



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2025 – 04:38 PM JST

PDB ID : 8ZFF / pdb_00008zff
EMDB ID : EMD-60059
Title : Structure of the Bacterial Ribosome without hypoxia-induced rRNA modifications
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Ito, T.; Suzuki, T.
Deposited on : 2024-05-07
Resolution : 2.59 Å(reported)
Based on initial model : 7K00

This is a wwPDB EM Validation Summary 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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

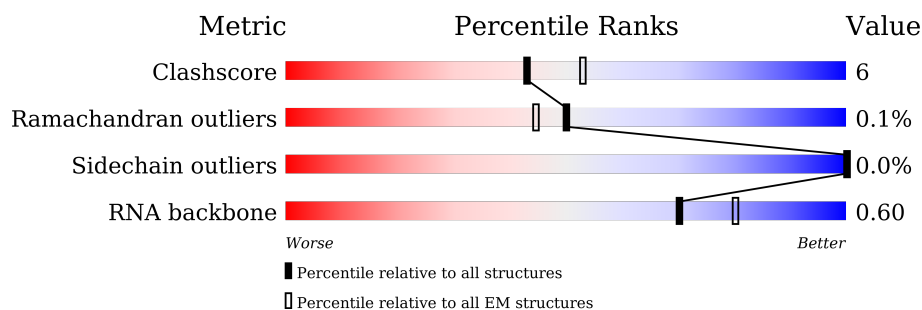
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.59 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 ≥ 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	1542	61% 33% . .
2	B	241	80% 12% 7%
3	C	233	73% 15% 12%
4	D	206	77% 22%
5	E	167	80% 13% 7%
6	F	135	53% 23% 24%
7	G	179	68% 18% 15%
8	H	130	82% 18% .

















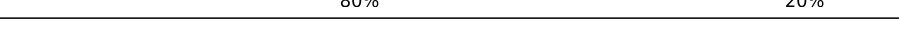
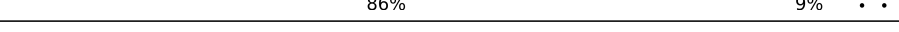
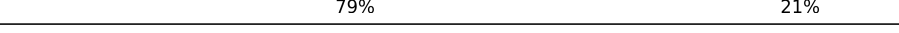


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Mol	Chain	Length	Quality of chain
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	

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Mol	Chain	Length	Quality of chain
34	m	127	 82% 11% 7%
35	n	117	 79% 21% .
36	o	115	 90% 10% .
37	p	118	 88% 11% .
38	q	103	 86% 14%
39	r	110	 85% 15%
40	s	100	 79% 14% 7%
41	t	104	 81% 16% ..
42	u	94	 86% 14%
43	v	85	 80% 12% 8%
44	w	78	 83% 15% .
45	x	63	 81% 17% .
46	y	59	 83% 15% .
47	z	57	 75% 23% .
48	0	55	 71% 22% 7%
49	1	46	 80% 20%
50	2	65	 86% 9% ..
51	3	38	 79% 21%
52	4	70	 54% 31% 14%
53	X	66	 9% 91%
54	Z	77	 56% 35% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MS6	1	82	X	-	-	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 140322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0
			32466	14487	5964	10503	1512		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2761	Total	C	N	O	P	0	0
			59301	26460	10925	19155	2761		

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	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
1	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 36 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 38 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 44 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL33.

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

- Molecule 49 is a protein called Large ribosomal subunit protein bL34.

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

- Molecule 50 is a protein called Large ribosomal subunit protein bL35.

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

- Molecule 51 is a protein called Large ribosomal subunit protein bL36A.

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

- Molecule 52 is a protein called Large ribosomal subunit protein bL31.

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	6	Total	C	N	O	P	0	0
			130	58	25	41	6		

- Molecule 54 is a RNA chain called P-site tRNA-fMet.

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

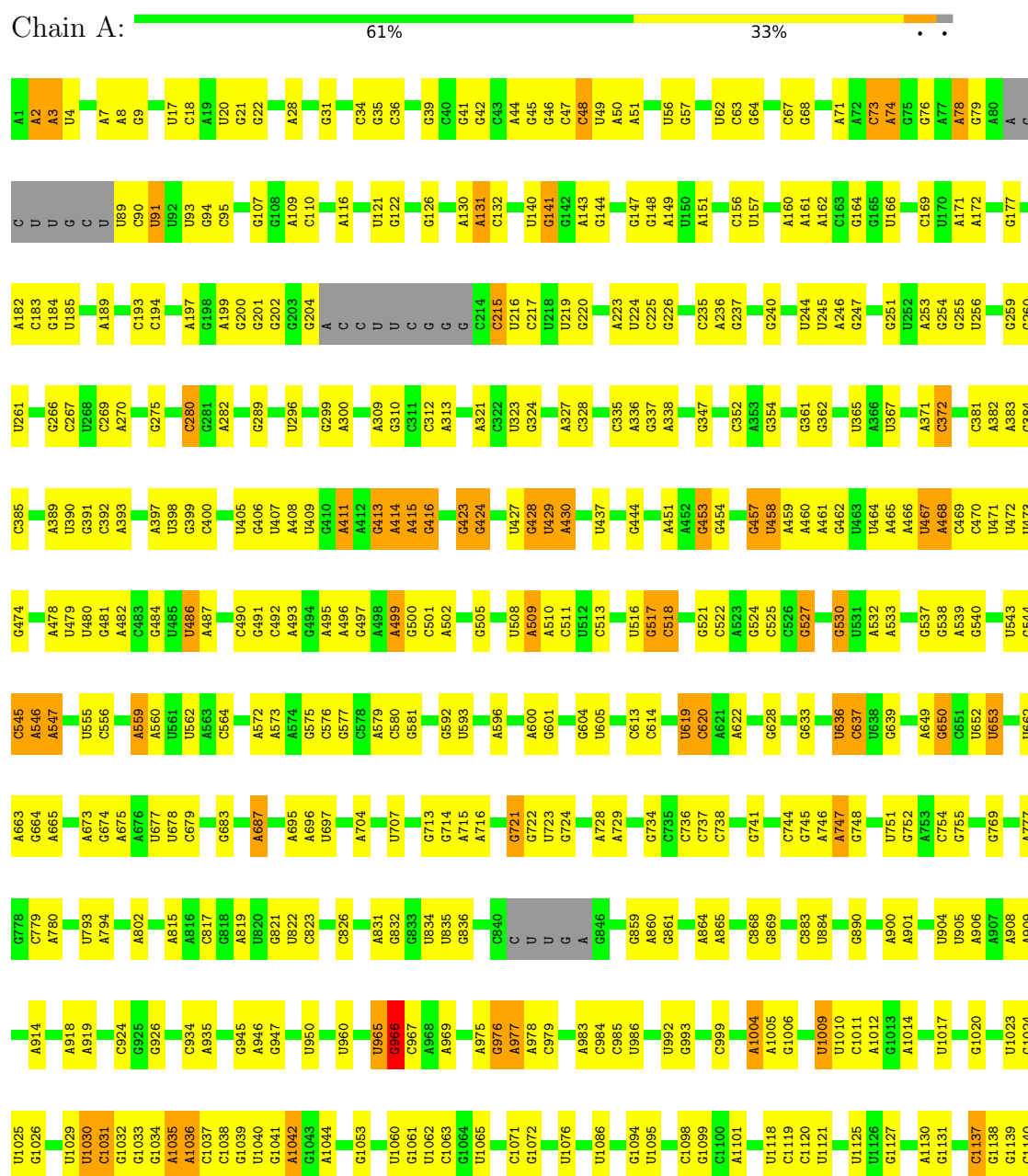
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

