



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2024 – 10:52 AM JST

PDB ID : 8Y37
EMDB ID : EMD-38874
Title : Cryo-EM structure of Staphylococcus aureus (15B196) 50S ribosome in complex with MCX-190.
Authors : Li, Y.; Lu, G.; Li, J.; Pei, X.; Lin, J.
Deposited on : 2024-01-28
Resolution : 2.53 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	: FAILED
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4.02b-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

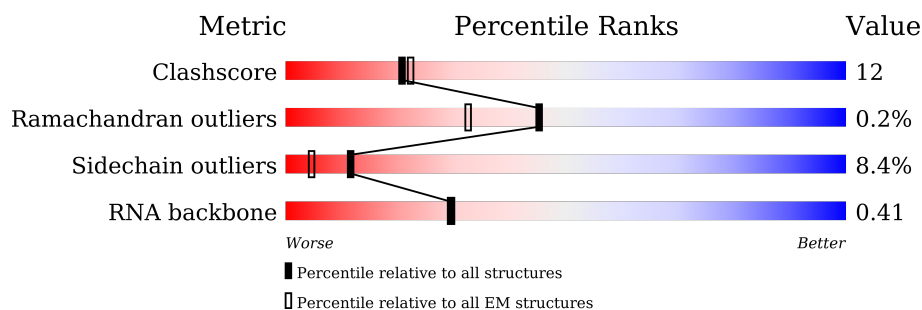
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	47	60% 36% .
2	2	43	79% 21%
3	3	64	73% 25% .
4	4	37	57% 41% .
5	A	2921	52% 39% 8% .
6	B	115	50% 38% 11%
7	C	274	65% 32% ..
8	D	215	65% 33% .

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Mol	Chain	Length	Quality of chain
9	E	206	
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	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 88301 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	2884	Total	C	N	O	P	0	0
			61838	27611	11307	20036	2884		

- 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		

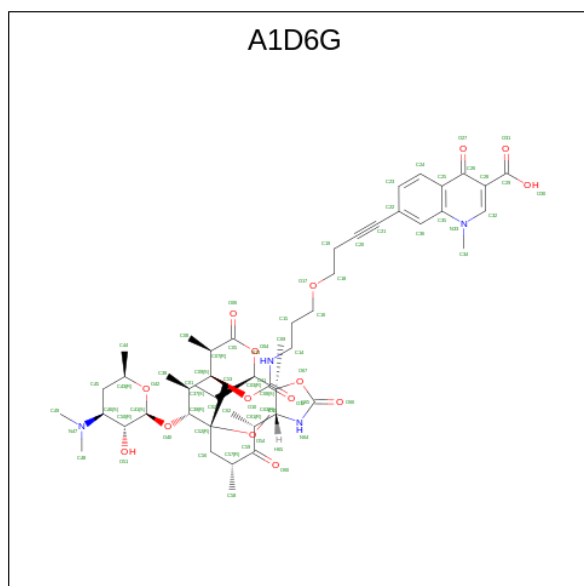
- Molecule 29 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	59	Total	C	N	O	S	0	0
			370	225	68	76	1		

- 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 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
31	A	1	Total	C	N	O	0
			69	50	4	15	

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 33 is water.

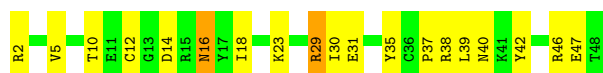
Mol	Chain	Residues	Atoms		AltConf
33	A	6	Total	O	0
			6	6	

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: 



- Molecule 2: Large ribosomal subunit protein bL34

Chain 2: 



- Molecule 3: Large ribosomal subunit protein bL35

Chain 3: 



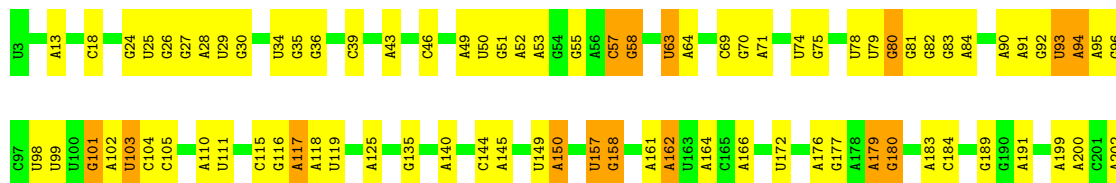
- Molecule 4: Large ribosomal subunit protein bL36

Chain 4: 



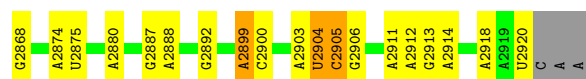
- Molecule 5: 23S ribosomal RNA

Chain A: 

