (4%)	30	30

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	142	ILE
16	P	60	THR
30	d	15	LYS
11	K	109	SER
13	M	59	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
21	U	46	GLN
29	c	29	GLN
25	Y	58	ASN
15	O	100	HIS
21	U	27	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2888/2897 (99%)	382 (13%)	16 (0%)
2	B	119/120 (99%)	7 (5%)	0
32	f	75/76 (98%)	31 (41%)	0
33	g	74/76 (97%)	48 (64%)	0
All	All	3156/3169 (99%)	468 (14%)	16 (0%)

5 of 468 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	15	G
1	A	34	U
1	A	45	G

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Mol	Chain	Res	Type
1	A	46	G

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2193	G
1	A	2158	A
1	A	1535	A
1	A	2130	U
1	A	1494	A

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

45 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	$\# Z  > 2$
33	2MG	g	10	33	18,26,27	1.53	3 (16%)	16,38,41	1.64	4 (25%)
1	PSU	A	1911	1	18,21,22	2.32	8 (44%)	22,30,33	1.84	4 (18%)
33	OMG	g	34	33	18,26,27	1.57	3 (16%)	19,38,41	1.52	4 (21%)
1	5MU	A	1939	1	19,22,23	2.67	7 (36%)	28,32,35	3.95	10 (35%)
1	OMC	A	2498	34,1	19,22,23	1.90	6 (31%)	26,31,34	0.96	1 (3%)
1	G7M	A	2069	1	20,26,27	2.24	5 (25%)	17,39,42	0.71	0
1	H2U	A	2449	1	18,21,22	4.07	5 (27%)	21,30,33	5.20	7 (33%)
1	PSU	A	1917	1	18,21,22	2.32	8 (44%)	22,30,33	1.82	4 (18%)
1	2MG	A	2445	1	18,26,27	3.39	7 (38%)	16,38,41	1.30	3 (18%)
33	PSU	g	39	33	18,21,22	1.84	5 (27%)	22,30,33	2.49	7 (31%)
32	5MU	f	54	32	19,22,23	1.65	3 (15%)	28,32,35	2.93	11 (39%)
1	3TD	A	1915	1	18,22,23	6.42	12 (66%)	22,32,35	1.93	4 (18%)
1	2MA	A	2503	34,1	19,25,26	1.20	1 (5%)	21,37,40	1.85	3 (14%)
32	5MC	f	32	32	18,22,23	0.97	2 (11%)	26,32,35	1.29	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	4SU	f	8	32	18,21,22	3.20	5 (27%)	26,30,33	3.64	10 (38%)
1	PSU	A	2504	1	18,21,22	2.39	8 (44%)	22,30,33	1.89	4 (18%)
1	OMG	A	2251	1,32	18,26,27	2.46	5 (27%)	19,38,41	1.15	3 (15%)
33	H2U	g	17	33	18,21,22	1.01	2 (11%)	21,30,33	3.29	5 (23%)
33	31M	g	76	1	38,44,45	4.34	18 (47%)	38,61,64	2.23	13 (34%)
1	PSU	A	955	1	18,21,22	2.44	8 (44%)	22,30,33	1.85	4 (18%)
1	5MC	A	1962	1	18,22,23	2.01	6 (33%)	26,32,35	1.16	2 (7%)
33	1MA	g	58	33	16,25,26	1.65	5 (31%)	18,37,40	2.30	5 (27%)
32	PSU	f	55	32	18,21,22	1.31	2 (11%)	22,30,33	1.91	4 (18%)
13	4D4	M	81	13	9,11,12	2.03	2 (22%)	8,13,15	2.10	4 (50%)
1	PSU	A	746	34,1	18,21,22	2.37	9 (50%)	22,30,33	1.80	4 (18%)
33	OMC	g	32	33	19,22,23	1.39	3 (15%)	26,31,34	2.13	2 (7%)
33	5MC	g	40	33	18,22,23	1.27	1 (5%)	26,32,35	2.12	10 (38%)
33	5MC	g	49	33	18,22,23	1.07	2 (11%)	26,32,35	1.72	4 (15%)
33	YYG	g	37	33	31,42,43	2.16	7 (22%)	33,62,65	2.03	10 (30%)
1	PSU	A	2457	1	18,21,22	2.46	8 (44%)	22,30,33	1.90	4 (18%)
33	5MU	g	54	33	19,22,23	1.54	3 (15%)	28,32,35	2.42	7 (25%)
1	PSU	A	2580	1	18,21,22	2.47	10 (55%)	22,30,33	1.90	5 (22%)
1	PSU	A	2605	1	18,21,22	2.39	8 (44%)	22,30,33	1.87	4 (18%)
33	7MG	g	46	33	22,26,27	2.13	4 (18%)	29,39,42	3.15	10 (34%)
1	2MG	A	1835	1	18,26,27	3.37	7 (38%)	16,38,41	1.35	3 (18%)
1	PSU	A	2604	1	18,21,22	2.40	8 (44%)	22,30,33	1.87	4 (18%)
33	M2G	g	26	33	20,27,28	1.57	3 (15%)	22,40,43	1.06	2 (9%)
1	1MG	A	745	1	18,26,27	2.80	4 (22%)	19,39,42	1.28	3 (15%)
1	OMU	A	2552	1	19,22,23	2.68	7 (36%)	26,31,34	1.86	6 (23%)
1	6MZ	A	1618	1	18,25,26	1.98	1 (5%)	16,36,39	2.19	4 (25%)
1	5MU	A	747	1	19,22,23	2.58	7 (36%)	28,32,35	3.81	11 (39%)
33	H2U	g	16	33	18,21,22	0.99	2 (11%)	21,30,33	1.90	2 (9%)
4	MEQ	D	150[A]	4	8,9,10	0.95	0	5,10,12	0.66	0
33	PSU	g	55	33	18,21,22	2.22	6 (33%)	22,30,33	2.47	8 (36%)
1	6MZ	A	2030	1	18,25,26	1.98	1 (5%)	16,36,39	2.59	4 (25%)