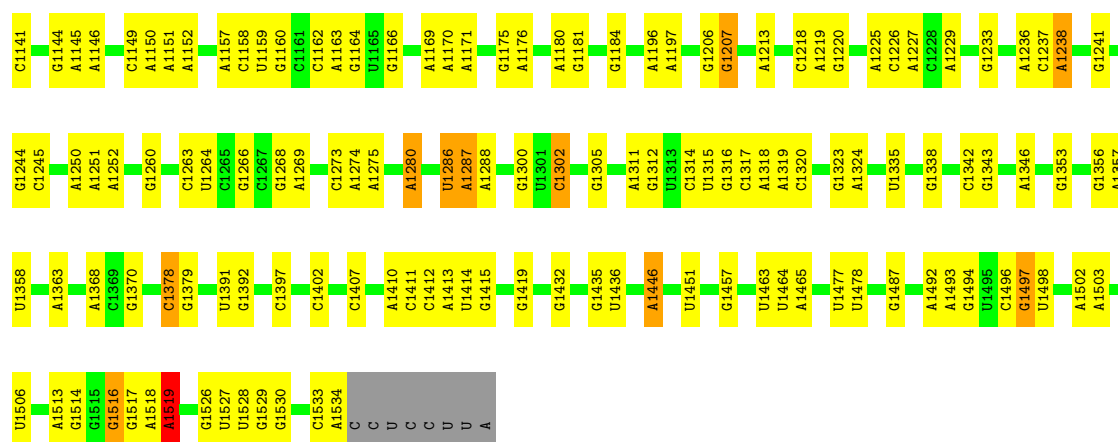
Mol	Chain	Residues	Atoms		AltConf
55	A	119	Total	Mg	0
			119	119	
55	a	328	Total	Mg	0
			328	328	
55	b	6	Total	Mg	0
			6	6	
55	c	1	Total	Mg	0
			1	1	
55	d	1	Total	Mg	0
			1	1	
55	z	1	Total	Mg	0
			1	1	
55	Z	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

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

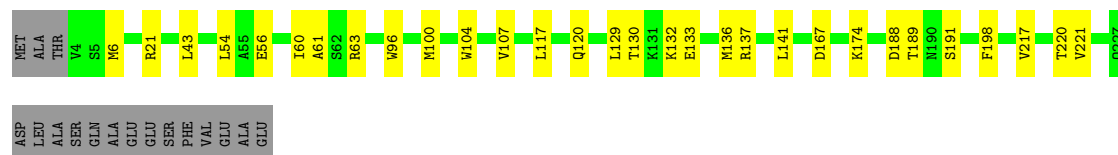
• Molecule 1: 16S rRNA





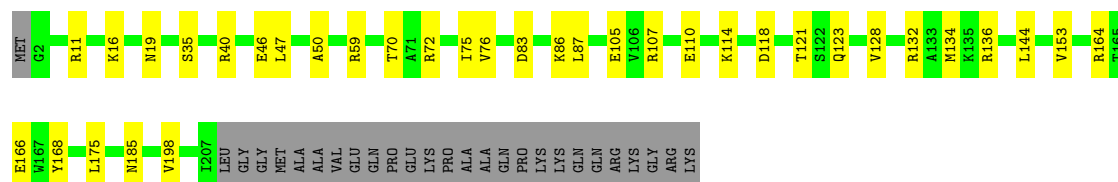
- Molecule 2: Small ribosomal subunit protein uS2

Chain B: 80% 12% 7%



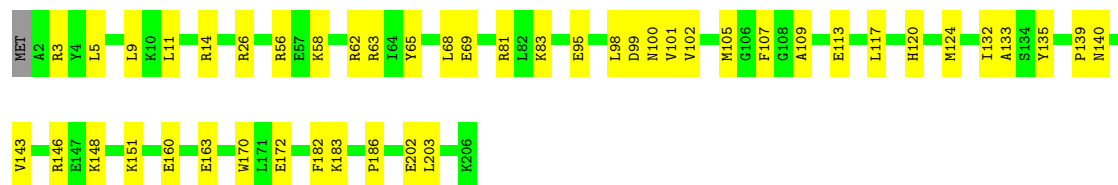
- Molecule 3: Small ribosomal subunit protein uS3

