wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 02:51 PM JST

PDB ID : 8Y39
EMDB ID : EMD-38876
Title : cryo-EM structure of Staphylococcus aureus(ATCC 29213) 70S ribosome in complex with MCX-190.
Authors : Li, Y.; Lu, G.; Li, J.; Pei, X.; Lin, J.
Deposited on : 2024-01-28
Resolution : 3.60 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

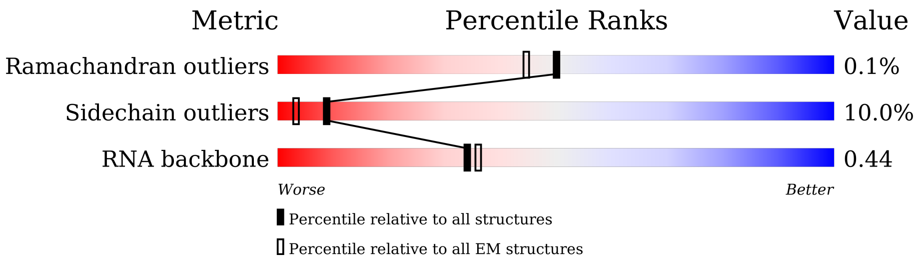
EMDB validation analysis : FAILED
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : FAILED
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

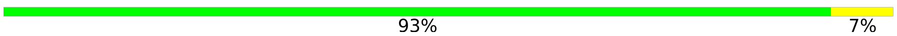
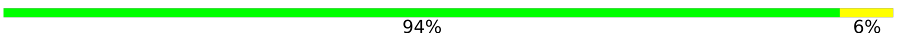
The reported resolution of this entry is 3.60 Å.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	2921	 66% 33% •
2	B	115	 60% 40%
3	C	274	 93% 7%
4	D	215	 90% 10%
5	E	206	 92% 8%
6	F	175	 78% 22%
7	G	175	 85% 15%
8	H	145	 94% 6%
9	I	122	 88% 11% •

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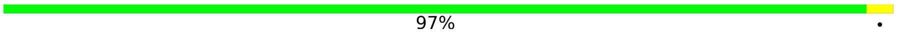
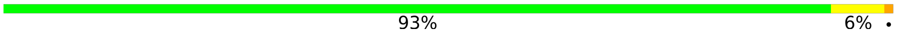
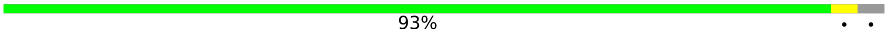
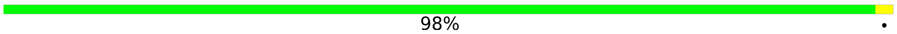
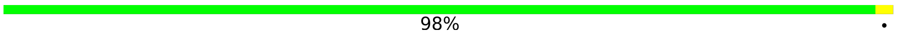
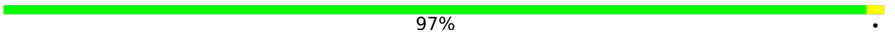
Mol	Chain	Length	Quality of chain
10	J	146	 92% 8%
11	K	137	 87% 13%
12	L	120	 97% •
13	M	119	 86% 14%
14	N	114	 83% 17%
15	O	116	 92% 8%
16	P	102	 93% 6% •
17	Q	117	 88% 8% •
18	R	89	 88% 12%
19	S	103	 90% 10%
20	T	94	 84% 16%
21	U	82	 91% 9%
22	V	58	 86% 14%
23	W	67	 79% 21%
24	X	58	 91% 9%
25	Y	59	 93% • •
26	Z	48	 98% •
27	1	47	 79% 21%
28	2	43	 98% •
29	3	64	 89% 11%
30	4	37	 84% 16%
31	a	1548	 71% 25% •
32	b	232	 92% 5% •
33	c	217	 90% • 7%
34	d	200	 97% •

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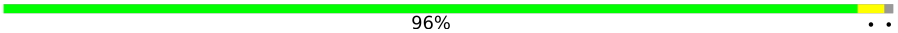
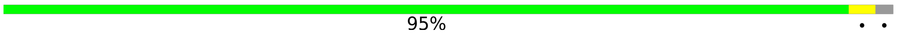
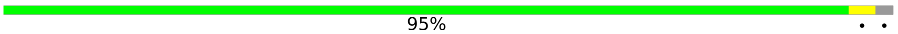
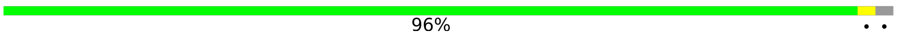
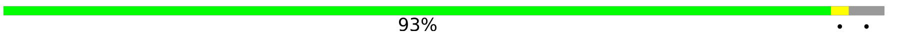
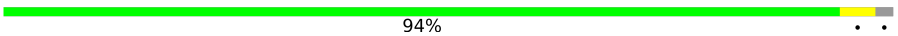
Mol	Chain	Length	Quality of chain
35	e	166	
36	f	98	
37	g	156	
38	h	132	
39	i	130	
40	j	102	
41	k	129	
42	l	149	
43	m	121	
44	n	61	
45	o	89	
46	p	91	
47	q	87	
48	r	80	
49	s	108	
50	t	83	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 138218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2885	61859	27619	11312	20043	2885	0	0

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

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

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 12 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 14 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 15 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 16 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 19 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 20 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 22 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 23 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 25 is a protein called Large ribosomal subunit protein bL31B.

