



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 11:23 AM JST

PDB ID : 8Y38
EMDB ID : EMD-38875
Title : Cryo-EM structure of Staphylococcus aureus 70S ribosome (strain 15B196) in complex with MCX-190.
Authors : Li, Y.; Lu, G.; Li, J.; Pei, X.; Lin, J.
Deposited on : 2024-01-28
Resolution : 2.58 Å(reported)

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

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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	: 4.02b-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)	: 2.39

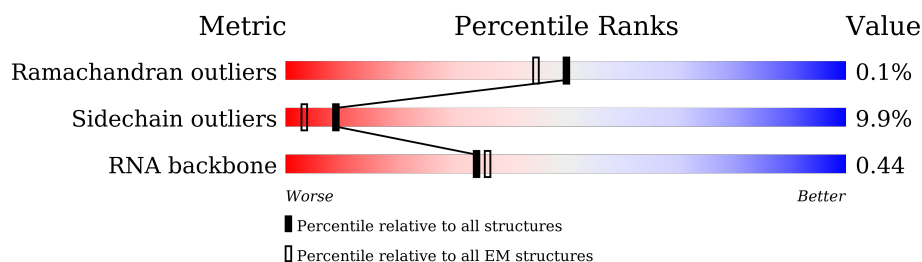
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 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	1	47	83% 17%
2	2	43	98% .
3	3	64	89% 11%
4	4	37	84% 16%
5	A	2921	66% 33% .
6	B	115	59% 41%
7	C	274	93% 7%
8	D	215	90% 10%
9	E	206	92% 8%




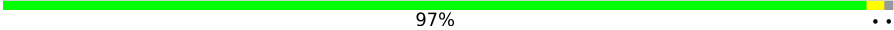





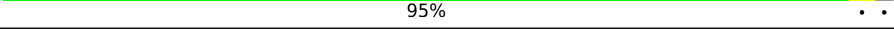
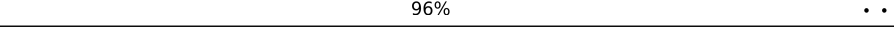
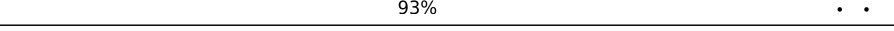

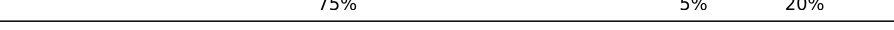

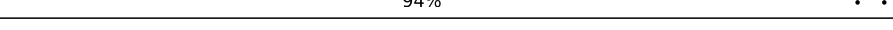
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Mol	Chain	Length	Quality of chain
10	F	175	
11	G	175	
12	H	145	
13	I	122	
14	J	146	
15	K	137	
16	L	120	
17	M	119	
18	N	114	
19	O	116	
20	P	102	
21	Q	117	
22	R	89	
23	S	103	
24	T	94	
25	U	82	
26	V	58	
27	W	67	
28	X	58	
29	Y	59	
30	Z	48	
31	a	1548	
32	b	232	
33	c	217	
34	d	200	

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Mol	Chain	Length	Quality of chain
35	e	166	 91% . 6%
36	f	98	 90% 7% .
37	g	156	 90% 10% .
38	h	132	 97% ..
39	i	130	 95% ..
40	j	102	 89% 6% 5%
41	k	129	 84% . 12%
42	l	149	 85% 5% . 9%
43	m	121	 90% 6% .
44	n	61	 95% ..
45	o	89	 96% ..
46	p	91	 93% . .
47	q	87	 83% 9% 8%
48	r	80	 75% 5% 20%
49	s	108	 70% 6% 24%
50	t	83	 94% . .

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 138224 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 bL33B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2885	Total	C	N	O	P	0	0
			61861	27621	11312	20043	2885		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	274	Total	C	N	O	S	0	0
			2090	1301	415	369	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1317	835	223	253	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	175	Total	C	N	O	S	0	0
			1259	788	239	229	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			891	557	174	159	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O		0	0
			889	563	175	151			

- Molecule 19 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 20 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	112	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 22 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 24 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	94	Total	C	N	O		0	0
			711	456	127	128			

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	82	Total	C	N	O		0	0
			615	380	121	114			

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	58	Total	C	N	O		0	0
			445	277	96	72			

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	67	Total	C	N	O		0	0
			541	333	102	106			

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	X	58	Total	C	N	O	0	0
			449	280	85	84		

- Molecule 29 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Y	57	Total	C	N	O	0	0
			353	214	65	74		

- Molecule 30 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	48	Total	C	N	O	S	0	0
			361	222	77	59	3		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1479	Total	C	N	O	P	0	0
			31706	14154	5809	10264	1479		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1032	N	C	conflict	GB 1747281577

- Molecule 32 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	224	Total	C	N	O	S	0	0
			1802	1149	314	332	7		

- Molecule 33 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	202	Total	C	N	O	S	0	0
			1596	1005	300	289	2		

- Molecule 34 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	199	Total	C	N	O	S	0	0
			1616	1020	302	292	2		

- Molecule 35 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	156	Total	C	N	O	S	0	0
			1160	731	212	215	2		

- Molecule 36 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	95	Total	C	N	O	S	0	0
			789	498	138	150	3		

- Molecule 37 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	155	Total	C	N	O	S	0	0
			1242	775	239	224	4		