Chain C: 73% 15% 12%



- Molecule 4: Small ribosomal subunit protein uS4

Chain D: 77% 22%

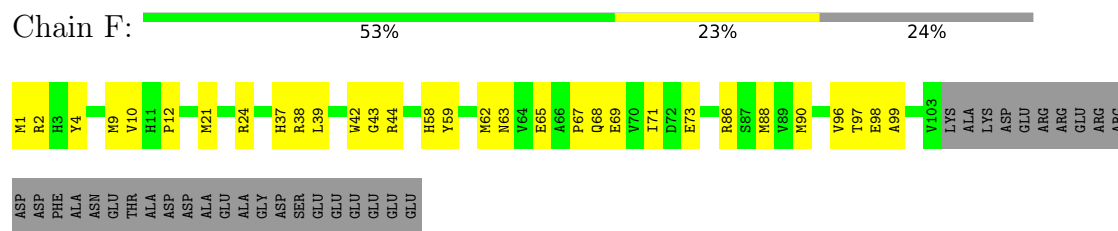


- Molecule 5: Small ribosomal subunit protein uS5

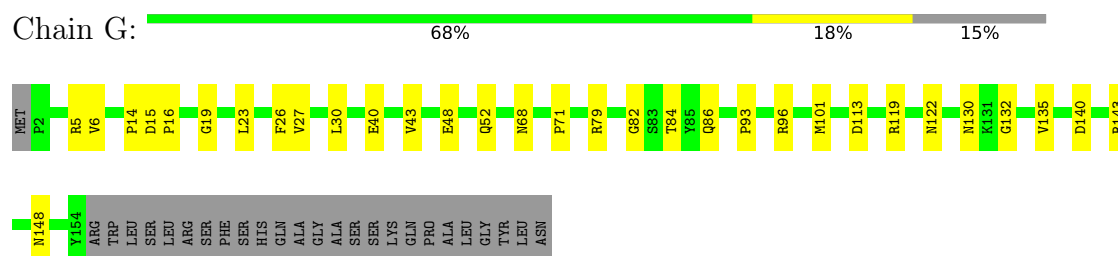
Chain E: 80% 13% 7%



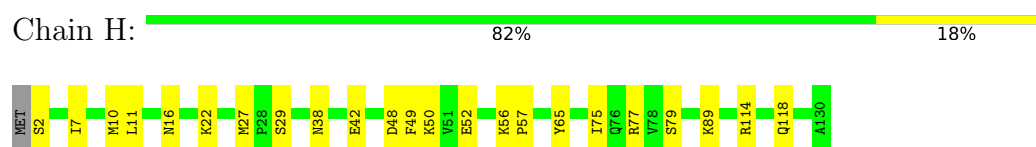
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform



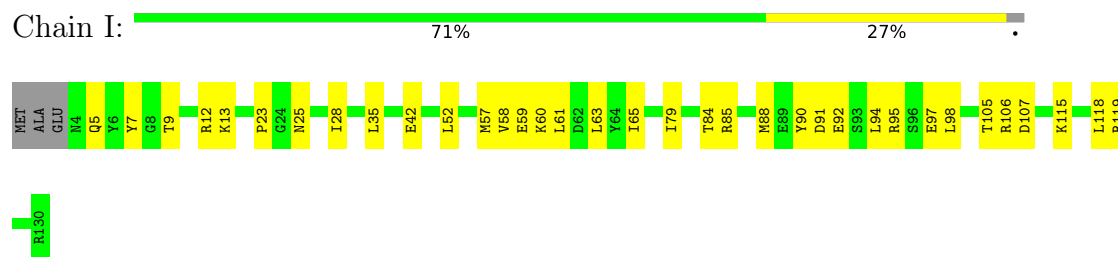
- Molecule 7: Small ribosomal subunit protein uS7



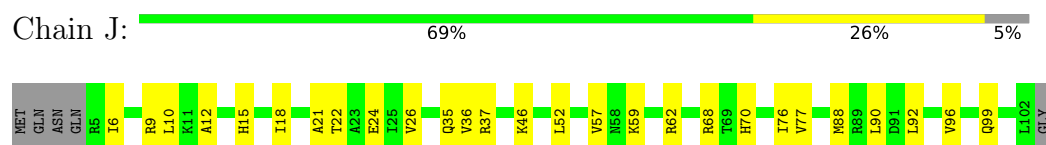
- Molecule 8: Small ribosomal subunit protein uS8



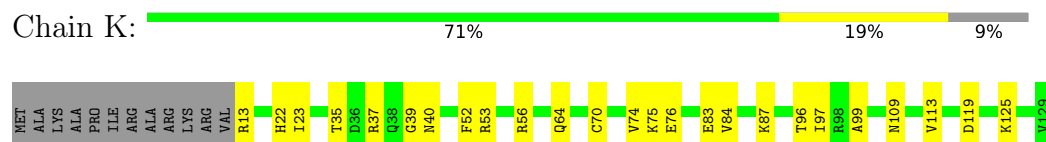
- Molecule 9: Small ribosomal subunit protein uS9




- Molecule 10: Small ribosomal subunit protein uS10



- Molecule 11: Small ribosomal subunit protein uS11



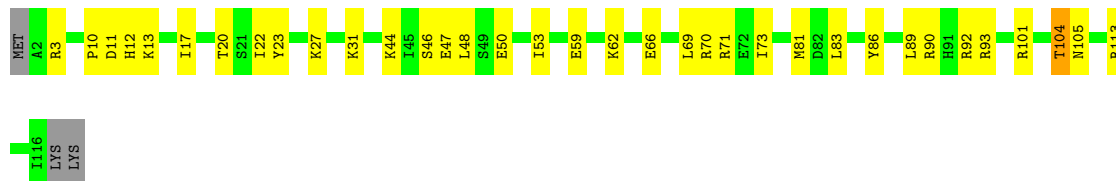
- Molecule 12: Small ribosomal subunit protein uS12

Chain L:  85% 15% .




- Molecule 13: Small ribosomal subunit protein uS13

Chain M:  68% 29% . .




- Molecule 14: Small ribosomal subunit protein uS14

Chain N:  79% 20% .



- Molecule 15: Small ribosomal subunit protein uS15

Chain O:  89% 10% .




- Molecule 16: Small ribosomal subunit protein bS16

Chain P:  76% 23% .



- Molecule 17: Small ribosomal subunit protein uS17

Chain Q:  80% 14% 6%



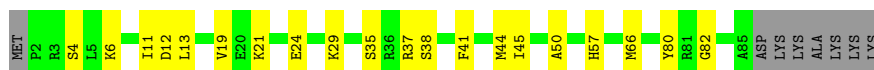
- Molecule 18: Small ribosomal subunit protein bS18

Chain R:  72% 16% 12%



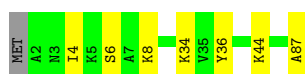
- Molecule 19: Small ribosomal subunit protein uS19