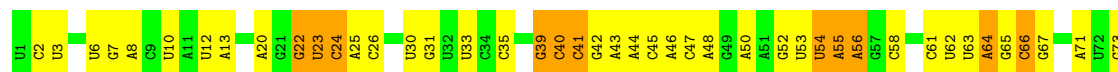


U1493	C1400	A1303	G1207	G1133	A1064	A972	G890	U	C674	A574	U482	G393	G291	U209
G1494	A1401	U1305	A1208	U1134	A1065	A973	A891	G	A677	G575	A489	G396	U292	A210
G1495	G1402	A1306	U1215	C1136	G1066	U974	U896	A757	A678	U576	A489	U397	U293	
G1496			U1216	U975		U976	U897	G774	A679	A577	A490	C398	G294	
A1497	G1405	G1307	U1217	G1137	A1070	U976	U898	A775	G681	U579	G492	U399	G297	G213
U1498	A1308	G1308	G1218	U1138	A1071	U977	U899	U786	A682	C580	G493	U400	U298	G215
U1499	A1415	A1310	G1219	A1140	A1072	A985	G900	U787	G683	A581	A493	U401	U299	A216
G1500	U1416	A1311	A1220	U1141	A1073	A989	G901	A788	U684	G582	G496	U402	G300	G217
A1501	A1421	A1312	G1225	A1142	U1077	A990	G902	U789	U686	A583	U497	U403	U301	G218
A1502	A1422	G1315	G1226	A1143	G1080	A991	G903	A788	U688	A591	C502	U404	A302	A219
U1503	C1423	U1316	U1227	U1145	A992	A992	G904	U792	U688	A592	A503	U405	G303	A220
U1504			A1228	A992	C993	C993		A797	A689	U593		G304	G221	G221
G			G1229	C993			C910					A406	A305	
A1506	G1426	C1326	G1229	G1000	G1083	G1000	A911			G409	A506		A305	
A1507	U1427	U1327	C1148	G1000	U1084	G1000	A911			G410	C507		A305	A225
C1508		G1328	U1149	U1085	U1085	U1085	U917	G802	A691	A411			U309	A225
G1509	A1432	G1329	C1235	U1150	U1086	U1086	U917	G805	G696	U510			C310	A226
U1510	U1433	U1330	G1236	G1151	G1087	U1087	C921	G809	U697	G511			U311	G227
C1511	U1434		U1237	U1152	A1004	A1004	G922	A810	U698	A512			A312	A228
U1512	C1435	C1336	G1245	G1153	A1005	A1005	G923	A810	U699	G513			U	A229
A1513	C1436	A1337	G1246	A1155	G1091	G1091	G924	G815	A700	G514			A	A230
		U1338	G1247	G1156	A1092	A1092	G925	G816	G701	G515			C	U231
		U1339	G1247	U1157	C1093	C1093	G926	G816	U702	A516			G	U232
		G1340	G1247	U1157	A1094	A1094	G927	G816	A703	A517			G317	U233
		A1341	C1254	G1158	A1095	A1095	C928	G820	A703	A518			A318	C234
		C1342	C1254	A1159	C1096	A1096	C929	G821	G707	A519			G319	G235
		U1343	U1258	C1160	U1097	U1097	C	G822	A621	G520			U320	
		A1344	U1259	U1163	A1098	A1098	U	G822	A622	G521			U321	U238
		G1345	G1260	U1163	G1100	G1100	U	A827	C623	U521			C322	
		U1346	G1261	G1166	A1101	A1101	U	A827	G711	G522			C323	U242
		G1347	G1265	G1169	U1102	U1102	C	A827	A715	A523			A324	U243
		U1348	G1265	G1169	G1103	G1103	U	A827	C716	A524			A325	A244
		C1349	G1273	G1174	U1104	U1104	G	A827	A719	A525			A326	
		A1357	G1274	G1175	U1105	U1105	G937	A834	G719	A526			G327	G248
		A1358	A1275	U1176	C1033	C1033	U939	U835	A720	A527			A329	G251
		A1359	G1276	C1177	G1036	G1036	U940	G837	A721	G528			C333	G252
		G1360	C1277	C1178	U1037	U1037	A941	G837	A722	A529			A334	G253
		G1361	C1278	G1180	C1038	C1038	C942	A838	U731	G534			A335	A254
		C1362	C1279	G1180	C1039	C1039	C943	G850	U738	A448			U336	G255
			U1280	G1183	U1040	U1040	C944	C851	U738	U449			G350	G267
		U1366		G1183	U1043	U1043	A945	U852	G746	U450			G351	A268
		C1370	A1284	C1184	A1044	A1044	G951	G853	G749	G452			A352	C270
			A1285	U1185	C1116	C1116	A952	U856	G749	A548			A353	C271
		U1378	G1286	A1186	U1117	U1117	A953	C857	U657	U549			A354	C272
		A1379	U1287	A1186	G1118	G1118	A954	U858	A658	A550			A273	A273
		G1380	A1192	A1192	C1119	C1119	A955	C859	A659	A553			A360	
		U1381		A1192	C1120	C1120	C957	U	U	A461			A363	A278
		A1471	G1290	C1197	C1051	C1051	C957	U	U	U462			A363	A279
		C1472	A1291	C1197	A1052	A1052	C957	U	U	U463			C280	
			A1291	C1197	A1053	A1053	C957	U	U	U464			A372	G283
		G1476	G1294	A1199	U1125	U1125	C960	A864	A	U556			A373	G284
		U1477	C1295	A1199	U1126	U1126	A961	A868	G	U556			A373	C284
		A1478	C1296	G1201	U1056	U1056	A962	A868	G	U556			A373	U285
		G1479	G1297	U1202	U1057	U1057	A963	U872	U	G565			A388	U286
				U1203	A1057	A1057	A964	U873	A	U666			A389	
		A1390		U1203	A1057	A1057	A965	U873	A	U667			A390	
		A1396	G1300	U1204	U1061	U1061	A965	G881	C	U668			A391	U289
		G1397	U1301	U1205	U1062	U1062	A965	C882	C	A672			A391	U290
			G1302	G1206	U1063	U1063	U970		C	G673			U392	