- Molecule 38 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	131	Total	C	N	O	S	0	0
			1031	652	183	192	4		

- Molecule 39 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	127	Total	C	N	O	S	0	0
			1007	624	201	181	1		

- Molecule 40 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	97	Total	C	N	O	S	0	0
			773	488	141	143	1		

- Molecule 41 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	114	Total	C	N	O	S	0	0
			844	520	160	161	3		

- Molecule 42 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 43 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	116	Total	C	N	O	S	0	0
			922	566	183	172	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 45 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	87	Total	C	N	O	S	0	0
			726	448	149	128	1		

- Molecule 46 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	87	Total	C	N	O	S	0	0
			688	433	127	127	1		

- Molecule 47 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			657	416	117	123	1		

- Molecule 48 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	64	Total	C	N	O	S	0	0
			525	336	98	88	3		

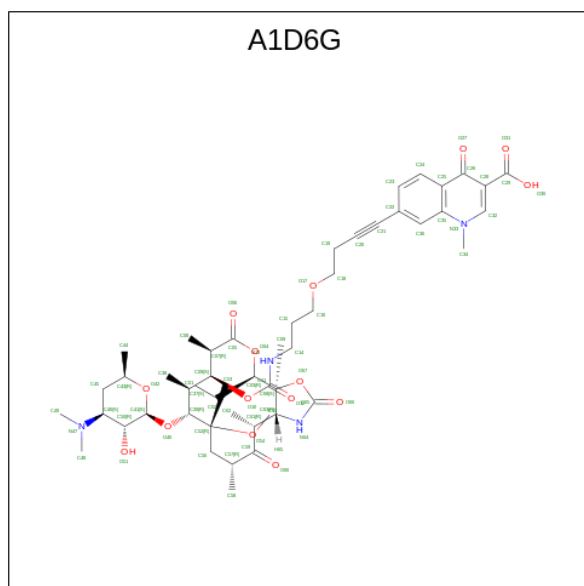
- Molecule 49 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			665	427	121	115	2		

- Molecule 50 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	81	Total	C	N	O	S	0	0
			611	370	120	119	2		

- Molecule 51 is 7-[4-[3-[(1 {S},2 {R},5 {R},6 {S},7 {S},8 {R},9 {R},11 {R},13 {R},14 {R})-8-[(2 {S},3 {R},4 {S},6 {R})-4-(dimethylamino)-6-methyl-3-oxidanyl-oxan-2-yl]oxy-2-ethyl-9-methoxy-1,5,7,9,11,13-hexamethyl-4,12,16-tris(oxidanylidene)-3,17-dioxo-15-azabicyclo [12.3.0]heptadecan-6-yl]oxycarbonylamino]propoxy]but-1-ynyl]-1-methyl-4-oxidanylidene-quinoline-3-carboxylic acid (three-letter code: A1D6G) (formula: C₅₀H₇₂N₄O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
51	A	1	Total	C	N	O	0
			69	50	4	15	

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	A	12	Total	Mg	0
			12	12	


- Molecule 53 is water.

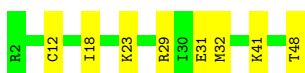
Mol	Chain	Residues	Atoms		AltConf
53	A	4	Total	O	0
			4	4	

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 bL33B

Chain 1:  83% 17%




- Molecule 2: Large ribosomal subunit protein bL34

Chain 2:  98%




- Molecule 3: Large ribosomal subunit protein bL35

Chain 3:  89% 11%



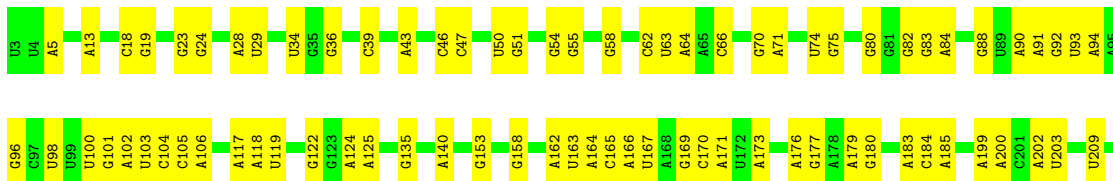
- Molecule 4: Large ribosomal subunit protein bL36