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

- Molecule 26 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 27 is a protein called Large ribosomal subunit protein bL33B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	1	47	390	238	78	70	4	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	2	43	367	225	89	52	1	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	3	64	521	324	113	82	2	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	4	37	296	186	60	45	5	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

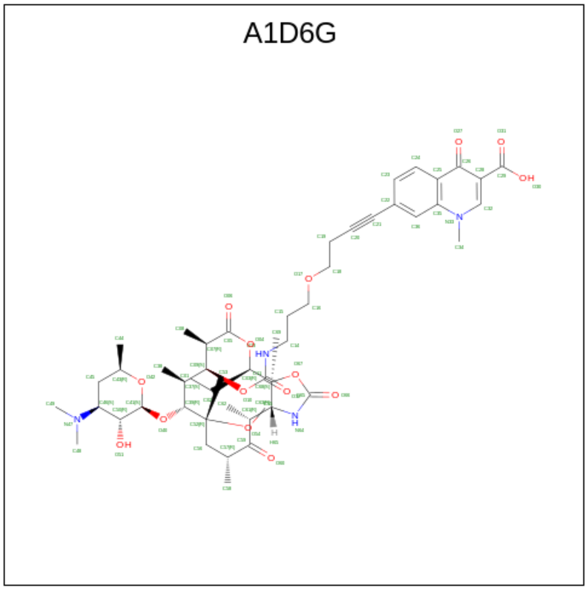
- Molecule 49 is a protein called Small ribosomal subunit protein uS19.

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

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

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

- 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-dioxa-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: $C_{50}H_{72}N_4O_{15}$).



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

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

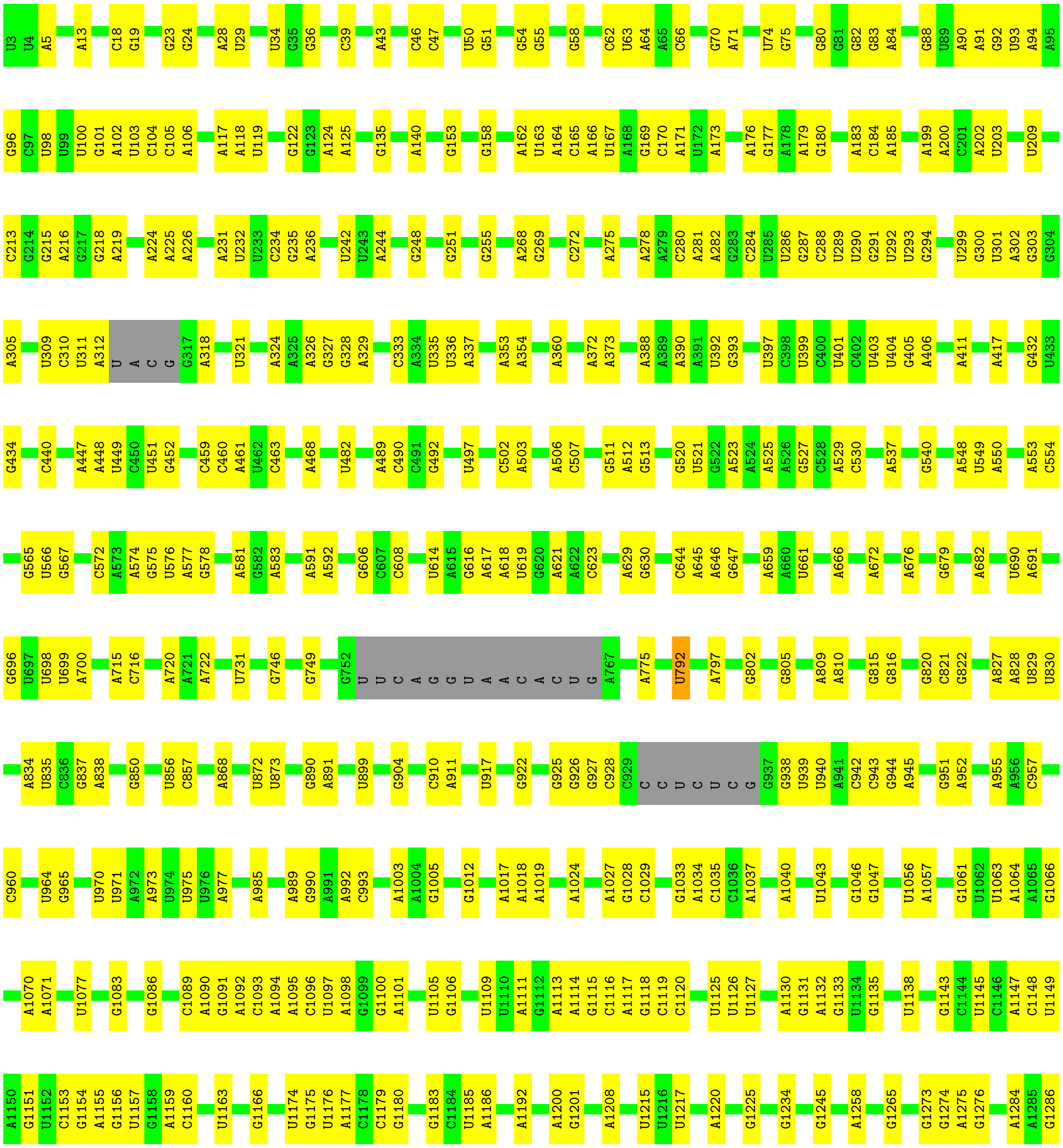
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
52	A	12	12	12	0