Chain S: 70% 22% 9%



- Molecule 20: Small ribosomal subunit protein bS20

Chain T: 91% 8%



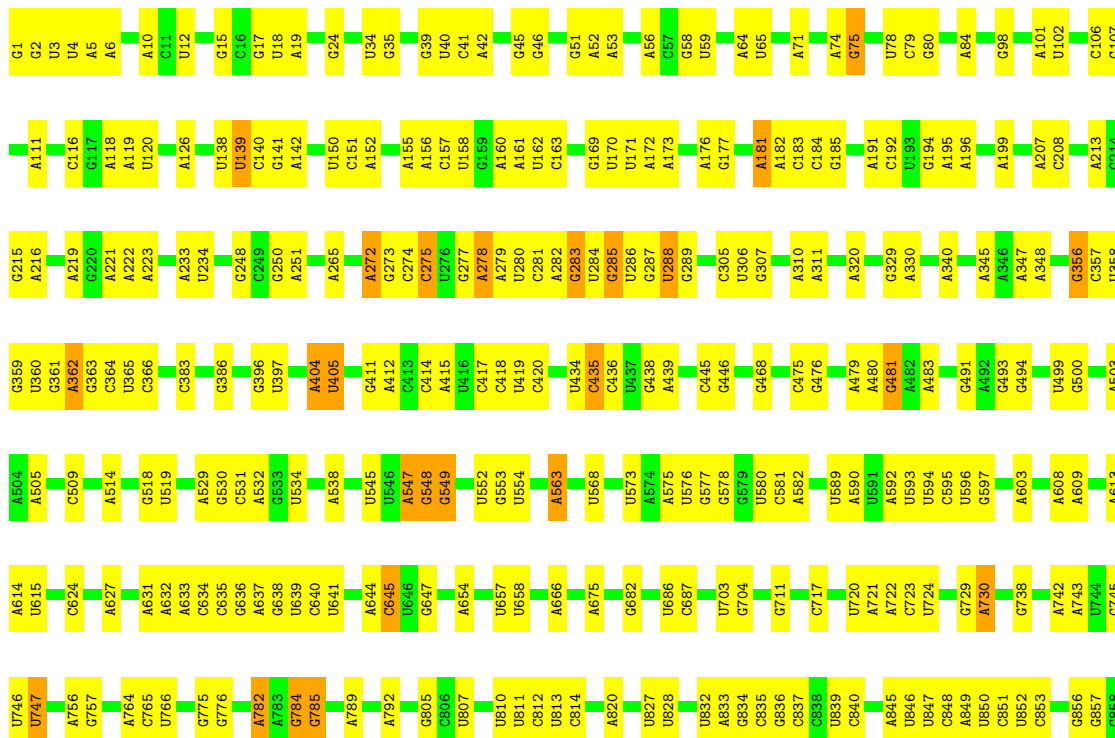
- Molecule 21: Small ribosomal subunit protein bS21

Chain U: 76% 23%

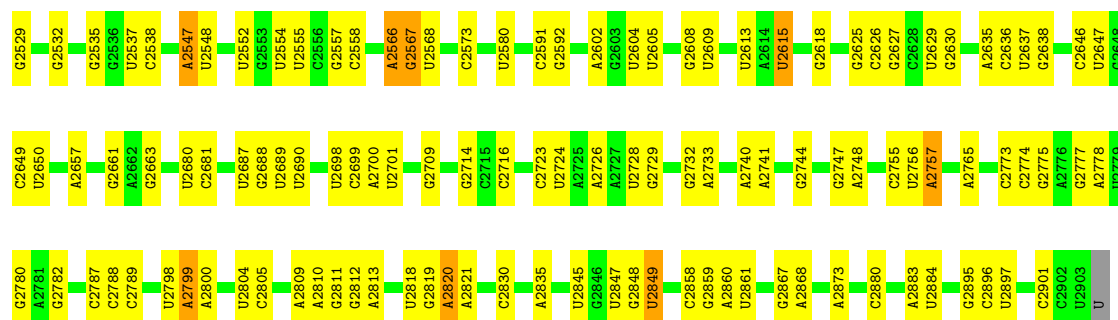


- Molecule 22: 23S rRNA

Chain a: 64% 28% 5%







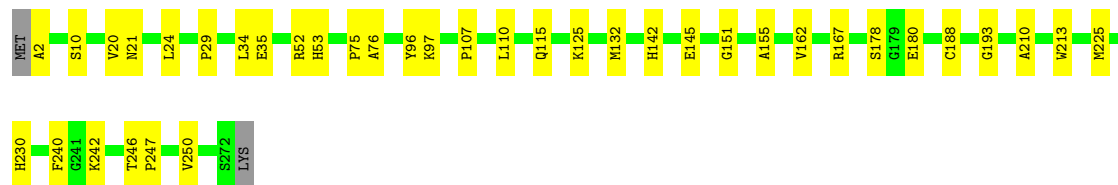
• Molecule 23: 5S rRNA

Chain b: 75% 23% ..



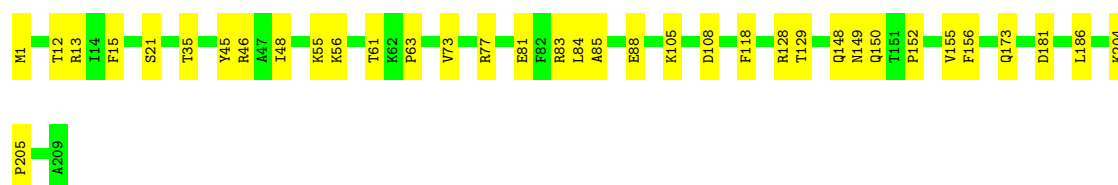
• Molecule 24: Large ribosomal subunit protein uL2

Chain c: 85% 14% .



• Molecule 25: Large ribosomal subunit protein uL3

Chain d: 83% 17%



• Molecule 26: Large ribosomal subunit protein uL4

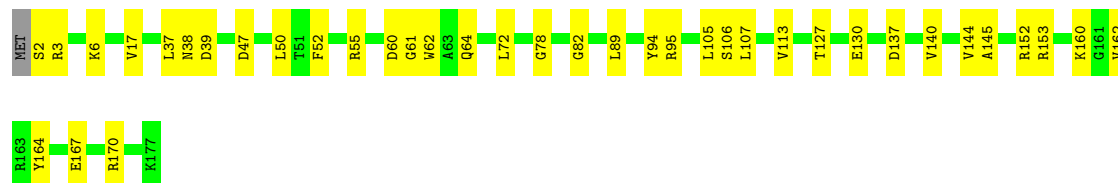
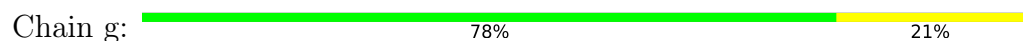
Chain e: 91% 9%



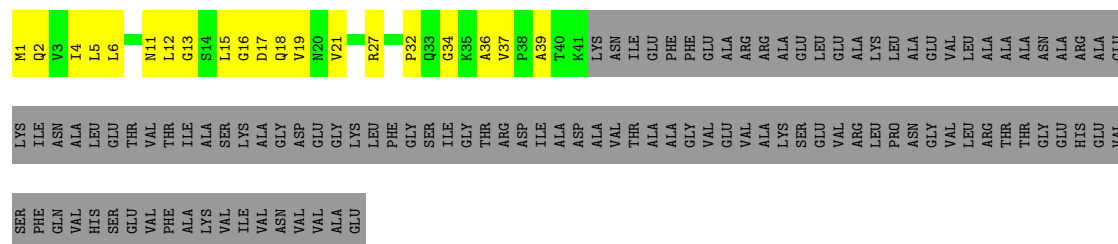
• Molecule 27: Large ribosomal subunit protein uL5

Chain f: 73% 26% .

