

wwPDB EM Validation Summary Report (i)

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)

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 (i) 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 (1)) 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.



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	А	2921	66%	33% •
2	В	115	60%	40%
3	С	274	93%	7%
4	D	215	90%	10%
5	Е	206	92%	8%
6	F	175	78%	22%
7	G	175	85%	15%
8	Н	145	94%	6%
9	Ι	122	88%	11% •

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Mol	Chain	Length	Quality of chain	
10	J	146	92%	8%
11	Κ	137	87%	13%
12	L	120	97%	•
13	М	119	86%	14%
14	Ν	114	83%	17%
15	О	116	92%	8%
16	Р	102	93%	6% •
17	Q	117	88%	8% •
18	R	89	88%	12%
19	S	103	90%	10%
20	Т	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	80%	11%
30	4	37	84%	16%
31	т 2	15/18	710/	25%
20	a h	929	/1%	20% •
- 32 - 22	U C	202	92%	5% •
<u>ა</u> კ	C	217	90%	• 7%
- 34	d	200	97%	•

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Mol	Chain	Length	Quality of chain	
35	е	166	91%	• 6%
36	f	98	89%	8% •
37	g	156	90%	10% •
38	h	132	96%	••
39	i	130	95%	• •
40	j	102	89%	6% 5%
41	k	129	84%	• 12%
42	1	149	85%	5%• 9%
43	m	121	91%	5% •
44	n	61	95%	•••
45	О	89	96%	•••
46	р	91	93%	• •
47	q	87	83%	9% 8%
48	r	80	75% 5%	20%
49	S	108	70% 6%	24%
50	t	83	94%	

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2 Entry composition (i)

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			AltConf	Trace			
1	А	2885	Total 61859	C 27619	N 11312	O 20043	Р 2885	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	115	Total 2445	C 1094	N 436	0 801	Р 114	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	274	Total 2090	C 1301	N 415	O 369	${ m S}{ m 5}$	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Е	206	Total 1572	C 986	N 288	O 296	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

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

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



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

Mol	Chain	Residues		Atoms					Trace
7	G	175	Total 1259	C 788	N 239	O 229	${ m S} { m 3}$	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
8	Н	145	Total	C 714	N 208	0	${ m S}_{ m 3}$	0	0
			1140	114	200	210	3		

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

Mol	Chain	Residues		At	oms			AltConf	Trace
9	Ι	122	Total 918	C 572	N 174	0 168	$\frac{S}{4}$	0	0

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

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

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

Mol	Chain	Residues		At	oms			AltConf	Trace
11	K	137	Total 1071	C 689	N 203	0 175	${S \atop 4}$	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	М	119	Total 891	$\begin{array}{c} \mathrm{C} \\ 557 \end{array}$	N 174	O 159	S 1	0	0

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



Mol	Chain	Residues		Ato	\mathbf{ms}		AltConf	Trace
14	Ν	114	Total 889	$\begin{array}{c} \mathrm{C} \\ 563 \end{array}$	N 175	O 151	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	0	116	Total 942	C 593	N 189	0 156	$\frac{S}{4}$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	Р	102	Total 790	C 503	N 142	0 144	S 1	0	0

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

Mol	Chain	Residues		Atoms					Trace
17	Q	112	Total 853	C 532	N 163	0 155	${ m S} { m 3}$	0	0

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

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

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

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
19	S	103	Total 770	C 486	N 142	0 141	S 1	0	0

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

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
20	Т	94	Total 711	C 456	N 127	O 128	0	0

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



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

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

Mol	Chain	Residues		Atom	ıs	AltConf	Trace	
22	V	58	Total 445	С 277	N 96	O 72	0	0

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

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

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

Mol	Chain	Residues		Atom	ıs	AltConf	Trace	
24	Х	58	Total 449	C 280	N 85	O 84	0	0

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

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
25	Y	57	Total 353	C 214	N 65	О 74	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
26	7	48	Total	С	Ν	Ο	S	0	0
20	2	40	361	222	77	59	3	0	0