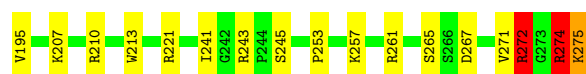
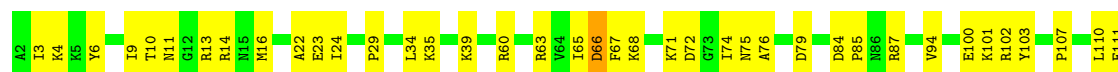




• Molecule 6: 5S ribosomal RNA



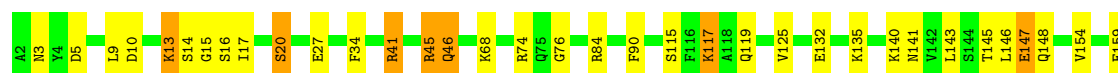
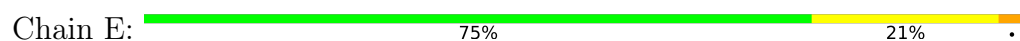
• Molecule 7: Large ribosomal subunit protein uL2



• Molecule 8: Large ribosomal subunit protein uL3



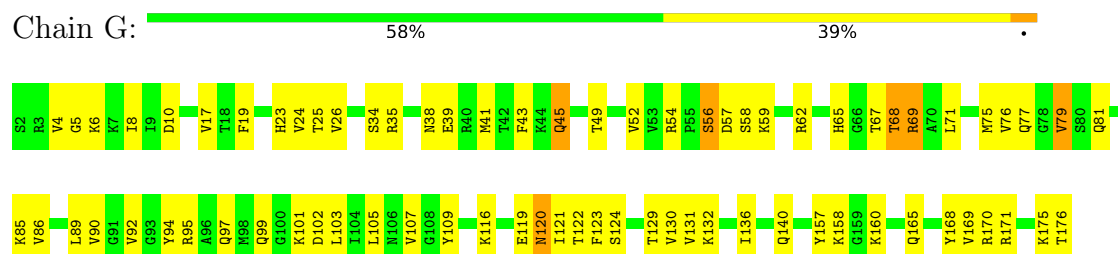
• Molecule 9: Large ribosomal subunit protein uL4



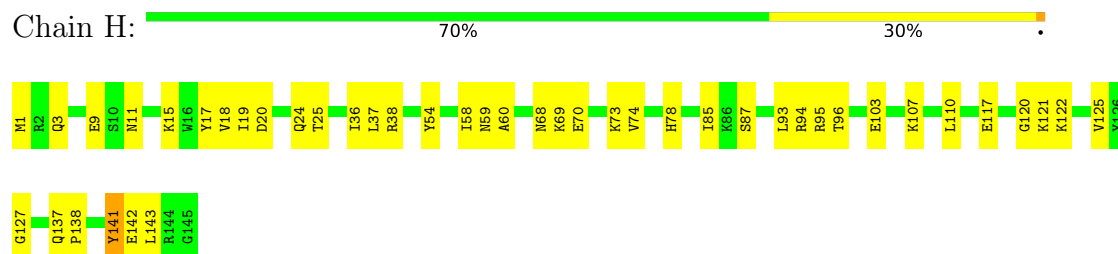
- Molecule 10: Large ribosomal subunit protein uL5



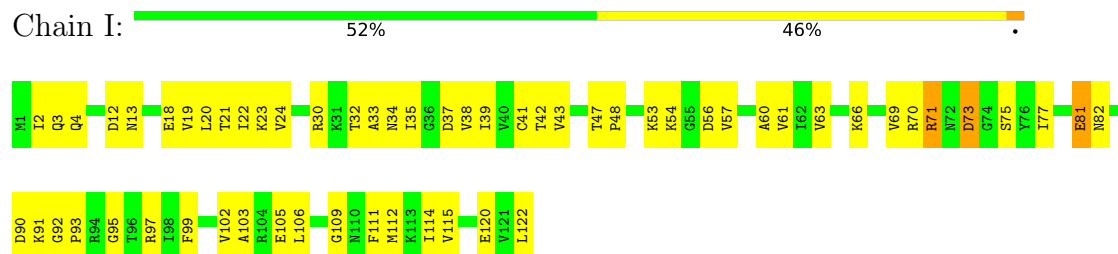
- Molecule 11: Large ribosomal subunit protein uL6