Chain 4:  84% 16%

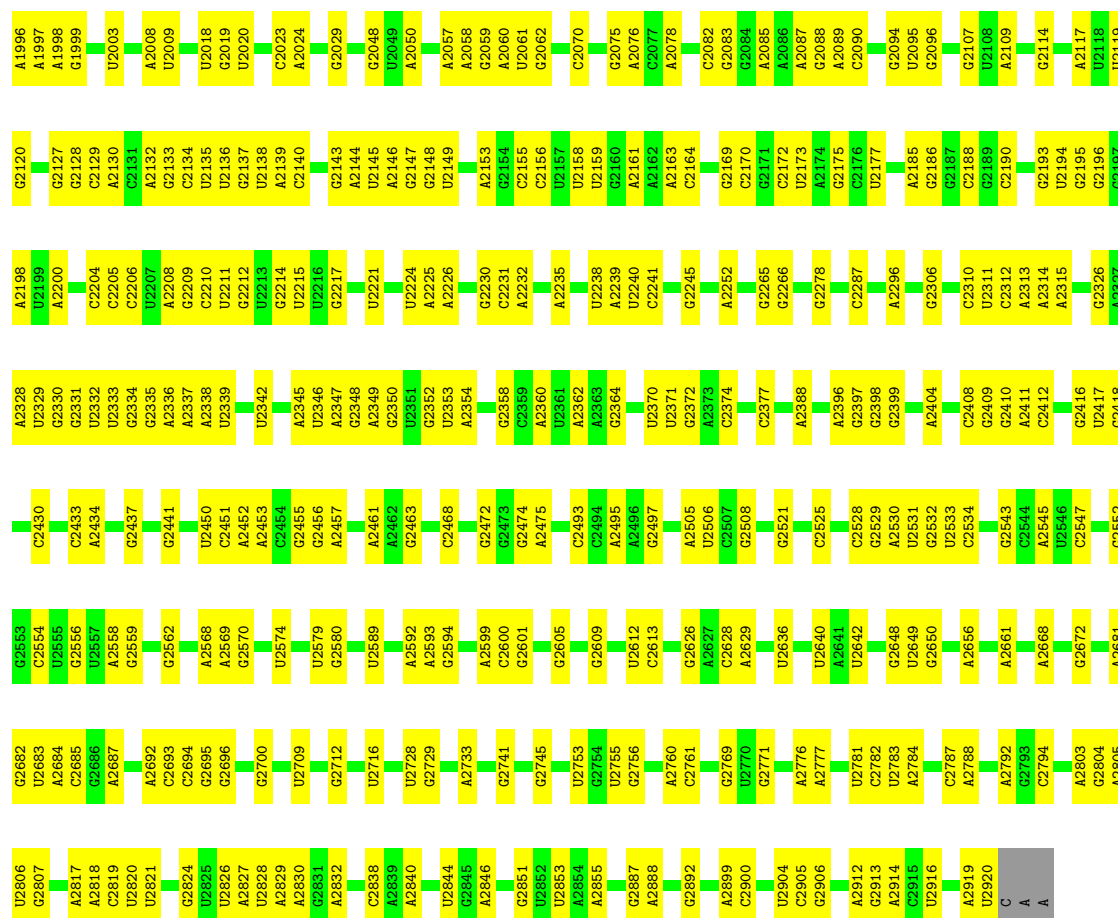


- Molecule 5: 23S ribosomal RNA

Chain A:  66% 33%

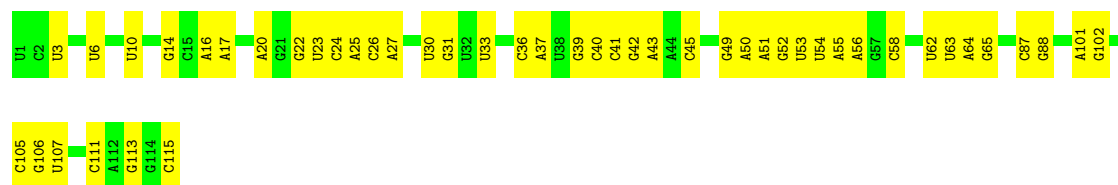


A1883	C1719	U1598	G1524	U1287	A1150	C960	A834	G696	G565	G434	A305	C213
A1886	U1737	G1599	U1525	G1290	G1151	U964	U986	U697	U566	C440	U309	G214
A1893	G1740	U1602	A1527	A1291	C1153	G965	C836	U699	G667	A440	C310	G215
G1894	U1757	A1605	G1528	G1294	G1155	U970	A837	A700	A447	A448	U311	G217
U1897	A1758	C1606	U1532	G1304	G1156	U971	G850	A715	C572	U449	A312	G218
C1898	G1759	G1613	A1527	U1455	U1157	A972	U856	C716	A574	A451	U	A219
U1899	G1760	A1616	G1528	U1457	G1158	A973	U856	A720	G575	G452	A	A224
A1903	G1761	A1616	G1528	U1457	C1160	U974	C857	A721	U576	G452	C	A225
A1904	U1762	A1616	G1528	U1457	C1160	U975	U857	A721	U577	G452	G	A226
G1905	U1763	A1616	G1528	U1457	C1160	U976	U857	A721	U577	G452	G	A226
A1908	U1764	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A318	A231
A1909	U1765	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	U821	U232
A1912	U1766	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A324	U233
C1919	U1767	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A325	G235
A1923	U1768	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A326	A236
G1933	U1769	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A327	A236
G1934	U1770	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A328	U242
U1938	U1771	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A329	U243
A1939	U1772	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A330	A244
A	U1773	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A331	G248
C	U1774	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A332	G251
U	U1775	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A333	G255
A	U1776	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A334	A268
U	U1777	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A335	G269
A	U1778	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A336	C272
C	U1779	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A337	A275
U	U1780	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A338	A278
A	U1781	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A339	A279
U	U1782	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A340	C280
A	U1783	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A341	A281
C	U1784	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A342	A282
U	U1785	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A343	G283
A	U1786	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A344	C284
C	U1787	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A345	U285
U	U1788	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A346	U286
A	U1789	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A347	G287
C	U1790	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A348	C288
U	U1791	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A349	U289
A	U1792	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A350	U290
C	U1793	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A351	G291
U	U1794	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A352	U292
A	U1795	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A353	G293
C	U1796	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A354	G294
U	U1797	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A355	U299
A	U1798	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A356	G300
C	U1799	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A357	U301
U	U1800	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A358	A302
A	U1801	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A359	G303
C	U1802	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A360	G304
U	U1803	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A361	
A	U1804	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A362	
C	U1805	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A363	
U	U1806	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A364	
A	U1807	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A365	
C	U1808	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A366	
U	U1809	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A367	
A	U1810	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A368	
C	U1811	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A369	
U	U1812	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A370	
A	U1813	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A371	
C	U1814	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A372	
U	U1815	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A373	
A	U1816	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A374	
C	U1817	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A375	
U	U1818	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A376	
A	U1819	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A377	
C	U1820	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A378	
U	U1821	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A379	
A	U1822	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A380	
C	U1823	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A381	
U	U1824	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A382	
A	U1825	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A383	
C	U1826	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A384	
U	U1827	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A385	
A	U1828	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A386	
C	U1829	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A387	
U	U1830	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A388	
A	U1831	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A389	
C	U1832	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A390	
U	U1833	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A391	
A	U1834	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A392	
C	U1835	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A393	
U	U1836	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A394	
A	U1837	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A395	
C	U1838	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A396	
U	U1839	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A397	
A	U1840	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A398	
C	U1841	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A399	
U	U1842	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A400	
A	U1843	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A401	
C	U1844	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A402	
U	U1845	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A403	
A	U1846	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A404	
C	U1847	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A405	
U	U1848	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A406	
A	U1849	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A407	
C	U1850	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A408	
U	U1851	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A409	
A	U1852	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A410	
C	U1853	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A411	
U	U1854	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A412	
A	U1855	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A413	
C	U1856	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A414	
U	U1857	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A415	
A	U1858	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A416	
C	U1859	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A417	
U	U1860	A1616	G1528	U1457	C1160	U977	U857	A721	U577	G452	A418	
A	U1861	A1616	G1528	U1457	C1160	U977	U857	A721				