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

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
27	1	47	Total 390	C 238	N 78	O 70	${S \atop 4}$	0	0

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



Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
28	2	43	Total 367	C 225	N 89	O 52	S 1	0	0

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

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
29	3	64	Total 521	C 324	N 113	O 82	${ m S} { m 2}$	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
30	4	37	Total 296	C 186	N 60	0 45	${f S}{5}$	0	0

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

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

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

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

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

Mol	Chain	Residues		At	AltConf	Trace			
33	с	202	Total 1596	C 1005	N 300	O 289	${S \over 2}$	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	199	Total 1616	C 1020	N 302	0 292	$\frac{S}{2}$	0	0

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



Mol	Chain	Residues		At	oms			AltConf	Trace
35	е	156	Total 1160	С 731	N 212	O 215	${ m S} { m 2}$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	f	95	Total 789	C 498	N 138	O 150	${ m S} { m 3}$	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	155	Total 1242	C 775	N 239	0 224	$\begin{array}{c} \mathrm{S} \\ \mathrm{4} \end{array}$	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	131	Total 1031	C 652	N 183	0 192	$\frac{S}{4}$	0	0

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

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

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

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

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
41	k	114	Total 844	C 520	N 160	0 161	${ m S} { m 3}$	0	0

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



Mol	Chain	Residues		At	oms			AltConf	Trace
42	1	135	Total 1058	$\begin{array}{c} \mathrm{C} \\ 658 \end{array}$	N 214	0 184	${ m S} { m 2}$	0	0

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

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

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

Mol	Chain	Residues		Ate	oms			AltConf	Trace
44	n	60	Total 501	C 317	N 100	O 79	${f S}{5}$	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
45	О	87	Total 726	C 448	N 149	0 128	S 1	0	0

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

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
46	р	87	Total 688	C 433	N 127	0 127	S 1	0	0

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

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
47	q	80	Total 657	C 416	N 117	0 123	S 1	0	0

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

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
48	r	64	Total 525	C 336	N 98	O 88	${ m S} { m 3}$	0	0

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



Mol	Chain	Residues		At	oms			AltConf	Trace
49	s	82	Total 665	$\begin{array}{c} \mathrm{C} \\ 427 \end{array}$	N 121	0 115	${ m S} { m 2}$	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
50	t	81	Total 611	C 370	N 120	0 119	${S \over 2}$	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[1 2.3.0]heptadecan-6-yl]oxycarbonylamino]propoxy]but-1-ynyl]-1-methyl-4-oxidanylidene-quin oline-3-carboxylic acid (three-letter code: A1D6G) (formula: $C_{50}H_{72}N_4O_{15}$).



Mol	Chain	Residues	A	Aton	ns		AltConf
51	А	1	Total	С	Ν	0	0
	**	±	69	50	4	15	

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

Mol	Chain	Residues	Atoms	AltConf
52	А	12	TotalMg1212	0



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.