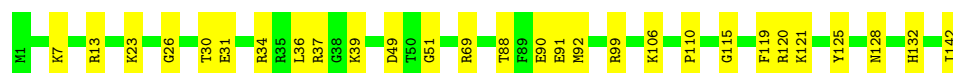
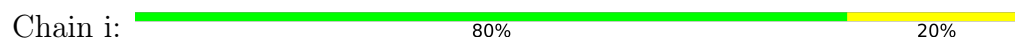
- Molecule 28: Large ribosomal subunit protein uL6



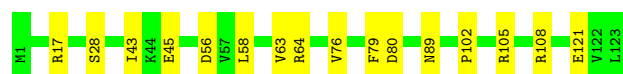
- Molecule 29: Large ribosomal subunit protein bL9



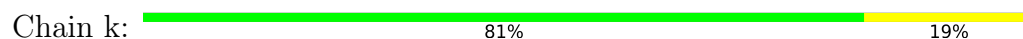
- Molecule 30: Large ribosomal subunit protein uL13



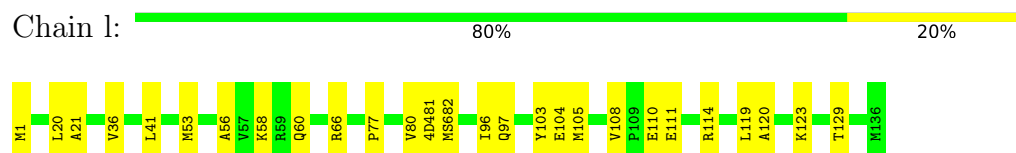
- Molecule 31: Large ribosomal subunit protein uL14



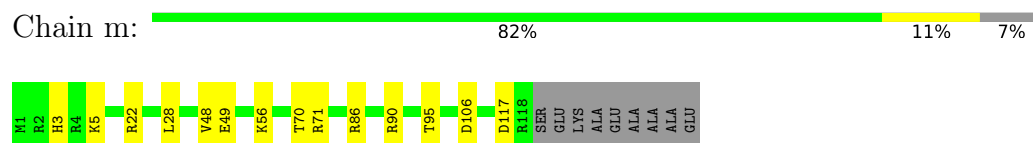
- Molecule 32: Large ribosomal subunit protein uL15



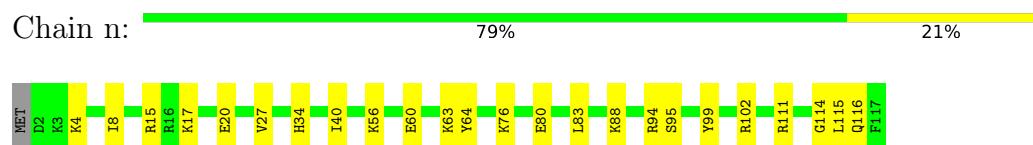
- Molecule 33: Large ribosomal subunit protein uL16



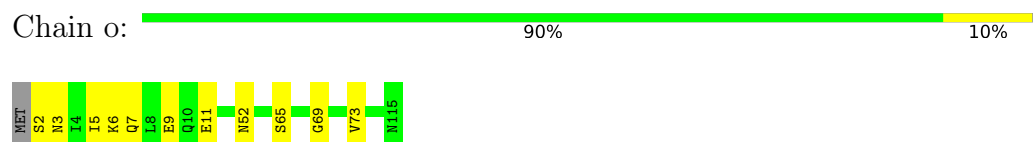
- Molecule 34: Large ribosomal subunit protein bL17



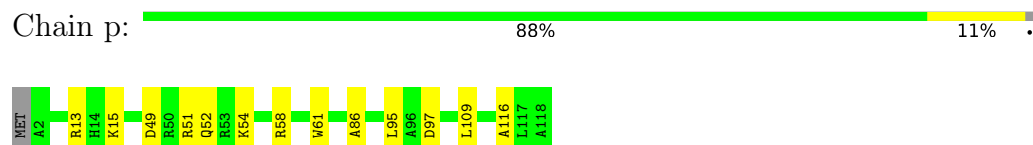
- Molecule 35: Large ribosomal subunit protein uL18



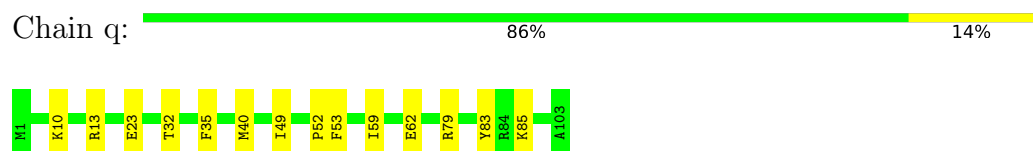
- Molecule 36: Large ribosomal subunit protein bL19



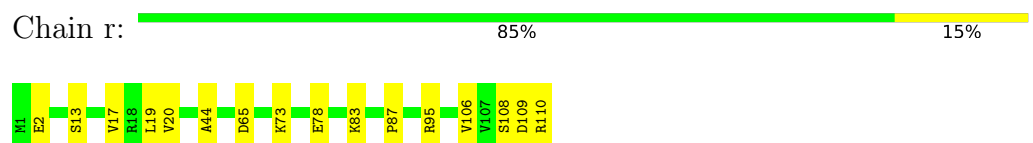
- Molecule 37: Large ribosomal subunit protein bL20




- Molecule 38: Large ribosomal subunit protein bL21



- Molecule 39: Large ribosomal subunit protein uL22




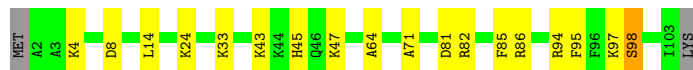
- Molecule 40: Large ribosomal subunit protein uL23

Chain s:  79% 14% 7%



- Molecule 41: Large ribosomal subunit protein uL24

Chain t:  81% 16% ..