• Molecule 6: 5S ribosomal RNA

Chain B: 59% 41%



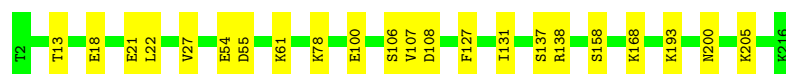
• Molecule 7: Large ribosomal subunit protein uL2

Chain C: 93% 7%



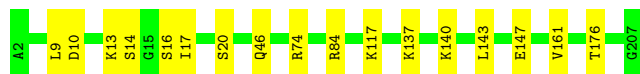
• Molecule 8: Large ribosomal subunit protein uL3

Chain D: 90% 10%




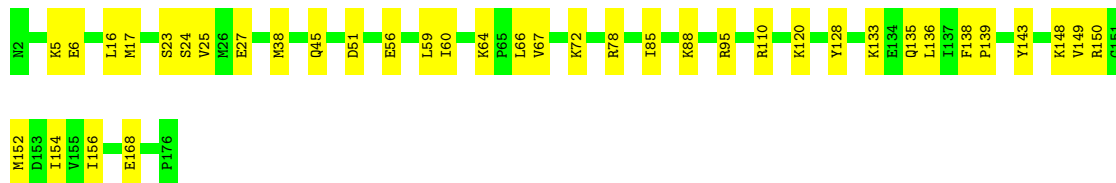
- Molecule 9: Large ribosomal subunit protein uL4

Chain E:  92% 8%




- Molecule 10: Large ribosomal subunit protein uL5

Chain F:  78% 22%



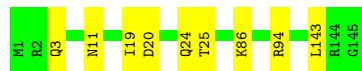
- Molecule 11: Large ribosomal subunit protein uL6

Chain G:  85% 15%




- Molecule 12: Large ribosomal subunit protein uL13

Chain H:  94% 6%



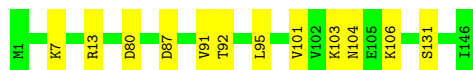
- Molecule 13: Large ribosomal subunit protein uL14

Chain I:  88% 11%




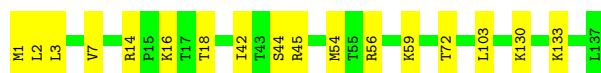
- Molecule 14: Large ribosomal subunit protein uL15

Chain J:  92% 8%



- Molecule 15: Large ribosomal subunit protein uL16

Chain K:  88% 12%



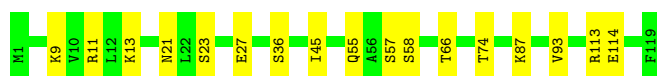
- Molecule 16: Large ribosomal subunit protein bL17

Chain L: 97% .



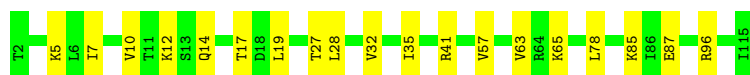
- Molecule 17: Large ribosomal subunit protein uL18

Chain M: 86% 14%



- Molecule 18: Large ribosomal subunit protein bL19

Chain N: 83% 17%



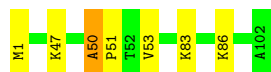
- Molecule 19: Large ribosomal subunit protein bL20

Chain O: 93% 7%



- Molecule 20: Large ribosomal subunit protein bL21

Chain P: 93% 6% .