 \bullet Molecule 1: 23S ribosomal RNA



U1287	G1290 A1291	G1294			G1309 A1310	A1311	A1312	A1337	U1338 111330	G1340	A1341	C1342 U1343	A1344	U1348	U1349	G1357		G1360	G1361 C1362		U1366	C1370	U1378		G1384	C1387	A1396	G1397	A1402	G1405		A1415 111416		A1421 A1422		A1432 U1433	U1434	A1440
A1443	A1450	U1451	01454	U1456	01457 A1458	A1459	01460 C1461	G1462	A1463	G1465		A14/1 C1472		G1476 U1477	A1478	G1479 G1480	A1481	U1482	A1483 G1484	10	G1487 A1488	A1489	61490	U1493	G1494	A1497	01498 01499	G1500	01504	G1505 C1506	A1507	C1508 G1509	U1510	C1511 U1512	A1513	A1517	G1522	G1523
C1524 U1525	G1526 A1527	G1528	01 <mark>532</mark> ^	4 U I	5 5	A1537	A1538 A1539	U1540	C1541	75010	G1550	U1551 U1552	A1553	A1554 G1555	G1556	C1557 11558	G1559	A1560	61561 C1562		01568 G1569	G1570		A1575	A1576 G1577	A1578	C1579 A1580	U1581 11582	G1583	U1584 G1585	U1586	C1587 111588	U1589	C1590 G1591	A1592	G1593 U1594	C1595 G1596	U1597
U1598 G1599	U1602	A1605	C1606	G1613	A1616		01623 C1624	U1625	A1626	41628 A1628	U1629	A1630 G1631	A1632	A1633 A1634	A1635	01636 41637	G1638	G1639	01640 G1641	2	C1651 A1652	A1653	A1054 C1655	C1656	G1657 A1658	C1659	A1660 C1661	A1662	A1666	A1678	A1679	G1687		A1690 G1691	C1692	U1707	G1717	G1718
C1719	U1737	G1740	U1757 A1759	G1759	G1760 G1761	U1762	01763 A1764	A1765	C1766	C1769	C1770		A1789	G1790 G1791	-	A1796 G1797		A1800	G1803	U1804	U1805 U1806	A1807	01808 C1809	A1810	A1811 A1812	A1813	G1826	C1827	A1829	111 835		U1843 G1844		A1856	C1870	U1871	A1874 A1875	G1876
A1883	A1886	A1893	G1894	U1897	C1898 U1899		A1903 A1904	G1905	A 1 0 0 8	C1909		A1912	C1919	A1923		G1933 G1934		U1938	A 1939	ט :	D Ø	U1944	A1946 A1946	C1947	G1948 G1949	U1950	C1951	A1954	G1956	G1957 111958		A1964 A1965	U1966	U1967	01982	C1992	A1993 C1994	G1995
A1 996 A1 997	A1 998 G1 999	U2003		U2009	U2018	G2019	U2020	C2023	A2024	G2029		G2048 U2049	A2050	A2057	A2058	G2059 A2060	U2061	G2062	C2070	12000	G2075 A2076	C2077	AZUTO	C2082	G2083	A2087	G2088 A2089	C2090	G2094	U2095 G2096		G2107 112108	A2109	G2114		A2117 U2118	U2119 G2120	
G2127 G2128	C2129 A2130	C2131 A2132	G2133	U2135	02136 G2137	U2138	A2139 C2140		G2143 A2144	N2145 U2145	A2146	G2147 G2148	U2149	A2153	G2154	C2155 C2156	U2157	U2158	02169 G2160	A2161	A2162 A2163	C2164	G2169	C2170	G2171 C2172	U2173	A2174 G2175	C2176		A2185 G2186	G2187	C2188 G2189	C2190	G2193	U2194	G2195 G2196	G2197 A2198	U2199
A2200	C2204 C2205	C2206 U2207	A2208	C2210	U2211 G2212	U2213	G2214 U2215	U2216	G2217	U2221		02224 A2225	A2226	G2230	C2231	A2232	A2235		02238 A2239	U2240	C2241	G2245	A2252	-	G2265 G2266		G2278	C2287	A2296	C 2306		C2310 112311	C2312	A2313 A2314	A2315	G2326	A2327 A2328	U2329
G2330 G2331	U2332 U2333	G2334 G2335	A2336 A2337	A2338	02339	U2342	A2345	U2346	A2347	42349 A2349	G2350	02351 G2352	U2353	A2354	G2 <mark>358</mark>	C2359 A2360	U2361	A2362	A2363 G2364		U2370 U2371	G2372	A23/3 C2374		C2377	A2388	A2396	G2397	G2399	A7404		C2408 C2409	G2410	A2411 C2412		G2416 U2417	G2418	C2430
C2433	A2434	G2437	G2441	U2450	C2451 A2452	A2453	C2454 G2455	G2456	A2457	A2461	A2462	6.2463	C2468	G2472	G2473	G2474 A2475		C2493	C2494 A2495	A2496	G2497	A2505	0.2506 C2507	G2508	G2521		C2525	C2528	A2530	U2531 G2532	U2533	C2534	G2543	C2544 A2545	U2546	C2547	G2552 G2553	C2554
<mark>U2555</mark> G2556	<mark>U2557</mark> A2558	G2559	G2562	A2568	A2569 G2570		U2574	U2579	G2580	U2589		A2592 A2593	G2594	A2599	<mark>C2600</mark>	G2601	G2605		6.097.5	U2612	C2613	G2626	A262/ C2628	A2629	U2636		U2640 A2641	U2642	G2648	U2649 G2650		A 2656	A2661	A2668		G2672	A2681 G2682	U2683
A2684 C2685	G2686 A2687	A2692	C2693	G2695	G2696	G2700	U2709		G2712	U2716		02728 G2729		A2733	G2 <mark>741</mark>	G2745		U2753	62754 U2755	G2756	A2760	C2761	G2769	U2770	G2771	A2776	A2777	02781	U2783	A2784	C2787	A2788	A2792	G2793 C2794		A2803 G2804	A2805 U2806	G2807
A2817	A2818 C2819	U2820 U2821		U2825	U2826 A2827	U2828	A2829 A2830	G2831	A2832	C2838	A2839	A 2840	U2844	G2845 A2846		G2851 112852	U2853	A2854	QC 878	G2887	A2888	G2892	A2899	C2900	U2904	C2905	62906	A2912	A2914	C2915 112916		A2919 112920	U	A A				