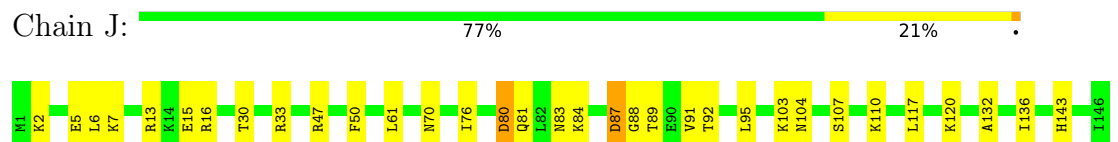
- Molecule 12: Large ribosomal subunit protein uL13



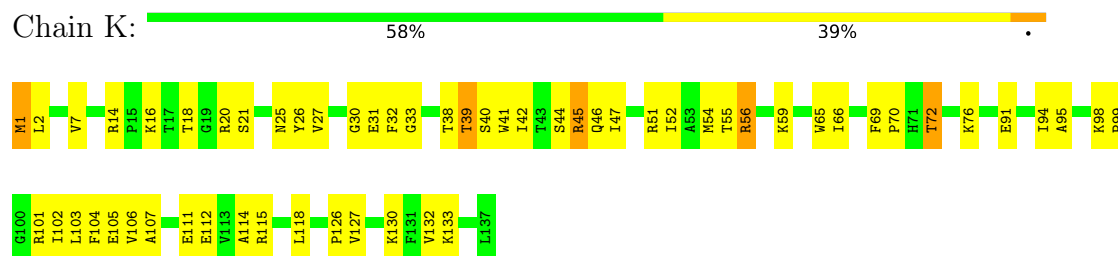
- Molecule 13: Large ribosomal subunit protein uL14



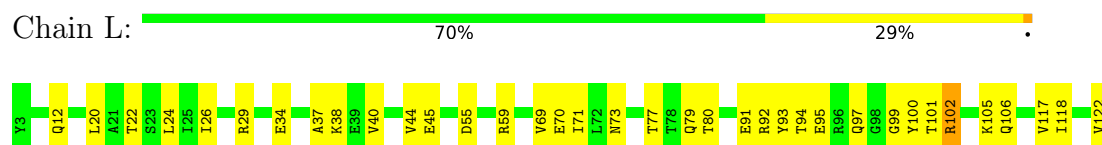
- Molecule 14: Large ribosomal subunit protein uL15



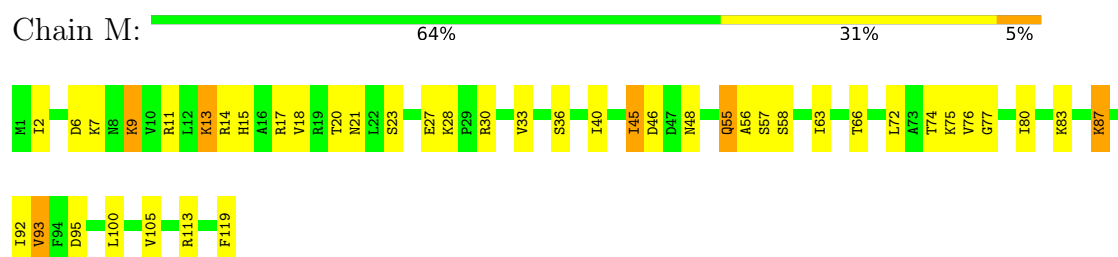
- Molecule 15: Large ribosomal subunit protein uL16



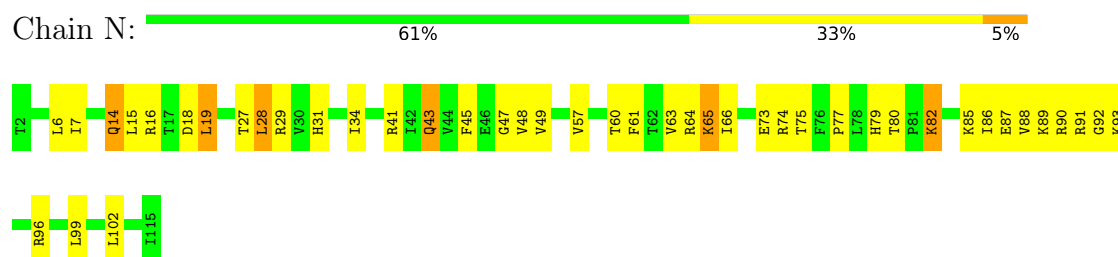
- Molecule 16: Large ribosomal subunit protein bL17