- Molecule 42: Large ribosomal subunit protein bL25

Chain u:  86% 14%




- Molecule 43: Large ribosomal subunit protein bL27

Chain v:  80% 12% 8%




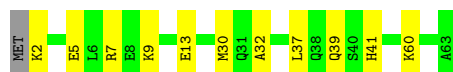
- Molecule 44: Large ribosomal subunit protein bL28

Chain w:  83% 15% .




- Molecule 45: Large ribosomal subunit protein uL29

Chain x:  81% 17% .



- Molecule 46: Large ribosomal subunit protein uL30

Chain y:  83% 15% .



- Molecule 47: Large ribosomal subunit protein bL32

MET	A2	V3	Q4	T9	R10	S11	K12	M15	H38	L39	I43	Y49	R50	G51	R52	K53	V54	I55	A56	K57
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- | |
|-----|
| MET |
| ALA |
| LYS |
| G4 |
| I5 |
| R6 |
| E7 |
| K8 |
| I9 |
| K10 |
| F20 |
| Y21 |
| T22 |
| K27 |
| R28 |
| T29 |
| K30 |
| E51 |
| A52 |
| K53 |
| I54 |
| LYS |

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|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| I5 | I6 | I7 | I8 | I9 | I10 | I11 | I12 | I13 | I14 | I15 | I16 | I17 | I18 | I19 | I20 | I21 | I22 | I23 | I24 | I25 | I26 | I27 | I28 | I29 | I30 | I31 | I32 | I33 | I34 | I35 | I36 | I37 | I38 | I39 | I40 | I41 | I42 | I43 | I44 | I45 | I46 | I47 | I48 | I49 | I50 | I51 | I52 | I53 | I54 | I55 | I56 | I57 | I58 | I59 | I60 | I61 | I62 | I63 | I64 | I65 | I66 | I67 | I68 | I69 | I70 | I71 | I72 | I73 | I74 | I75 | I76 | I77 | I78 | I79 | I80 | I81 | I82 | I83 | I84 | I85 | I86 | I87 | I88 | I89 | I90 | I91 | I92 | I93 | I94 | I95 | I96 | I97 | I98 | I99 | I100 |
|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|

- G G C A A A A A A A C C A A A A A A A A G G A A A A A U A G37 G42 U U C A A A A G U C G A A A A A U C C U A C U
- A C U

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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	244856	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (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: 6MZ, 5MU, 4SU, MS6, OMC, 5MC, OMG, MEQ, OMU, D2T, 2MG, UR3, IAS, 4OC, H2U, G7M, 2MA, 1MG, PSU, 4D4, MG, 3TD, MA6

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	0.35	0/36073	0.30	0/56264
2	B	0.21	0/1784	0.32	0/2403
3	C	0.26	0/1651	0.36	0/2225
4	D	0.27	0/1665	0.37	0/2227
5	E	0.30	0/1165	0.37	0/1568
6	F	0.26	0/858	0.42	0/1160
7	G	0.22	0/1219	0.36	0/1635
8	H	0.31	0/989	0.38	0/1326
9	I	0.27	0/1034	0.42	0/1375
10	J	0.27	0/796	0.43	0/1077
11	K	0.27	0/884	0.35	0/1191
12	L	0.31	0/960	0.40	0/1286
13	M	0.27	0/900	0.45	0/1204
14	N	0.28	0/817	0.43	0/1088
15	O	0.29	0/722	0.38	0/964
16	P	0.31	0/653	0.39	0/877
17	Q	0.28	0/650	0.36	0/871
18	R	0.28	0/553	0.38	0/742
19	S	0.24	0/685	0.39	0/922
20	T	0.29	0/676	0.35	0/895
21	U	0.19	0/597	0.35	0/792
22	a	0.40	0/65842	0.31	0/102711
23	b	0.33	0/2850	0.27	0/4444
24	c	0.36	0/2121	0.39	0/2852
25	d	0.36	0/1576	0.35	0/2119
26	e	0.31	0/1571	0.35	0/2113
27	f	0.27	0/1434	0.36	0/1926
28	g	0.25	0/1343	0.42	0/1816
29	h	0.23	0/306	0.40	0/413
30	i	0.34	0/1152	0.35	0/1551
31	j	0.35	0/955	0.36	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	k	0.34	0/1062	0.39	0/1413
33	l	0.34	0/1073	0.37	0/1433
34	m	0.37	0/958	0.42	0/1281
35	n	0.29	0/902	0.39	0/1209
36	o	0.34	0/929	0.34	0/1242
37	p	0.38	0/960	0.37	0/1278
38	q	0.35	0/829	0.38	0/1107
39	r	0.34	0/864	0.39	0/1156
40	s	0.30	0/744	0.45	0/994
41	t	0.28	0/787	0.49	2/1051 (0.2%)
42	u	0.29	0/766	0.36	0/1025
43	v	0.35	0/599	0.36	0/792
44	w	0.34	0/635	0.40	0/848
45	x	0.25	0/502	0.38	0/667
46	y	0.33	0/453	0.36	0/605
47	z	0.34	0/450	0.36	0/599
48	0	0.28	0/424	0.31	0/565
49	1	0.38	0/380	0.43	0/498
50	2	0.37	0/513	0.42	0/676
51	3	0.36	0/303	0.38	0/397
52	4	0.21	0/488	0.41	0/649
53	X	0.29	0/145	0.26	0/224
54	Z	0.28	0/1725	0.26	0/2687
All	All	0.36	0/150972	0.33	2/225712 (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
13	M	0	1
33	l	1	0
50	2	0	1
All	All	1	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	t	98	SER	CA-C-N	5.71	132.44	121.54
41	t	98	SER	C-N-CA	5.71	132.44	121.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	l	82	MS6	C

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	31	HIS	Peptide
13	M	104	THR	Peptide