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
33	2MG	g	10	33	-	0/5/27/28	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
33	OMG	g	34	33	-	3/5/27/28	0/3/3/3
1	5MU	A	1939	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2498	34,1	-	0/9/27/28	0/2/2/2
1	G7M	A	2069	1	-	1/3/25/26	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3
33	PSU	g	39	33	-	3/7/25/26	0/2/2/2
32	5MU	f	54	32	-	1/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	0/7/25/26	0/2/2/2
1	2MA	A	2503	34,1	-	1/3/25/26	0/3/3/3
32	5MC	f	32	32	-	0/7/25/26	0/2/2/2
32	4SU	f	8	32	-	0/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
1	OMG	A	2251	1,32	-	1/5/27/28	0/3/3/3
33	H2U	g	17	33	-	5/7/38/39	0/2/2/2
33	31M	g	76	1	-	6/27/49/50	0/4/4/4
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
33	1MA	g	58	33	-	2/3/25/26	0/3/3/3
32	PSU	f	55	32	-	0/7/25/26	0/2/2/2
13	4D4	M	81	13	-	3/11/12/14	-
1	PSU	A	746	34,1	-	2/7/25/26	0/2/2/2
33	OMC	g	32	33	-	0/9/27/28	0/2/2/2
33	5MC	g	40	33	-	0/7/25/26	0/2/2/2
33	5MC	g	49	33	-	3/7/25/26	0/2/2/2
33	YYG	g	37	33	-	16/20/42/43	0/3/4/4
1	PSU	A	2457	1	-	0/7/25/26	0/2/2/2
33	5MU	g	54	33	-	2/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
33	7MG	g	46	33	-	3/7/37/38	0/3/3/3
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
33	M2G	g	26	33	-	0/7/29/30	0/3/3/3
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	OMU	A	2552	1	-	0/9/27/28	0/2/2/2
1	6MZ	A	1618	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	A	747	1	-	0/7/25/26	0/2/2/2
33	H2U	g	16	33	-	3/7/38/39	0/2/2/2
4	MEQ	D	150[A]	4	-	4/8/9/11	-
33	PSU	g	55	33	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	2/5/27/28	0/3/3/3

The worst 5 of 237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	C2'-C1'	-18.07	1.30	1.53
33	g	76	31M	C2'-C1'	-16.92	1.28	1.53
1	A	1915	3TD	O4'-C1'	14.21	1.63	1.43
33	g	76	31M	O4'-C1'	12.06	1.57	1.41
1	A	2449	H2U	O4-C4	10.10	1.43	1.23

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2449	H2U	C4-N3-C2	-15.23	113.16	125.79
33	g	17	H2U	C4-N3-C2	-13.77	114.37	125.79
1	A	2449	H2U	O2-C2-N1	-11.49	108.68	123.11
33	g	46	7MG	N9-C4-N3	10.82	141.66	125.47
32	f	8	4SU	C4-N3-C2	-10.44	117.20	127.34

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	150[A]	MEQ	N-CA-CB-CG
13	M	81	4D4	NE-CD-CG-CB
1	A	746	PSU	C2'-C1'-C5-C4
1	A	2251	OMG	C1'-C2'-O2'-CM2
33	g	17	H2U	O4'-C1'-N1-C6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1939	5MU	1	0
1	A	1915	3TD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2251	OMG	1	0
1	A	2604	PSU	1	0
1	A	2030	6MZ	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 179 ligands modelled in this entry, 178 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	$\# Z  > 2$
35	DI0	A	3175	-	58,61,61	1.62	11 (18%)	77,92,92	1.65	20 (25%)

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
35	DI0	A	3175	-	-	10/70/121/121	0/3/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	3175	DI0	CAF-CAE	-5.60	1.39	1.51
35	A	3175	DI0	OBI-CAG	-4.12	1.33	1.43
35	A	3175	DI0	OAU-CBG	-3.41	1.38	1.44
35	A	3175	DI0	OAY-CAC	-3.13	1.35	1.43
35	A	3175	DI0	CBC-CBB	2.86	1.58	1.54