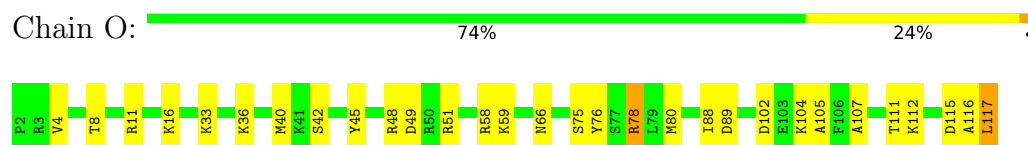
- Molecule 17: Large ribosomal subunit protein uL18



- Molecule 18: Large ribosomal subunit protein bL19

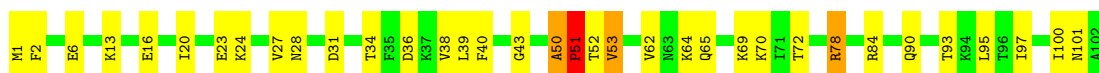


- Molecule 19: Large ribosomal subunit protein bL20



- Molecule 20: Large ribosomal subunit protein bL21

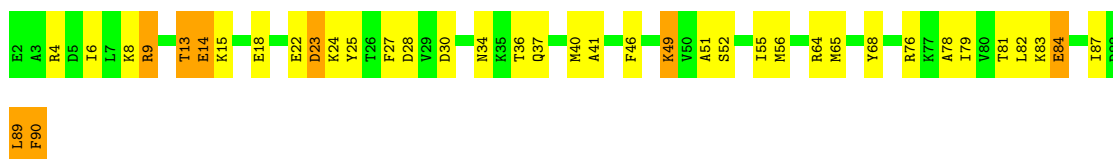




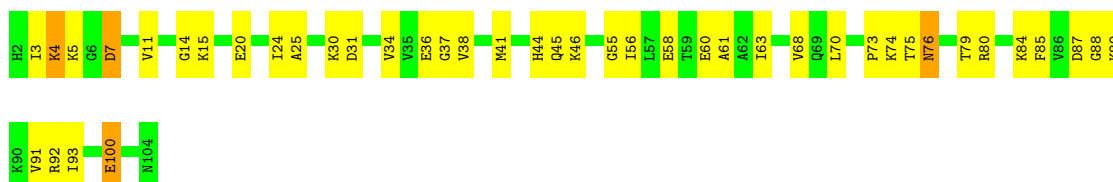
- Molecule 21: Large ribosomal subunit protein uL22



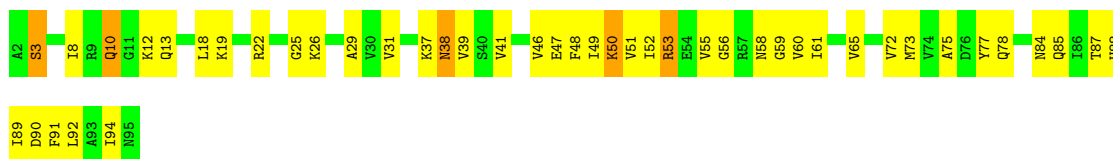
- Molecule 22: Large ribosomal subunit protein uL23



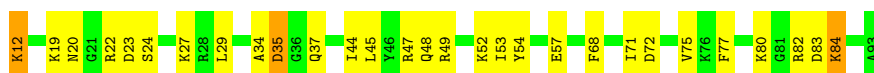
- Molecule 23: Large ribosomal subunit protein uL24



- Molecule 24: Large ribosomal subunit protein bL25

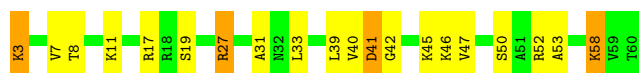


- Molecule 25: Large ribosomal subunit protein bL27

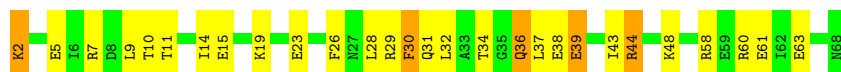


- Molecule 26: Large ribosomal subunit protein bL28

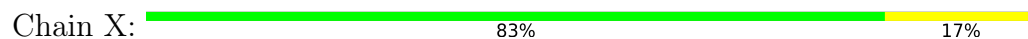




- Molecule 27: Large ribosomal subunit protein uL29



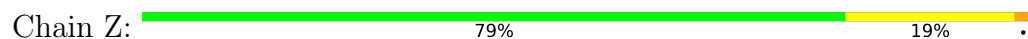
- Molecule 28: Large ribosomal subunit protein uL30



- Molecule 29: Large ribosomal subunit protein bL31B



- Molecule 30: Large ribosomal subunit protein bL32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68392	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: A1D6G, OMG, 2MA, 5MU, MA6, 2MG, MG