5.2 Too-close contacts [i](#)

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	32466	0	16359	351	0
2	B	1753	0	1780	19	0
3	C	1624	0	1696	19	0
4	D	1643	0	1707	36	0
5	E	1152	0	1196	17	0
6	F	839	0	833	24	0
7	G	1203	0	1254	22	0
8	H	979	0	1031	17	0
9	I	1022	0	1070	30	0
10	J	786	0	828	19	0
11	K	877	0	884	16	0
12	L	957	0	1017	17	0
13	M	891	0	952	31	0
14	N	805	0	844	12	0
15	O	714	0	734	7	0
16	P	643	0	661	11	0
17	Q	641	0	682	9	0
18	R	544	0	565	9	0
19	S	668	0	693	15	0
20	T	670	0	719	5	0
21	U	589	0	629	10	0
22	a	59301	0	29850	524	0
23	b	2549	0	1291	15	0
24	c	2082	0	2154	26	0
25	d	1566	0	1618	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	e	1552	0	1619	10	0
27	f	1410	0	1444	37	0
28	g	1323	0	1371	26	0
29	h	303	0	327	15	0
30	i	1129	0	1162	19	0
31	j	946	0	1023	11	0
32	k	1053	0	1129	21	0
33	l	1075	0	1145	16	0
34	m	945	0	989	9	0
35	n	892	0	923	14	0
36	o	917	0	962	8	0
37	p	947	0	1019	12	0
38	q	816	0	839	10	0
39	r	857	0	922	10	0
40	s	738	0	807	9	0
41	t	779	0	831	14	0
42	u	753	0	780	10	0
43	v	592	0	607	6	0
44	w	625	0	652	8	0
45	x	501	0	531	7	0
46	y	449	0	488	5	0
47	z	444	0	458	9	0
48	0	417	0	451	8	0
49	1	377	0	418	9	0
50	2	504	0	572	7	0
51	3	302	0	343	6	0
52	4	480	0	482	18	0
53	X	130	0	66	0	0
54	Z	1645	0	842	16	0
55	A	119	0	0	0	0
55	Z	1	0	0	0	0
55	a	328	0	0	0	0
55	b	6	0	0	0	0
55	c	1	0	0	0	0
55	d	1	0	0	0	0
55	z	1	0	0	0	0
All	All	140322	0	94249	1465	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 1465 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:414:A:HO2'	1:A:415:A:H8	0.99	0.97
22:a:1047:G:HO2'	22:a:1110:G:H1	1.13	0.97
1:A:76:G:H1	1:A:93:U:H3	1.11	0.97
22:a:1870:C:HO2'	22:a:1871:A:H8	0.99	0.95
22:a:2100:G:H1	22:a:2189:U:H3	0.95	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
3	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
4	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
5	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
6	F	101/135 (75%)	95 (94%)	6 (6%)	0	100	100
7	G	151/179 (84%)	139 (92%)	12 (8%)	0	100	100
8	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
9	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
10	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	13	29
11	K	113/129 (88%)	105 (93%)	8 (7%)	0	100	100
12	L	120/124 (97%)	111 (92%)	9 (8%)	0	100	100
13	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	Q	77/84 (92%)	77 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
19	S	82/92 (89%)	82 (100%)	0	0	100	100
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
24	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
25	d	206/209 (99%)	202 (98%)	3 (2%)	1 (0%)	25	47
26	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
27	f	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
28	g	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
29	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
30	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
31	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
32	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
33	l	132/136 (97%)	131 (99%)	1 (1%)	0	100	100
34	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
35	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
36	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
37	p	115/118 (98%)	115 (100%)	0	0	100	100
38	q	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
39	r	108/110 (98%)	108 (100%)	0	0	100	100
40	s	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
41	t	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
42	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
43	v	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
44	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
45	x	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	54 (100%)	0	0	100	100
48	0	49/55 (89%)	49 (100%)	0	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	8	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
All	All	5481/5913 (93%)	5281 (96%)	197 (4%)	3 (0%)	50	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	d	149	ASN
10	J	57	VAL
50	2	32	ILE

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	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	89/98 (91%)	89 (100%)	0	100	100
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
24	c	216/218 (99%)	216 (100%)	0	100	100
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	137/138 (99%)	137 (100%)	0	100	100
29	h	32/114 (28%)	32 (100%)	0	100	100
30	i	116/116 (100%)	115 (99%)	1 (1%)	75	90
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	107/107 (100%)	107 (100%)	0	100	100
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	86 (100%)	0	100	100
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100
39	r	93/93 (100%)	93 (100%)	0	100	100
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	83 (100%)	0	100	100
42	u	78/78 (100%)	78 (100%)	0	100	100
43	v	59/63 (94%)	59 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	54 (100%)	0	100	100
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100
48	0	46/49 (94%)	46 (100%)	0	100	100
49	1	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	55/62 (89%)	55 (100%)	0	100	100
All	All	4573/4825 (95%)	4572 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	i	128	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
28	g	73	ASN
36	o	66	ASN
28	g	88	GLN
33	l	13	HIS
40	s	70	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1542 (97%)	201 (13%)	6 (0%)
22	a	2757/2904 (94%)	301 (10%)	0
23	b	118/120 (98%)	13 (11%)	0
53	X	5/66 (7%)	0	0
54	Z	76/77 (98%)	10 (13%)	0
All	All	4464/4709 (94%)	525 (11%)	6 (0%)

5 of 525 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	A
1	A	4	U
1	A	7	A
1	A	9	G

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	636	U
1	A	1030	U
1	A	1035	A
1	A	517	G
1	A	429	U