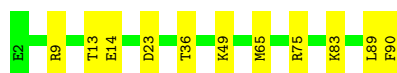
- Molecule 21: Large ribosomal subunit protein uL22

Chain Q: 88% 8% .

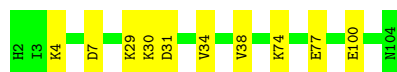
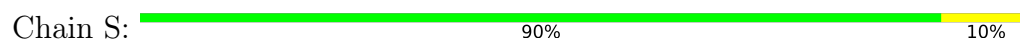


- Molecule 22: Large ribosomal subunit protein uL23

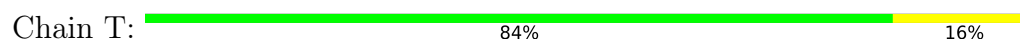
Chain R: 88% 12%



- Molecule 23: Large ribosomal subunit protein uL24



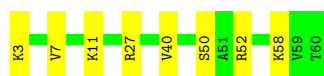
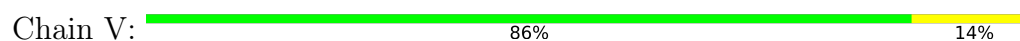
- Molecule 24: Large ribosomal subunit protein bL25



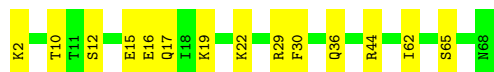
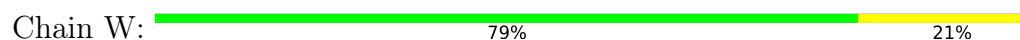
- Molecule 25: Large ribosomal subunit protein bL27



- Molecule 26: Large ribosomal subunit protein bL28



- Molecule 27: Large ribosomal subunit protein uL29



- Molecule 28: Large ribosomal subunit protein uL30



- Molecule 29: Large ribosomal subunit protein bL31B

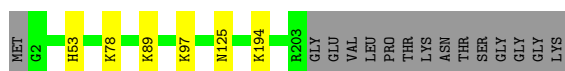
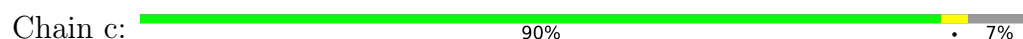




- Molecule 32: Small ribosomal subunit protein uS2



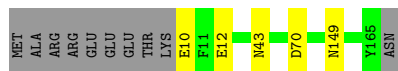
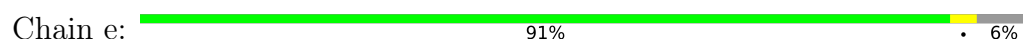
- Molecule 33: Small ribosomal subunit protein uS3



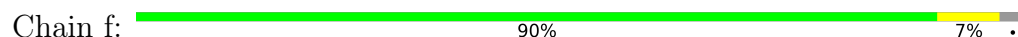
- Molecule 34: Small ribosomal subunit protein uS4



- Molecule 35: Small ribosomal subunit protein uS5



- Molecule 36: Small ribosomal subunit protein bS6



- Molecule 37: Small ribosomal subunit protein uS7



- Molecule 38: Small ribosomal subunit protein uS8





- Molecule 39: Small ribosomal subunit protein uS9

Chain i: 95% ..



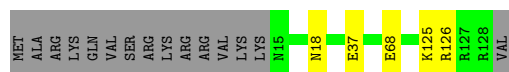
- Molecule 40: Small ribosomal subunit protein uS10

Chain j: 89% 6% 5%



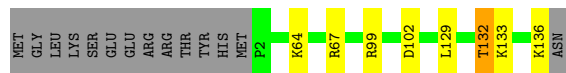
- Molecule 41: Small ribosomal subunit protein uS11

Chain k: 84% . 12%



- Molecule 42: Small ribosomal subunit protein uS12

Chain l: 85% 5% . 9%



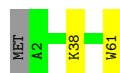
- Molecule 43: Small ribosomal subunit protein uS13

Chain m: 90% 6% .



- Molecule 44: Small ribosomal subunit protein uS14B

Chain n: 95% ..



- Molecule 45: Small ribosomal subunit protein uS15

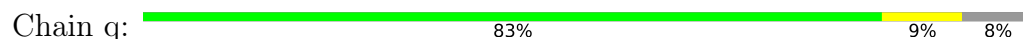
Chain o: 96% ..



- Molecule 46: Small ribosomal subunit protein bS16



- Molecule 47: Small ribosomal subunit protein uS17



- Molecule 48: Small ribosomal subunit protein bS18



- Molecule 49: Small ribosomal subunit protein uS19



- Molecule 50: Small ribosomal subunit protein bS20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47560	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
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: 2MG, A1D6G, 5MU, MA6, 2MA, MG, OMG