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	0.88	0/530
2	2	0.44	0/371	0.71	0/484
3	3	0.57	0/526	0.80	0/690
4	4	0.74	0/299	0.90	0/393
5	A	0.54	0/69095	0.83	3/107748 (0.0%)
6	B	0.51	0/2733	0.86	1/4257 (0.0%)
7	C	0.59	0/2125	0.86	0/2853
8	D	0.65	0/1651	0.82	0/2215
9	E	0.66	0/1595	0.82	2/2154 (0.1%)
10	F	0.48	0/1332	0.78	0/1798
11	G	0.59	0/1277	0.77	0/1731
12	H	0.43	0/1165	0.67	0/1570
13	I	0.57	0/925	0.76	0/1242
14	J	0.39	0/1100	0.63	0/1467
15	K	0.52	0/1095	0.68	0/1472
16	L	0.43	0/936	0.69	0/1253
17	M	0.58	0/900	0.79	0/1205
18	N	0.41	0/901	0.67	0/1209
19	O	0.39	0/954	0.65	0/1264
20	P	0.50	0/800	0.73	1/1070 (0.1%)
21	Q	0.49	0/861	0.73	0/1161
22	R	0.48	0/723	0.68	0/966
23	S	0.46	0/779	0.70	0/1043
24	T	0.41	0/719	0.65	0/969
25	U	0.50	0/621	0.71	0/825
26	V	0.69	0/451	0.84	0/603
27	W	0.33	0/542	0.67	0/722
28	X	0.32	0/451	0.55	0/606
29	Y	0.36	0/378	0.63	0/521
30	Z	0.58	0/367	0.81	0/490
All	All	0.54	0/96067	0.81	7/144511 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
7	C	0	2
9	E	0	2
20	P	0	2
All	All	0	7

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
9	E	46	GLN	CB-CA-C	-7.80	94.81	110.40
20	P	51	PRO	N-CA-C	-6.95	94.04	112.10
9	E	46	GLN	N-CA-CB	6.32	121.97	110.60
5	A	278	A	OP1-P-O3'	5.97	118.34	105.20
5	A	440	C	OP2-P-O3'	5.15	116.53	105.20

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	29	ARG	Sidechain
7	C	272	ARG	Sidechain
7	C	274	ARG	Sidechain
9	E	41	ARG	Sidechain
9	E	45	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	390	0	395	32	0
2	2	367	0	415	7	0
3	3	521	0	586	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4	296	0	340	16	0
5	A	61838	0	31093	513	0
6	B	2445	0	1240	40	0
7	C	2090	0	2201	106	0
8	D	1627	0	1667	79	0
9	E	1572	0	1619	49	0
10	F	1317	0	1323	195	0
11	G	1259	0	1221	94	0
12	H	1143	0	1134	51	0
13	I	918	0	981	68	0
14	J	1086	0	1125	30	0
15	K	1071	0	1123	73	0
16	L	932	0	983	34	0
17	M	891	0	925	38	0
18	N	889	0	937	52	0
19	O	942	0	1014	44	0
20	P	790	0	830	34	0
21	Q	853	0	905	29	0
22	R	715	0	748	64	0
23	S	770	0	809	47	0
24	T	711	0	740	52	0
25	U	615	0	622	26	0
26	V	445	0	466	23	0
27	W	541	0	563	38	0
28	X	449	0	491	9	0
29	Y	370	0	243	36	0
30	Z	361	0	361	9	0
31	A	69	0	0	1	0
32	A	12	0	0	0	0
33	A	6	0	0	1	0
All	All	88301	0	57100	1695	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 1695 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:59:LYS:HD3	11:G:62:ARG:NH2	1.59	1.15
19:O:89:ASP:OD1	19:O:89:ASP:O	1.65	1.14
21:Q:66:THR:HG22	21:Q:66:THR:O	1.39	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:6:ILE:HD11	28:X:47:ILE:HD11	1.28	1.14
11:G:54:ARG:NH1	11:G:62:ARG:HG2	1.64	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	30 (86%)	5 (14%)	0	100	100
7	C	272/274 (99%)	241 (89%)	29 (11%)	2 (1%)	19	33
8	D	213/215 (99%)	196 (92%)	17 (8%)	0	100	100
9	E	204/206 (99%)	187 (92%)	17 (8%)	0	100	100
10	F	173/175 (99%)	140 (81%)	31 (18%)	2 (1%)	11	19
11	G	173/175 (99%)	155 (90%)	18 (10%)	0	100	100
12	H	143/145 (99%)	129 (90%)	14 (10%)	0	100	100
13	I	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
14	J	144/146 (99%)	136 (94%)	8 (6%)	0	100	100
15	K	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
16	L	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
17	M	117/119 (98%)	106 (91%)	11 (9%)	0	100	100
18	N	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
19	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
20	P	100/102 (98%)	94 (94%)	4 (4%)	2 (2%)	6	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Q	110/117 (94%)	104 (94%)	6 (6%)	0	100	100
22	R	87/89 (98%)	82 (94%)	5 (6%)	0	100	100
23	S	101/103 (98%)	91 (90%)	10 (10%)	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	57/59 (97%)	52 (91%)	4 (7%)	1 (2%)	7	12
30	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
All	All	3071/3132 (98%)	2819 (92%)	245 (8%)	7 (0%)	45	62

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	Y	2	LYS
7	C	126	VAL
20	P	51	PRO
10	F	76	THR
20	P	50	ALA