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	3175	DI0	OAL-CAW-CBT	4.88	116.70	107.40
35	A	3175	DI0	CBT-CAW-CAD	-4.69	106.31	115.20
35	A	3175	DI0	OBK-CAN-CAX	4.22	110.07	103.81
35	A	3175	DI0	CAP-CAH-CAJ	-3.35	109.30	114.05
35	A	3175	DI0	CBR-CAP-CBC	-2.75	106.45	111.09

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	3175	DI0	NAQ-CBA-CBS-OBW
35	A	3175	DI0	NAQ-CAK-CBB-CBC
35	A	3175	DI0	CAJ-CAH-CAP-OBJ
35	A	3175	DI0	OBX-CCC-CCD-OBW
35	A	3175	DI0	OAL-CAW-CBT-CCF

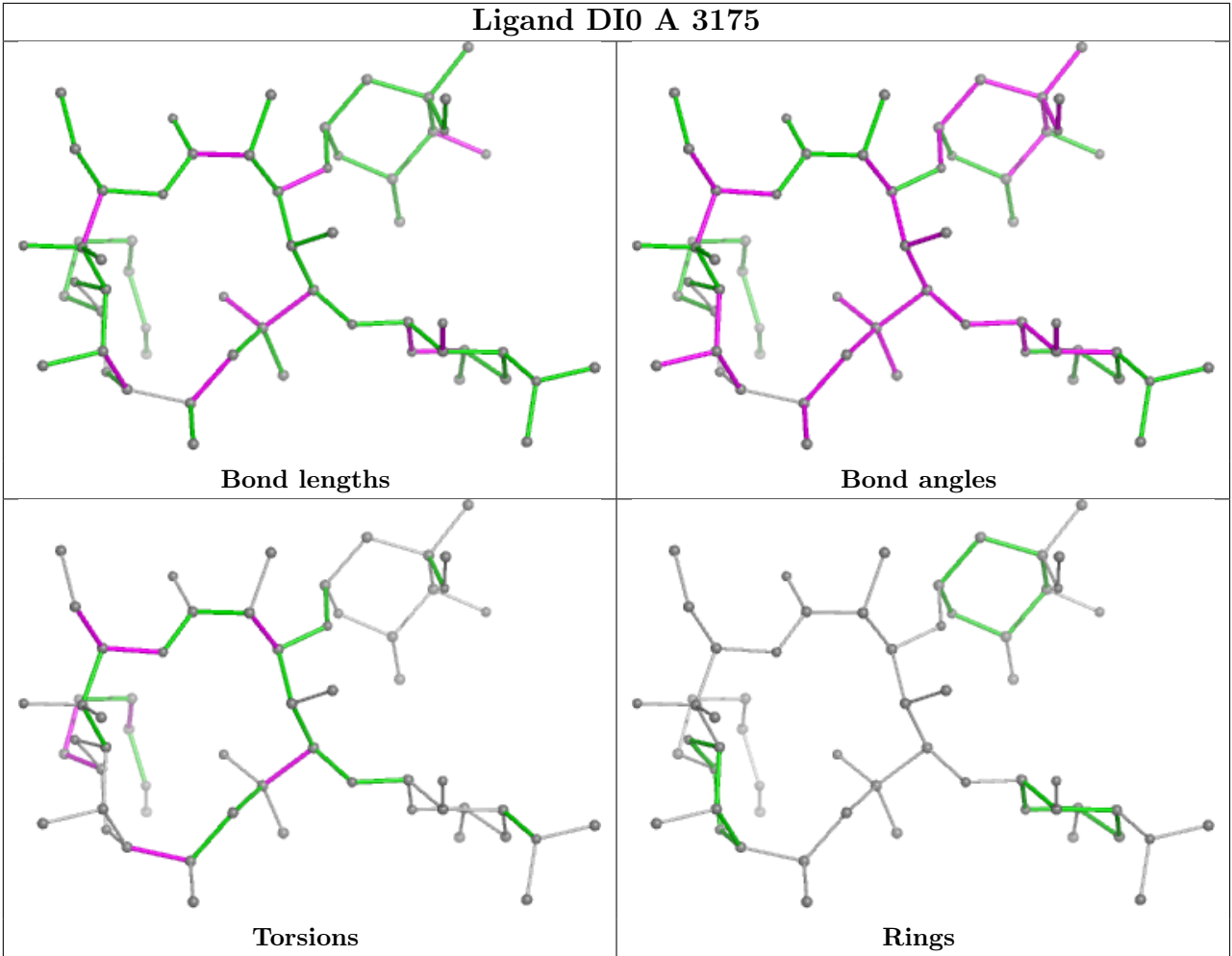
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	3175	DI0	1	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
33	g	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	885:C	O3'	892:A	P	11.25
1	A	1915:3TD	O3'	1916:A	P	1.31

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	g	75:C	O3'	76:31M	P	1.09