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	1	0.60	0/395	0.85	0/530
2	2	0.44	0/371	0.71	0/484
3	3	0.61	0/526	0.81	0/690
4	4	0.73	0/299	0.91	0/393
5	A	0.52	0/69122	0.80	1/107793 (0.0%)
6	B	0.35	0/2733	0.71	0/4257
7	C	0.65	0/2125	0.87	0/2853
8	D	0.71	0/1651	0.83	0/2215
9	E	0.66	0/1595	0.76	0/2154
10	F	0.46	0/1332	0.79	0/1798
11	G	0.59	0/1277	0.78	0/1731
12	H	0.51	0/1165	0.71	0/1570
13	I	0.65	0/925	0.81	0/1242
14	J	0.46	0/1100	0.69	0/1467
15	K	0.64	0/1095	0.76	0/1472
16	L	0.46	0/936	0.69	0/1253
17	M	0.59	0/900	0.77	0/1205
18	N	0.59	0/901	0.76	0/1209
19	O	0.43	0/954	0.64	0/1264
20	P	0.51	0/800	0.72	1/1070 (0.1%)
21	Q	0.61	0/861	0.78	0/1161
22	R	0.53	0/723	0.71	0/966
23	S	0.48	0/779	0.73	0/1043
24	T	0.45	0/719	0.66	0/969
25	U	0.55	0/621	0.76	0/825
26	V	0.71	0/451	0.85	0/603
27	W	0.52	0/542	0.70	0/722
28	X	0.51	0/451	0.62	0/606
29	Y	0.37	0/361	0.67	0/500
30	Z	0.58	0/367	0.81	0/490
31	a	0.24	0/35498	0.83	0/55345
32	b	0.26	0/1829	0.53	0/2455

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.23	0/1618	0.50	0/2173
34	d	0.25	0/1646	0.49	0/2211
35	e	0.28	0/1174	0.53	0/1584
36	f	0.27	0/800	0.57	0/1073
37	g	0.24	0/1262	0.51	0/1698
38	h	0.27	0/1043	0.50	0/1401
39	i	0.25	0/1023	0.59	0/1374
40	j	0.25	0/785	0.51	0/1060
41	k	0.29	0/859	0.57	0/1161
42	l	0.27	0/1075	0.57	0/1439
43	m	0.24	0/929	0.59	0/1246
44	n	0.25	0/511	0.53	0/678
45	o	0.23	0/735	0.52	0/982
46	p	0.27	0/699	0.53	0/942
47	q	0.29	0/665	0.57	0/889
48	r	0.29	0/534	0.63	0/715
49	s	0.26	0/683	0.55	0/916
50	t	0.23	0/611	0.46	0/817
All	All	0.45	0/150056	0.78	2/224694 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1555	G	C3'-C2'-C1'	-5.28	97.28	101.50
20	P	50	ALA	C-N-CD	5.13	139.18	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	45/47 (96%)	41 (91%)	4 (9%)	0	100	100
2	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
3	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
4	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
7	C	272/274 (99%)	245 (90%)	26 (10%)	1 (0%)	30	50
8	D	213/215 (99%)	200 (94%)	13 (6%)	0	100	100
9	E	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
10	F	173/175 (99%)	144 (83%)	28 (16%)	1 (1%)	22	41
11	G	173/175 (99%)	157 (91%)	16 (9%)	0	100	100
12	H	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
13	I	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	33
14	J	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
15	K	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
16	L	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
17	M	117/119 (98%)	107 (92%)	10 (8%)	0	100	100
18	N	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
19	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
20	P	100/102 (98%)	93 (93%)	5 (5%)	2 (2%)	6	11
21	Q	110/117 (94%)	105 (96%)	5 (4%)	0	100	100
22	R	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
23	S	101/103 (98%)	88 (87%)	13 (13%)	0	100	100
24	T	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
25	U	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
26	V	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
27	W	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
28	X	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
29	Y	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
30	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
32	b	222/232 (96%)	212 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	c	200/217 (92%)	190 (95%)	10 (5%)	0	100	100
34	d	197/200 (98%)	187 (95%)	10 (5%)	0	100	100
35	e	154/166 (93%)	149 (97%)	5 (3%)	0	100	100
36	f	93/98 (95%)	87 (94%)	6 (6%)	0	100	100
37	g	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	h	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
39	i	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
40	j	95/102 (93%)	89 (94%)	6 (6%)	0	100	100
41	k	112/129 (87%)	102 (91%)	10 (9%)	0	100	100
42	l	133/149 (89%)	122 (92%)	10 (8%)	1 (1%)	16	33
43	m	114/121 (94%)	105 (92%)	9 (8%)	0	100	100
44	n	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
45	o	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
46	p	85/91 (93%)	84 (99%)	1 (1%)	0	100	100
47	q	78/87 (90%)	74 (95%)	4 (5%)	0	100	100
48	r	62/80 (78%)	60 (97%)	2 (3%)	0	100	100
49	s	80/108 (74%)	73 (91%)	7 (9%)	0	100	100
50	t	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
All	All	5323/5563 (96%)	4979 (94%)	338 (6%)	6 (0%)	50	69

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	P	51	PRO
13	I	98	ILE
10	F	139	PRO
20	P	50	ALA
42	l	132	THR