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%)	41 (93%)	3 (7%)	13	25
2	2	39/39 (100%)	38 (97%)	1 (3%)	41	66
3	3	55/55 (100%)	50 (91%)	5 (9%)	7	14
4	4	35/35 (100%)	29 (83%)	6 (17%)	1	3
7	C	220/221 (100%)	204 (93%)	16 (7%)	11	22
8	D	173/173 (100%)	160 (92%)	13 (8%)	11	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	E	168/168 (100%)	153 (91%)	15 (9%)	8	15
10	F	139/154 (90%)	121 (87%)	18 (13%)	3	6
11	G	123/153 (80%)	107 (87%)	16 (13%)	3	6
12	H	122/123 (99%)	117 (96%)	5 (4%)	26	47
13	I	100/100 (100%)	92 (92%)	8 (8%)	10	19
14	J	109/112 (97%)	104 (95%)	5 (5%)	23	42
15	K	108/114 (95%)	95 (88%)	13 (12%)	4	7
16	L	96/101 (95%)	92 (96%)	4 (4%)	25	46
17	M	86/95 (90%)	71 (83%)	15 (17%)	1	2
18	N	93/100 (93%)	84 (90%)	9 (10%)	6	12
19	O	96/96 (100%)	92 (96%)	4 (4%)	25	46
20	P	84/86 (98%)	82 (98%)	2 (2%)	44	68
21	Q	89/94 (95%)	82 (92%)	7 (8%)	10	19
22	R	78/80 (98%)	70 (90%)	8 (10%)	6	11
23	S	81/88 (92%)	77 (95%)	4 (5%)	21	40
24	T	75/82 (92%)	67 (89%)	8 (11%)	5	10
25	U	60/64 (94%)	53 (88%)	7 (12%)	4	8
26	V	44/49 (90%)	37 (84%)	7 (16%)	2	3
27	W	58/60 (97%)	53 (91%)	5 (9%)	8	16
28	X	52/52 (100%)	50 (96%)	2 (4%)	28	51
29	Y	23/56 (41%)	20 (87%)	3 (13%)	3	6
30	Z	36/44 (82%)	35 (97%)	1 (3%)	38	63
All	All	2486/2639 (94%)	2276 (92%)	210 (8%)	11	17

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	K	18	THR
18	N	14	GLN
27	W	2	LYS
15	K	56	ARG
17	M	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
18	N	43	GLN
23	S	76	ASN
24	T	88	HIS
22	R	37	GLN
12	H	137	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	2875/2921 (98%)	939 (32%)	87 (3%)
6	B	114/115 (99%)	38 (33%)	4 (3%)
All	All	2989/3036 (98%)	977 (32%)	91 (3%)

5 of 977 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	13	A
5	A	18	C
5	A	28	A
5	A	34	U
5	A	36	G

5 of 91 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	1593	G
5	A	2225	A
5	A	1628	A
5	A	1789	A
5	A	2353	U

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	5MU	A	792	5	19,22,23	1.48	5 (26%)	28,32,35	2.24	8 (28%)
5	OMG	A	2278	5	18,26,27	1.06	1 (5%)	19,38,41	1.21	3 (15%)
5	MA6	A	2085	5	18,26,27	1.03	2 (11%)	19,38,41	2.04	5 (26%)
5	2MA	A	2530	32,5	17,25,26	1.07	0	17,37,40	1.29	3 (17%)
5	5MU	A	1966	5	19,22,23	1.66	5 (26%)	28,32,35	2.32	8 (28%)
5	2MG	A	2472	5	18,26,27	1.19	1 (5%)	16,38,41	1.17	2 (12%)

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	5MU	A	792	5	-	0/7/25/26	0/2/2/2
5	OMG	A	2278	5	-	1/5/27/28	0/3/3/3
5	MA6	A	2085	5	-	3/7/29/30	0/3/3/3
5	2MA	A	2530	32,5	-	0/3/25/26	0/3/3/3
5	5MU	A	1966	5	-	0/7/25/26	0/2/2/2
5	2MG	A	2472	5	-	0/5/27/28	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	-3.63	1.32	1.37
5	A	1966	5MU	C4-N3	-3.30	1.32	1.38
5	A	792	5MU	C4-N3	-3.28	1.32	1.38
5	A	1966	5MU	C6-C5	3.11	1.39	1.34
5	A	2278	OMG	C6-N1	-3.07	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	5.86	122.67	114.89
5	A	2085	MA6	C9-N6-C6	-5.78	102.00	119.51
5	A	1966	5MU	C5-C4-N3	5.40	119.92	115.31
5	A	792	5MU	N3-C2-N1	5.31	121.94	114.89
5	A	1966	5MU	C4-N3-C2	-5.12	120.73	127.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2085	MA6	C5-C6-N6-C9
5	A	2085	MA6	C5-C6-N6-C10
5	A	2278	OMG	C1'-C2'-O2'-CM2
5	A	2085	MA6	N1-C6-N6-C9