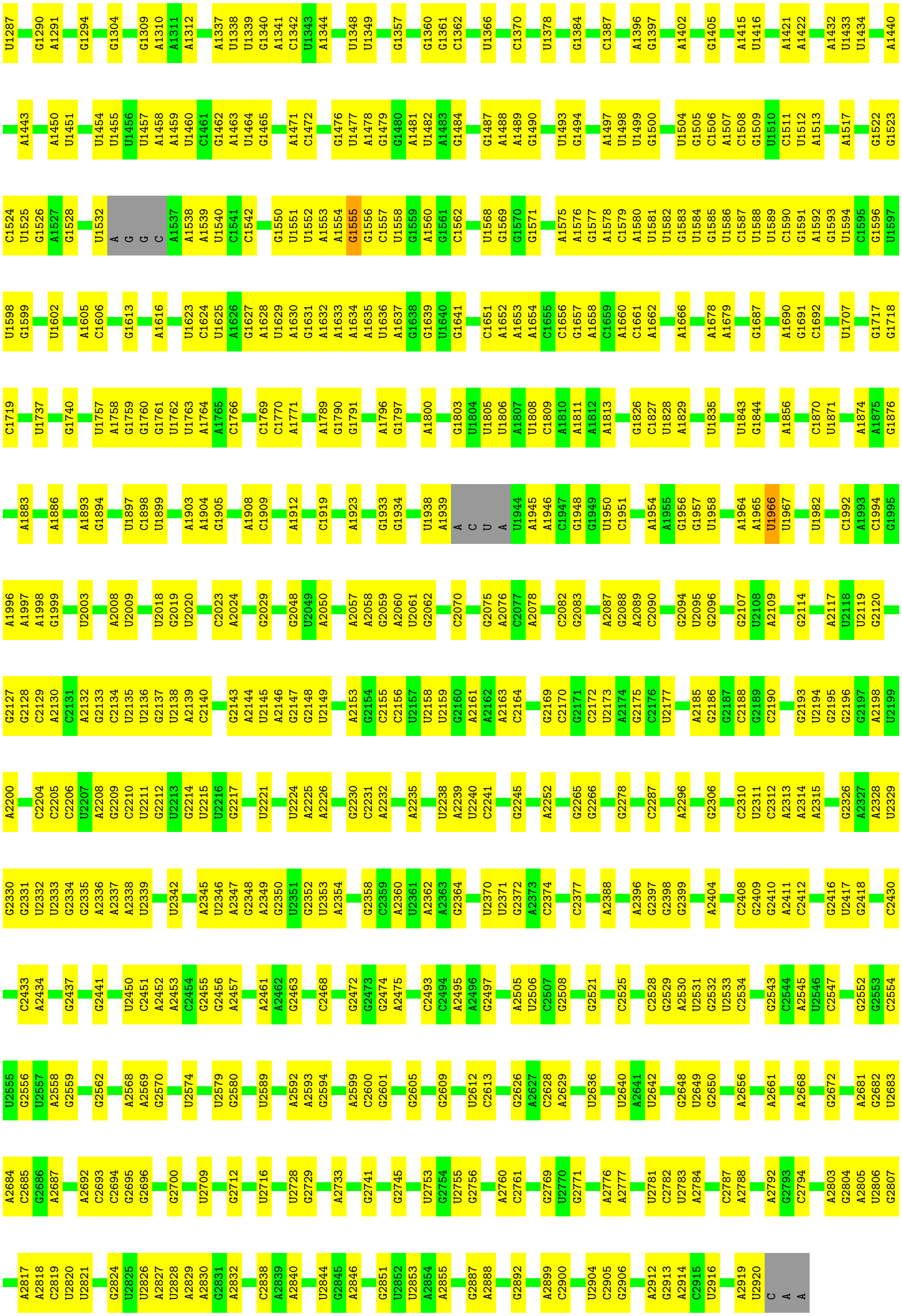
3 Residue-property plots ⓘ

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

- Molecule 1: 23S ribosomal RNA

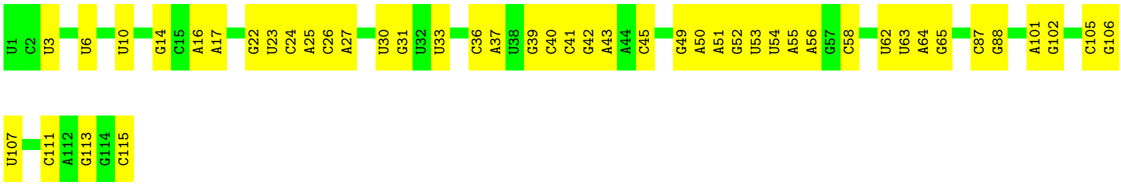
Chain A:





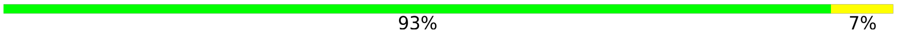
- Molecule 2: 5S ribosomal RNA

Chain B:



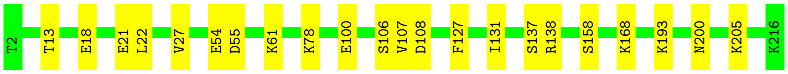
- Molecule 3: Large ribosomal subunit protein uL2

Chain C:



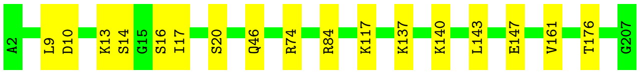
- Molecule 4: Large ribosomal subunit protein uL3

Chain D:



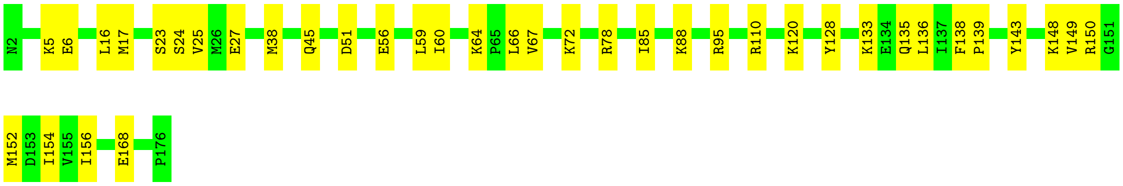
- Molecule 5: Large ribosomal subunit protein uL4

Chain E:



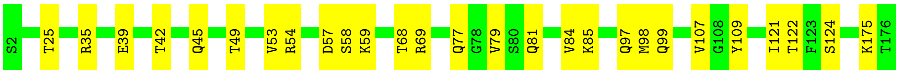
- Molecule 6: Large ribosomal subunit protein uL5

Chain F:



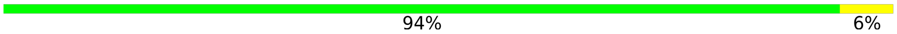
- Molecule 7: Large ribosomal subunit protein uL6

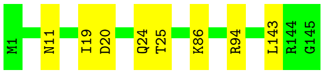
Chain G:



- Molecule 8: Large ribosomal subunit protein uL13

Chain H:



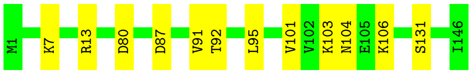


- Molecule 9: Large ribosomal subunit protein uL14

Chain I:

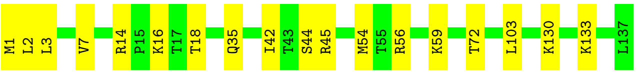
- Molecule 10: Large ribosomal subunit protein uL15

Chain J:



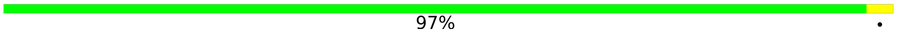
- Molecule 11: Large ribosomal subunit protein uL16

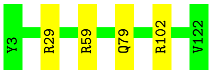
Chain K:



- Molecule 12: Large ribosomal subunit protein bL17

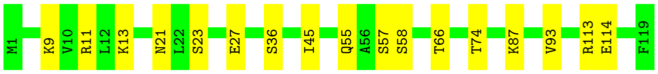
Chain L:





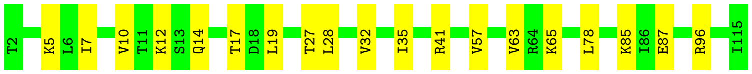
- Molecule 13: Large ribosomal subunit protein uL18

Chain M:



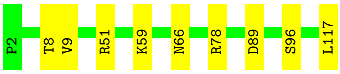
- Molecule 14: Large ribosomal subunit protein bL19

Chain N:



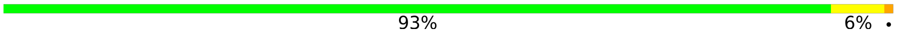
- Molecule 15: Large ribosomal subunit protein bL20

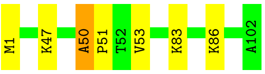
Chain O:



- Molecule 16: Large ribosomal subunit protein bL21

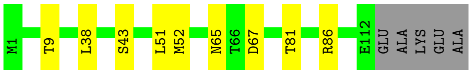
Chain P:





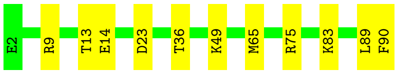
- Molecule 17: Large ribosomal subunit protein uL22

Chain Q:



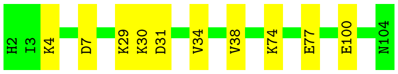
- Molecule 18: Large ribosomal subunit protein uL23

Chain R:



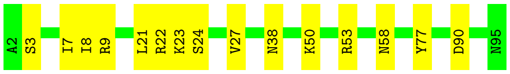
- Molecule 19: Large ribosomal subunit protein uL24

Chain S:



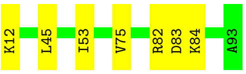
- Molecule 20: Large ribosomal subunit protein bL25

Chain T:



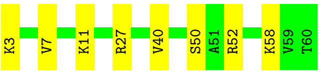
- Molecule 21: Large ribosomal subunit protein bL27

Chain U:



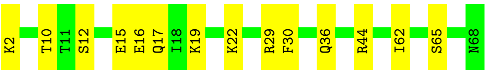
- Molecule 22: Large ribosomal subunit protein bL28

Chain V:



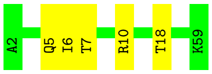
- Molecule 23: Large ribosomal subunit protein uL29

Chain W:



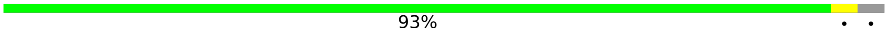
- Molecule 24: Large ribosomal subunit protein uL30

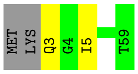
Chain X:



- Molecule 25: Large ribosomal subunit protein bL31B

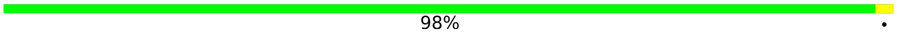
Chain Y:

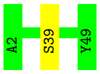




- Molecule 26: Large ribosomal subunit protein bL32

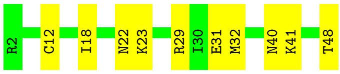
Chain Z:





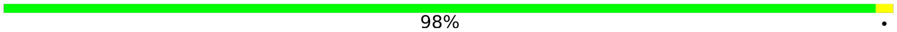
- Molecule 27: Large ribosomal subunit protein bL33B

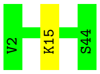
Chain 1:



- Molecule 28: Large ribosomal subunit protein bL34

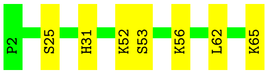
Chain 2:





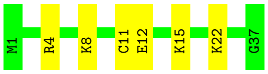
- Molecule 29: Large ribosomal subunit protein bL35

Chain 3:



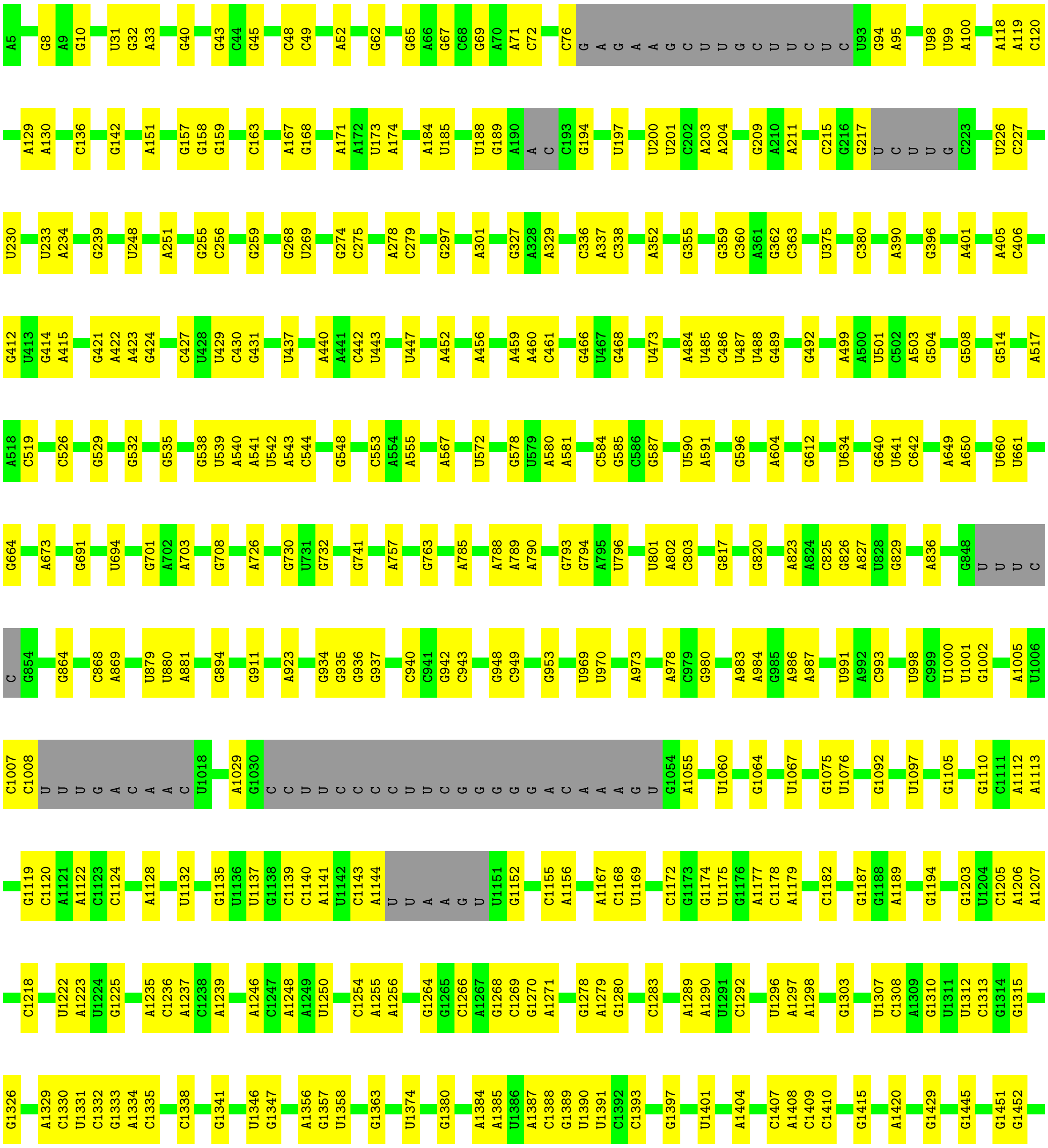
- Molecule 30: Large ribosomal subunit protein bL36

Chain 4:



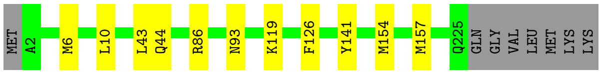
- Molecule 31: 16S ribosomal RNA

Chain a:



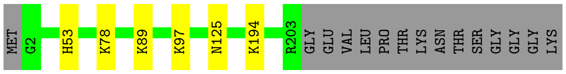
- Molecule 32: Small ribosomal subunit protein uS2

Chain b:



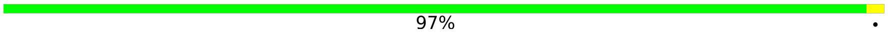
- Molecule 33: Small ribosomal subunit protein uS3

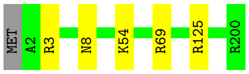
Chain c:



- Molecule 34: Small ribosomal subunit protein uS4

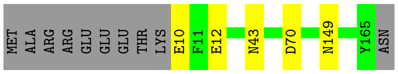
Chain d:





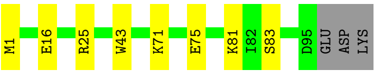
- Molecule 35: Small ribosomal subunit protein uS5

Chain e:



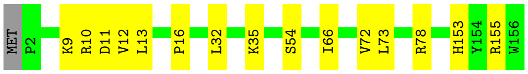
- Molecule 36: Small ribosomal subunit protein bS6

Chain f:



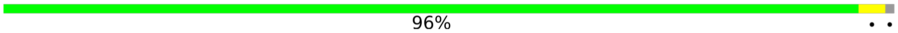
- Molecule 37: Small ribosomal subunit protein uS7

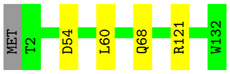
Chain g:



- Molecule 38: Small ribosomal subunit protein uS8

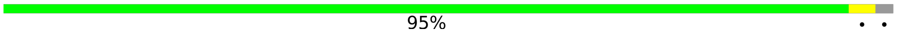
Chain h:

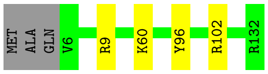




- Molecule 39: Small ribosomal subunit protein uS9

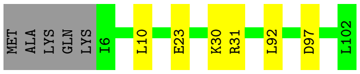
Chain i:





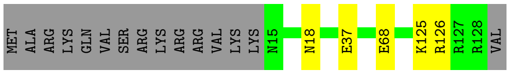
- Molecule 40: Small ribosomal subunit protein uS10

Chain j:



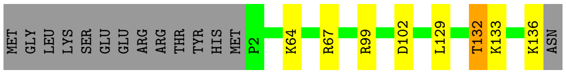
- Molecule 41: Small ribosomal subunit protein uS11

Chain k:



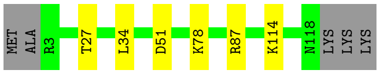
- Molecule 42: Small ribosomal subunit protein uS12

Chain l:



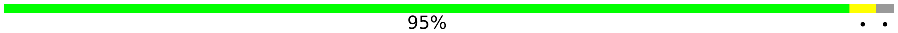
- Molecule 43: Small ribosomal subunit protein uS13

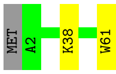
Chain m:



- Molecule 44: Small ribosomal subunit protein uS14B

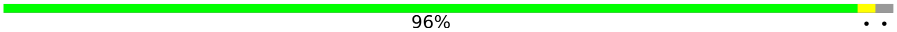
Chain n:

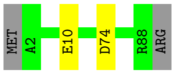




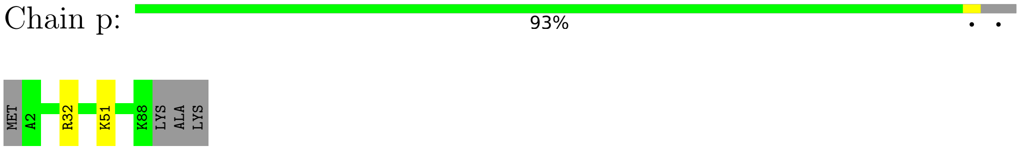
- Molecule 45: Small ribosomal subunit protein uS15

Chain o:

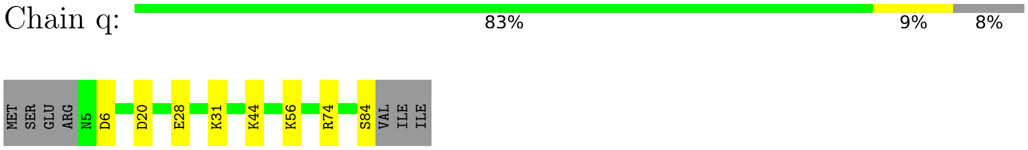




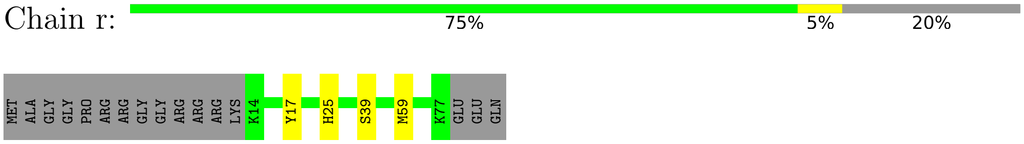
- Molecule 46: Small ribosomal subunit protein bS16



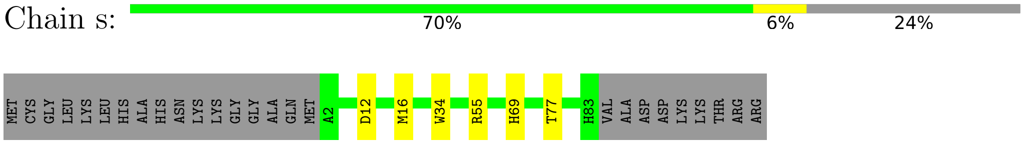
- Molecule 47: Small ribosomal subunit protein uS17



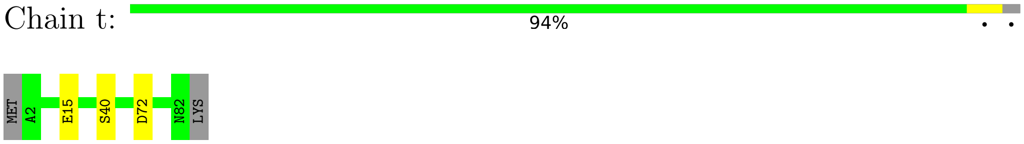
- Molecule 48: Small ribosomal subunit protein bS18



- 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	27177	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 $(e^-/\text{Å}^2)$	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: MG, OMG, 2MG, 5MU, 2MA, A1D6G

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	0.53	0/69148	0.80	1/107836 (0.0%)
2	B	0.36	0/2733	0.72	0/4257
3	C	0.65	0/2125	0.87	0/2853
4	D	0.71	0/1651	0.83	0/2215
5	E	0.67	0/1595	0.76	0/2154
6	F	0.46	0/1332	0.79	0/1798
7	G	0.59	0/1277	0.77	0/1731
8	H	0.51	0/1165	0.71	0/1570
9	I	0.65	0/925	0.81	0/1242
10	J	0.46	0/1100	0.69	0/1467
11	K	0.64	0/1095	0.76	0/1472
12	L	0.46	0/936	0.69	0/1253
13	M	0.59	0/900	0.77	0/1205
14	N	0.59	0/901	0.76	0/1209
15	O	0.44	0/954	0.64	0/1264
16	P	0.51	0/800	0.72	1/1070 (0.1%)
17	Q	0.61	0/861	0.78	0/1161
18	R	0.53	0/723	0.71	0/966
19	S	0.48	0/779	0.73	0/1043
20	T	0.45	0/719	0.67	0/969
21	U	0.55	0/621	0.77	0/825
22	V	0.71	0/451	0.86	0/603
23	W	0.51	0/542	0.70	0/722
24	X	0.51	0/451	0.63	0/606
25	Y	0.37	0/361	0.67	0/500
26	Z	0.58	0/367	0.81	0/490
27	1	0.61	0/395	0.85	0/530
28	2	0.44	0/371	0.71	0/484
29	3	0.61	0/526	0.82	1/690 (0.1%)
30	4	0.73	0/299	0.91	0/393
31	a	0.25	0/35498	0.84	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	0.24	0/1618	0.50	0/2173
34	d	0.25	0/1646	0.50	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	0.51	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	0.52	0/678
45	o	0.24	0/735	0.53	0/982
46	p	0.27	0/699	0.53	0/942
47	q	0.29	0/665	0.57	0/889
48	r	0.30	0/534	0.63	0/715
49	s	0.26	0/683	0.55	0/916
50	t	0.24	0/611	0.46	0/817
All	All	0.45	0/150082	0.78	3/224737 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1555	G	C3'-C2'-C1'	-5.30	97.26	101.50
16	P	50	ALA	C-N-CD	5.12	139.16	128.40
29	3	25	SER	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles ⓘ