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	1	44/45 (98%)	36 (82%)	8 (18%)	1	2
2	2	39/39 (100%)	38 (97%)	1 (3%)	41	65
3	3	55/55 (100%)	48 (87%)	7 (13%)	3	6
4	4	35/35 (100%)	29 (83%)	6 (17%)	1	2
7	C	220/221 (100%)	202 (92%)	18 (8%)	9	19
8	D	173/173 (100%)	151 (87%)	22 (13%)	3	6
9	E	168/168 (100%)	151 (90%)	17 (10%)	6	11
10	F	139/154 (90%)	102 (73%)	37 (27%)	0	0
11	G	123/153 (80%)	96 (78%)	27 (22%)	1	1
12	H	122/123 (99%)	113 (93%)	9 (7%)	11	23
13	I	100/100 (100%)	85 (85%)	15 (15%)	2	4
14	J	109/112 (97%)	97 (89%)	12 (11%)	5	9
15	K	108/114 (95%)	91 (84%)	17 (16%)	2	3
16	L	96/101 (95%)	92 (96%)	4 (4%)	25	48
17	M	86/95 (90%)	69 (80%)	17 (20%)	1	1
18	N	93/100 (93%)	74 (80%)	19 (20%)	1	1
19	O	96/96 (100%)	88 (92%)	8 (8%)	9	18
20	P	84/86 (98%)	79 (94%)	5 (6%)	16	33
21	Q	89/94 (95%)	80 (90%)	9 (10%)	6	11
22	R	78/80 (98%)	67 (86%)	11 (14%)	3	5
23	S	81/88 (92%)	71 (88%)	10 (12%)	4	7
24	T	75/82 (92%)	60 (80%)	15 (20%)	1	1
25	U	60/64 (94%)	53 (88%)	7 (12%)	4	8
26	V	44/49 (90%)	36 (82%)	8 (18%)	1	2
27	W	58/60 (97%)	44 (76%)	14 (24%)	0	1
28	X	52/52 (100%)	47 (90%)	5 (10%)	7	13
29	Y	21/56 (38%)	19 (90%)	2 (10%)	7	13
30	Z	36/44 (82%)	35 (97%)	1 (3%)	38	63
32	b	194/201 (96%)	182 (94%)	12 (6%)	15	31
33	c	164/175 (94%)	158 (96%)	6 (4%)	29	53
34	d	174/175 (99%)	169 (97%)	5 (3%)	37	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	e	122/131 (93%)	117 (96%)	5 (4%)	26	49
36	f	83/86 (96%)	76 (92%)	7 (8%)	9	18
37	g	131/132 (99%)	116 (88%)	15 (12%)	4	8
38	h	112/113 (99%)	109 (97%)	3 (3%)	40	64
39	i	105/107 (98%)	101 (96%)	4 (4%)	28	52
40	j	87/91 (96%)	81 (93%)	6 (7%)	13	26
41	k	90/104 (86%)	85 (94%)	5 (6%)	17	36
42	l	117/130 (90%)	109 (93%)	8 (7%)	13	27
43	m	100/104 (96%)	93 (93%)	7 (7%)	12	25
44	n	52/53 (98%)	50 (96%)	2 (4%)	28	52
45	o	79/81 (98%)	77 (98%)	2 (2%)	42	66
46	p	74/77 (96%)	72 (97%)	2 (3%)	40	64
47	q	75/82 (92%)	67 (89%)	8 (11%)	5	10
48	r	57/68 (84%)	53 (93%)	4 (7%)	12	25
49	s	71/91 (78%)	65 (92%)	6 (8%)	8	17
50	t	67/69 (97%)	64 (96%)	3 (4%)	23	45
All	All	4438/4709 (94%)	3997 (90%)	441 (10%)	9	12

5 of 441 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	N	65	LYS
24	T	24	SER
50	t	15	GLU
42	l	64	LYS
19	O	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
37	g	142	HIS
37	g	148	ASN
49	s	22	GLN
41	k	119	ASN
24	T	88	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1470/1548 (94%)	382 (25%)	0
5	A	2877/2921 (98%)	941 (32%)	78 (2%)
6	B	114/115 (99%)	46 (40%)	4 (3%)
All	All	4461/4584 (97%)	1369 (30%)	82 (1%)

5 of 1369 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	5	A
5	A	13	A
5	A	18	C
5	A	19	G
5	A	23	G

5 of 82 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	1826	G
5	A	2533	U
5	A	2094	G
5	A	2347	A
5	A	2829	A

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

6 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	$\# Z > 2$
5	2MA	A	2530	52,5	17,25,26	1.08	0	17,37,40	1.29	3 (17%)
5	5MU	A	792	5	19,22,23	1.48	5 (26%)	28,32,35	2.25	8 (28%)
5	5MU	A	1966	5	19,22,23	1.67	5 (26%)	28,32,35	2.32	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OMG	A	2278	5	18,26,27	1.07	1 (5%)	19,38,41	1.21	3 (15%)
5	2MG	A	2472	5	18,26,27	1.19	1 (5%)	16,38,41	1.18	2 (12%)
5	MA6	A	2085	5	18,26,27	1.06	2 (11%)	19,38,41	1.76	5 (26%)

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
5	2MA	A	2530	52,5	-	0/3/25/26	0/3/3/3
5	5MU	A	792	5	-	0/7/25/26	0/2/2/2
5	5MU	A	1966	5	-	0/7/25/26	0/2/2/2
5	OMG	A	2278	5	-	1/5/27/28	0/3/3/3
5	2MG	A	2472	5	-	0/5/27/28	0/3/3/3
5	MA6	A	2085	5	-	2/7/29/30	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2472	2MG	C6-N1	-3.64	1.32	1.37
5	A	1966	5MU	C4-N3	-3.27	1.32	1.38
5	A	792	5MU	C4-N3	-3.27	1.32	1.38
5	A	1966	5MU	C6-C5	3.14	1.39	1.34
5	A	2278	OMG	C6-N1	-3.10	1.33	1.37