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
1	2MG	A	1516	1	18,26,27	2.07	6 (33%)	16,38,41	1.49	4 (25%)
22	PSU	a	1917	22	18,21,22	1.01	1 (5%)	22,30,33	1.86	5 (22%)
54	PSU	Z	56	54	18,21,22	1.06	1 (5%)	22,30,33	1.86	5 (22%)
22	3TD	a	1915	22	18,22,23	4.06	6 (33%)	22,32,35	1.74	3 (13%)
22	5MC	a	1962	22	18,22,23	3.54	7 (38%)	26,32,35	1.09	2 (7%)
22	G7M	a	2069	22,55	20,26,27	2.57	7 (35%)	17,39,42	1.13	1 (5%)
22	OMU	a	2552	22	19,22,23	2.69	6 (31%)	26,31,34	1.82	5 (19%)
22	PSU	a	746	22,55	18,21,22	1.07	2 (11%)	22,30,33	1.71	3 (13%)
1	2MG	A	1207	1	18,26,27	2.13	6 (33%)	16,38,41	1.46	4 (25%)
22	2MA	a	2503	22,55	19,25,26	3.24	8 (42%)	21,37,40	2.74	3 (14%)
22	OMG	a	2251	22,54	18,26,27	2.66	8 (44%)	19,38,41	1.49	4 (21%)
22	6MZ	a	1618	22	18,25,26	1.94	3 (16%)	16,36,39	2.10	3 (18%)
33	MS6	l	82	33	7,7,8	4.42	2 (28%)	6,7,9	2.29	2 (33%)
1	G7M	A	527	1	20,26,27	2.64	7 (35%)	17,39,42	1.07	1 (5%)
54	H2U	Z	21	54	18,21,22	1.05	2 (11%)	21,30,33	0.74	0
11	IAS	K	119	11	6,7,8	1.02	0	6,8,10	1.26	1 (16%)
33	4D4	l	81	33	9,11,12	1.51	2 (22%)	8,13,15	2.04	3 (37%)
22	H2U	a	2449	22	18,21,22	1.29	3 (16%)	21,30,33	1.03	1 (4%)
22	PSU	a	2580	22	18,21,22	1.11	3 (16%)	22,30,33	2.09	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	D2T	L	89	12	7,9,10	1.40	0	6,11,13	2.06	3 (50%)
22	PSU	a	2604	22	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
22	PSU	a	2504	22	18,21,22	1.04	1 (5%)	22,30,33	1.82	4 (18%)
1	2MG	A	966	1	18,26,27	2.11	6 (33%)	16,38,41	1.49	3 (18%)
1	PSU	A	516	1,55	18,21,22	1.03	1 (5%)	22,30,33	1.68	5 (22%)
1	4OC	A	1402	1,55	20,23,24	2.93	8 (40%)	26,32,35	1.01	2 (7%)
54	5MU	Z	55	54	19,22,23	4.64	6 (31%)	28,32,35	3.67	9 (32%)
1	5MC	A	967	1	18,22,23	3.68	8 (44%)	26,32,35	1.02	1 (3%)
54	4SU	Z	8	54	18,21,22	4.10	8 (44%)	26,30,33	2.27	4 (15%)
22	5MU	a	1939	22	19,22,23	4.51	7 (36%)	28,32,35	3.82	10 (35%)
22	5MU	a	747	22	19,22,23	4.54	7 (36%)	28,32,35	3.79	10 (35%)
1	5MC	A	1407	1	18,22,23	3.54	8 (44%)	26,32,35	1.02	2 (7%)
1	UR3	A	1498	1	19,22,23	2.60	7 (36%)	26,32,35	1.33	1 (3%)
22	OMC	a	2498	22,55	19,22,23	2.75	8 (42%)	26,31,34	0.86	0
22	1MG	a	745	22	18,26,27	2.51	5 (27%)	19,39,42	1.43	3 (15%)
22	2MG	a	2445	22	18,26,27	2.06	6 (33%)	16,38,41	1.52	4 (25%)
22	PSU	a	2457	22	18,21,22	1.08	2 (11%)	22,30,33	2.02	6 (27%)
54	OMC	Z	33	54	19,22,23	2.84	8 (42%)	26,31,34	0.75	0
25	MEQ	d	150	25	8,9,10	1.10	0	5,10,12	1.50	2 (40%)
1	MA6	A	1518	1	18,26,27	1.09	1 (5%)	19,38,41	1.63	3 (15%)
22	PSU	a	955	22	18,21,22	1.08	2 (11%)	22,30,33	1.92	5 (22%)
22	PSU	a	2605	22	18,21,22	1.02	2 (11%)	22,30,33	1.89	3 (13%)
22	6MZ	a	2030	22	18,25,26	1.91	2 (11%)	16,36,39	2.40	3 (18%)
1	MA6	A	1519	1	18,26,27	1.06	1 (5%)	19,38,41	1.69	3 (15%)
22	2MG	a	1835	22	18,26,27	2.04	6 (33%)	16,38,41	1.49	4 (25%)
22	PSU	a	1911	22	18,21,22	1.02	1 (5%)	22,30,33	1.84	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
54	PSU	Z	56	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	3TD	a	1915	22	-	2/7/25/26	0/2/2/2
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
22	G7M	a	2069	22,55	-	1/3/25/26	0/3/3/3
22	OMU	a	2552	22	-	1/9/27/28	0/2/2/2
22	PSU	a	746	22,55	-	1/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
22	2MA	a	2503	22,55	-	1/3/25/26	0/3/3/3
22	OMG	a	2251	22,54	-	1/5/27/28	0/3/3/3
22	6MZ	a	1618	22	-	0/5/27/28	0/3/3/3
33	MS6	l	82	33	1/1/1/2	1/4/6/8	-
1	G7M	A	527	1	-	3/3/25/26	0/3/3/3
54	H2U	Z	21	54	-	7/7/38/39	0/2/2/2
11	IAS	K	119	11	-	0/7/7/8	-
33	4D4	l	81	33	-	3/11/12/14	-
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
12	D2T	L	89	12	-	3/7/12/14	-
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2504	22	-	2/7/25/26	0/2/2/2
1	2MG	A	966	1	-	2/5/27/28	0/3/3/3
1	PSU	A	516	1,55	-	2/7/25/26	0/2/2/2
1	4OC	A	1402	1,55	-	1/9/29/30	0/2/2/2
54	5MU	Z	55	54	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
54	4SU	Z	8	54	-	0/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
22	OMC	a	2498	22,55	-	0/9/27/28	0/2/2/2
22	1MG	a	745	22	-	0/3/25/26	0/3/3/3
22	2MG	a	2445	22	-	2/5/27/28	0/3/3/3
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
54	OMC	Z	33	54	-	0/9/27/28	0/2/2/2
25	MEQ	d	150	25	-	2/8/9/11	-
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	6MZ	a	2030	22	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3
22	2MG	a	1835	22	-	0/5/27/28	0/3/3/3
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2

The worst 5 of 192 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C6-C5	12.17	1.49	1.35
33	l	82	MS6	C-S	-11.34	1.57	1.81
54	Z	55	5MU	C6-N1	10.58	1.56	1.38
54	Z	55	5MU	C2-N1	10.35	1.55	1.38
22	a	747	5MU	C6-N1	10.25	1.55	1.38

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	747	5MU	C5-C4-N3	12.47	125.95	115.31
22	a	1939	5MU	C5-C4-N3	12.46	125.95	115.31
54	Z	55	5MU	C5-C4-N3	12.28	125.79	115.31
22	a	1939	5MU	C5-C6-N1	-10.87	112.16	123.34
22	a	747	5MU	C5-C6-N1	-10.71	112.33	123.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	l	82	MS6	C

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	2MG	O4'-C4'-C5'-O5'
1	A	966	2MG	C3'-C4'-C5'-O5'
54	Z	21	H2U	O4'-C4'-C5'-O5'
54	Z	21	H2U	C3'-C4'-C5'-O5'
54	Z	21	H2U	O4'-C1'-N1-C6

There are no ring outliers.

10 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1516	2MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	Z	56	PSU	1	0
22	a	1915	3TD	1	0
1	A	1207	2MG	1	0
54	Z	21	H2U	1	0
1	A	966	2MG	1	0
54	Z	55	5MU	1	0
22	a	1939	5MU	1	0
22	a	2030	6MZ	2	0
1	A	1519	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 457 ligands modelled in this entry, 457 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.