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	
3	C	272/274 (99%)	245 (90%)	26 (10%)	1 (0%)	30	63
4	D	213/215 (99%)	200 (94%)	13 (6%)	0	100	100
5	E	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
6	F	173/175 (99%)	144 (83%)	28 (16%)	1 (1%)	22	55
7	G	173/175 (99%)	157 (91%)	16 (9%)	0	100	100
8	H	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
9	I	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	51
10	J	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
11	K	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
12	L	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
13	M	117/119 (98%)	107 (92%)	10 (8%)	0	100	100
14	N	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
15	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
16	P	100/102 (98%)	93 (93%)	5 (5%)	2 (2%)	6	34
17	Q	110/117 (94%)	105 (96%)	5 (4%)	0	100	100
18	R	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
19	S	101/103 (98%)	88 (87%)	13 (13%)	0	100	100
20	T	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
21	U	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
22	V	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
23	W	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
24	X	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
25	Y	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
26	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
27	1	45/47 (96%)	41 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
30	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
32	b	222/232 (96%)	211 (95%)	11 (5%)	0	100	100
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%)	150 (97%)	4 (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	51
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%)	4978 (94%)	339 (6%)	6 (0%)	50	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	51	PRO
9	I	98	ILE
6	F	139	PRO
16	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	
3	C	220/221 (100%)	202 (92%)	18 (8%)	9	34
4	D	173/173 (100%)	151 (87%)	22 (13%)	3	19
5	E	168/168 (100%)	151 (90%)	17 (10%)	6	27
6	F	139/154 (90%)	102 (73%)	37 (27%)	0	3
7	G	123/153 (80%)	96 (78%)	27 (22%)	1	5
8	H	122/123 (99%)	114 (93%)	8 (7%)	14	42
9	I	100/100 (100%)	85 (85%)	15 (15%)	2	15
10	J	109/112 (97%)	97 (89%)	12 (11%)	5	25
11	K	108/114 (95%)	90 (83%)	18 (17%)	2	11
12	L	96/101 (95%)	92 (96%)	4 (4%)	25	54
13	M	86/95 (90%)	69 (80%)	17 (20%)	1	7
14	N	93/100 (93%)	74 (80%)	19 (20%)	1	6
15	O	96/96 (100%)	87 (91%)	9 (9%)	7	30
16	P	84/86 (98%)	79 (94%)	5 (6%)	16	45
17	Q	89/94 (95%)	80 (90%)	9 (10%)	6	27
18	R	78/80 (98%)	67 (86%)	11 (14%)	3	17
19	S	81/88 (92%)	71 (88%)	10 (12%)	4	20
20	T	75/82 (92%)	60 (80%)	15 (20%)	1	6
21	U	60/64 (94%)	53 (88%)	7 (12%)	4	23
22	V	44/49 (90%)	36 (82%)	8 (18%)	1	8
23	W	58/60 (97%)	44 (76%)	14 (24%)	0	4
24	X	52/52 (100%)	47 (90%)	5 (10%)	7	29
25	Y	21/56 (38%)	19 (90%)	2 (10%)	7	30
26	Z	36/44 (82%)	35 (97%)	1 (3%)	38	64
27	1	44/45 (98%)	34 (77%)	10 (23%)	0	4
28	2	39/39 (100%)	38 (97%)	1 (3%)	41	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	3	55/55 (100%)	49 (89%)	6 (11%)	5	25
30	4	35/35 (100%)	29 (83%)	6 (17%)	1	10
32	b	194/201 (96%)	183 (94%)	11 (6%)	17	46
33	c	164/175 (94%)	158 (96%)	6 (4%)	29	58
34	d	174/175 (99%)	169 (97%)	5 (3%)	37	63
35	e	122/131 (93%)	117 (96%)	5 (4%)	26	55
36	f	83/86 (96%)	75 (90%)	8 (10%)	7	29
37	g	131/132 (99%)	116 (88%)	15 (12%)	4	23
38	h	112/113 (99%)	108 (96%)	4 (4%)	30	59
39	i	105/107 (98%)	101 (96%)	4 (4%)	28	57
40	j	87/91 (96%)	81 (93%)	6 (7%)	13	40
41	k	90/104 (86%)	85 (94%)	5 (6%)	17	47
42	l	117/130 (90%)	109 (93%)	8 (7%)	13	41
43	m	100/104 (96%)	94 (94%)	6 (6%)	16	45
44	n	52/53 (98%)	50 (96%)	2 (4%)	28	57
45	o	79/81 (98%)	77 (98%)	2 (2%)	42	66
46	p	74/77 (96%)	72 (97%)	2 (3%)	40	65
47	q	75/82 (92%)	67 (89%)	8 (11%)	5	26
48	r	57/68 (84%)	53 (93%)	4 (7%)	12	40
49	s	71/91 (78%)	65 (92%)	6 (8%)	8	33
50	t	67/69 (97%)	64 (96%)	3 (4%)	23	53
All	All	4438/4709 (94%)	3995 (90%)	443 (10%)	9	28

5 of 443 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	51	LEU
22	V	52	ARG
49	s	69	HIS
41	k	68	GLU
18	R	13	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	43	GLN
49	s	22	GLN
20	T	88	HIS
41	k	119	ASN
33	c	88	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2878/2921 (98%)	941 (32%)	78 (2%)
2	B	114/115 (99%)	45 (39%)	4 (3%)
31	a	1470/1548 (94%)	382 (25%)	0
All	All	4462/4584 (97%)	1368 (30%)	82 (1%)

5 of 1368 RNA backbone outliers are listed below:

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

5 of 82 RNA pucker outliers are listed below:

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

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

5 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	2MA	A	2530	52,1	17,25,26	1.07	0	17,37,40	1.29	3 (17%)
1	2MG	A	2472	1	18,26,27	1.19	1 (5%)	16,38,41	1.17	2 (12%)
1	5MU	A	792	1	19,22,23	1.48	5 (26%)	28,32,35	2.24	8 (28%)
1	OMG	A	2278	1	18,26,27	1.08	1 (5%)	19,38,41	1.22	3 (15%)
1	5MU	A	1966	1	19,22,23	1.66	5 (26%)	28,32,35	2.33	8 (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
1	2MA	A	2530	52,1	-	0/3/25/26	0/3/3/3
1	2MG	A	2472	1	-	0/5/27/28	0/3/3/3
1	5MU	A	792	1	-	0/7/25/26	0/2/2/2
1	OMG	A	2278	1	-	1/5/27/28	0/3/3/3
1	5MU	A	1966	1	-	0/7/25/26	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2472	2MG	C6-N1	-3.61	1.32	1.37
1	A	792	5MU	C4-N3	-3.27	1.32	1.38
1	A	1966	5MU	C4-N3	-3.22	1.32	1.38
1	A	2278	OMG	C6-N1	-3.16	1.33	1.37
1	A	1966	5MU	C6-C5	3.12	1.39	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1966	5MU	N3-C2-N1	5.91	122.73	114.89
1	A	1966	5MU	C5-C4-N3	5.42	119.94	115.31
1	A	792	5MU	N3-C2-N1	5.30	121.93	114.89
1	A	1966	5MU	C4-N3-C2	-5.20	120.62	127.35
1	A	792	5MU	C4-N3-C2	-5.07	120.79	127.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2278	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	2.37	23 (32%)	96,107,107	1.76	25 (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
51	A1D6G	A	3000	52	-	11/82/113/113	0/5/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A	3000	A1D6G	C65-N64	8.53	1.45	1.33
51	A	3000	A1D6G	C11-N13	7.12	1.49	1.34
51	A	3000	A1D6G	O10-C11	4.94	1.43	1.35
51	A	3000	A1D6G	C22-C21	4.64	1.55	1.44
51	A	3000	A1D6G	O67-C65	4.63	1.43	1.36

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	A	3000	A1D6G	O42-C43-C45	4.15	115.49	109.14
51	A	3000	A1D6G	C52-C39-C37	-4.13	107.29	113.61
51	A	3000	A1D6G	C02-C03-C68	-3.97	109.76	115.23
51	A	3000	A1D6G	O10-C11-N13	3.94	118.03	111.11
51	A	3000	A1D6G	C44-C43-C45	-3.84	107.37	113.40

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

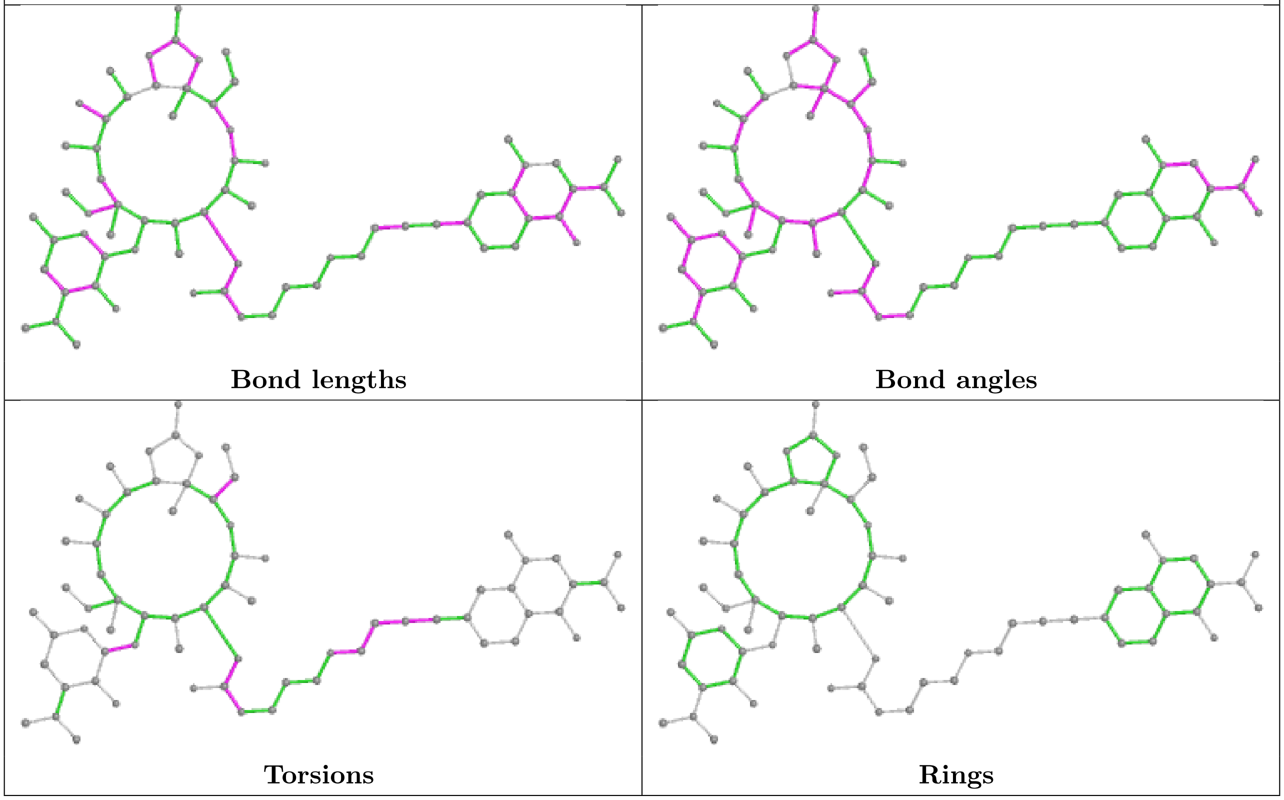
Mol	Chain	Res	Type	Atoms
51	A	3000	A1D6G	O10-C11-N13-C14
51	A	3000	A1D6G	O12-C11-N13-C14
51	A	3000	A1D6G	C19-C20-C21-C22
51	A	3000	A1D6G	N13-C11-O10-C09
51	A	3000	A1D6G	C18-C19-C20-C21

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 then 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.

Ligand A1D6G A 3000



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.