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1966	5MU	N3-C2-N1	5.87	122.69	114.89
5	A	1966	5MU	C5-C4-N3	5.40	119.92	115.31
5	A	792	5MU	N3-C2-N1	5.33	121.97	114.89
5	A	1966	5MU	C4-N3-C2	-5.13	120.71	127.35
5	A	792	5MU	C4-N3-C2	-5.10	120.75	127.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2085	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
5	A	2278	OMG	C1'-C2'-O2'-CM2
5	A	2085	MA6	N1-C6-N6-C10

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 13 ligands modelled in this entry, 12 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
51	A1D6G	A	3000	52	70,73,73	2.38	24 (34%)	96,107,107	1.76	27 (28%)

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
51	A1D6G	A	3000	52	-	11/82/113/113	0/5/5/5

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A	3000	A1D6G	C65-N64	8.48	1.45	1.33
51	A	3000	A1D6G	C11-N13	7.15	1.50	1.34
51	A	3000	A1D6G	O10-C11	5.00	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A	3000	A1D6G	O67-C65	4.66	1.43	1.36
51	A	3000	A1D6G	C22-C21	4.61	1.55	1.44

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	A	3000	A1D6G	C52-C39-C37	-4.16	107.24	113.61
51	A	3000	A1D6G	O42-C43-C45	4.12	115.45	109.14
51	A	3000	A1D6G	C02-C03-C68	-3.95	109.79	115.23
51	A	3000	A1D6G	O10-C11-N13	3.94	118.03	111.11
51	A	3000	A1D6G	C44-C43-C45	-3.83	107.38	113.40

There are no chirality outliers.

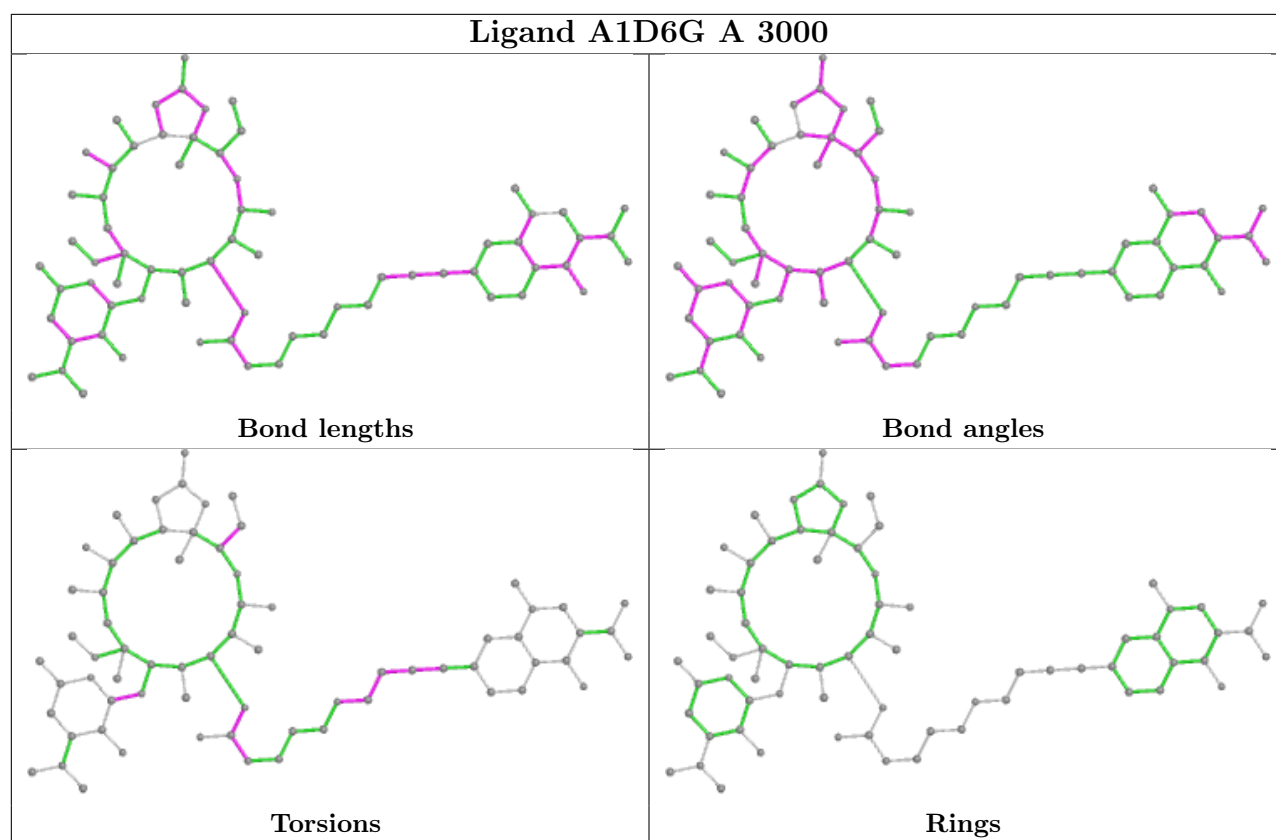
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	A	3000	A1D6G	C18-C19-C20-C21
51	A	3000	A1D6G	O10-C11-N13-C14
51	A	3000	A1D6G	O12-C11-N13-C14
51	A	3000	A1D6G	C19-C20-C21-C22
51	A	3000	A1D6G	N13-C11-O10-C09

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.