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	792	5MU	1	0
5	A	2278	OMG	1	0
5	A	2085	MA6	3	0

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
31	A1D6G	A	3000	32	70,73,73	2.33	22 (31%)	96,107,107	1.60	20 (20%)

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
31	A1D6G	A	3000	32	-	8/82/113/113	0/5/5/5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	3000	A1D6G	C65-N64	8.42	1.45	1.33
31	A	3000	A1D6G	C11-N13	7.17	1.50	1.34
31	A	3000	A1D6G	O10-C11	5.47	1.44	1.35
31	A	3000	A1D6G	O67-C65	4.56	1.43	1.36
31	A	3000	A1D6G	C22-C21	4.54	1.55	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	3000	A1D6G	O10-C11-N13	4.78	119.50	111.11
31	A	3000	A1D6G	C44-C43-C45	-3.79	107.44	113.40
31	A	3000	A1D6G	C02-C03-C68	-3.71	110.11	115.23
31	A	3000	A1D6G	O12-C11-N13	-3.58	119.48	124.96
31	A	3000	A1D6G	O42-C43-C45	3.40	114.34	109.14

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

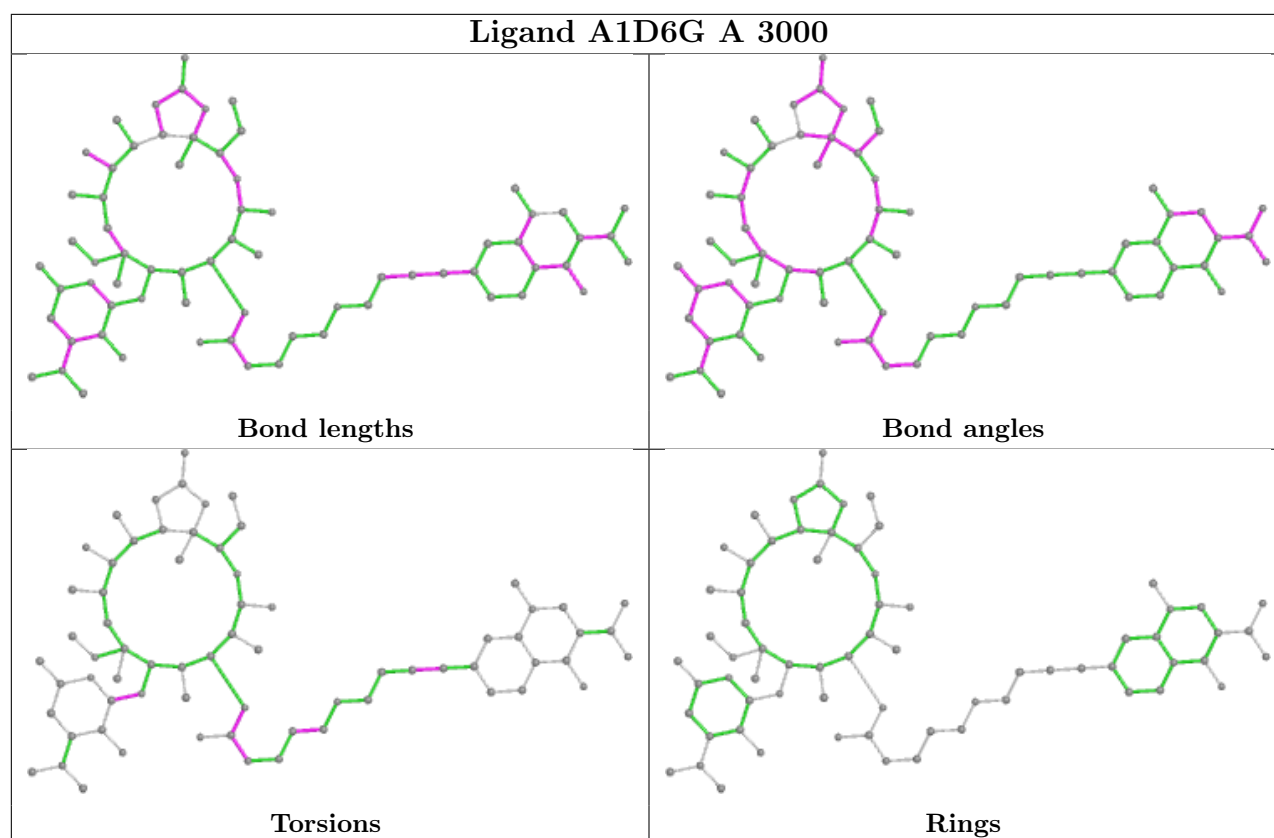
Mol	Chain	Res	Type	Atoms
31	A	3000	A1D6G	O10-C11-N13-C14
31	A	3000	A1D6G	O12-C11-N13-C14
31	A	3000	A1D6G	C19-C20-C21-C22
31	A	3000	A1D6G	N13-C11-O10-C09
31	A	3000	A1D6G	O42-C41-O40-C39

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	3000	A1D6G	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.