 \bullet Molecule 2: 5S ribosomal RNA

Chain B:

60%



Mail Mail U10 U10 U11 U11 U12 U13 U13 U14 U14 U15 U13 U13 U14 U14 U13 U14 U14 U15 U15 U14 U14 U15 U14 U14 U14 U15 U14 U16 U14 U16 U14 U16



• Molecule 3: Large ribosomal subunit protein uL2



• Molecule 8: Large ribosomal subunit protein uL13

Chain H: 94% 6%





• Molecule 9: Large ribosomal subunit protein uL14

Chain I:	88%	11% •
M1 I2 03 814 814 N34 N34 N34 T65	860 860 868 870 871 871 871 871 881 881 198 8120 8120 1122	
• Molecule 10:	: Large ribosomal subunit protein uL15	
Chain J:	92%	8%
M1 K7 R13 B80 D80	192 192 192 196 196 196 196 196 196 196 196 196	
• Molecule 11:	: Large ribosomal subunit protein uL16	
Chain K:	87%	13%
M1 L2 L3 L3 K14 P15 F17 T17	118 435 844 844 844 845 844 855 844 855 845 84	
• Molecule 12:	: Large ribosomal subunit protein bL17	
Chain L:	97%	·
Y3 R29 R59 Q79 R102		
• Molecule 13:	: Large ribosomal subunit protein uL18	
Chain M:	86%	14%
M1 K9 V10 K11 L12 K13 K13 K13 C12 C12	2.23 E27 336 336 456 456 857 857 857 857 857 857 857 857 857 857	
• Molecule 14:	: Large ribosomal subunit protein bL19	
Chain N:	83%	17%
12 K5 L6 L6 L6 T1 T11 K12 K12 K12	414 117 117 128 128 135 135 135 135 135 135 135 135 135 135	
• Molecule 15:	: Large ribosomal subunit protein bL20	
Chain O:	92%	8%



P2 T8 V9 R51 R51 R78 R78 B96 S96 S96 S96 S96

• Molecule 16: Large ribosomal subunit protein bL21





• Molecule 23: Large ribosomal subunit protein uL29

Chain W:	79%	21%
K2 111 110 111 111 111 111 111 111 111 11	R44 162 865 865	
• Molecule 24: Large rib	osomal subunit protein uL30	
Chain X:	91%	9%
A2 16 17 110 869 K869		
• Molecule 25: Large rib	osomal subunit protein bL31B	
Chain Y:	93%	• •
129 121 121 121 121 121 121 121 121 121		
• Molecule 26: Large rib	osomal subunit protein bL32	
Chain Z:	98%	•
A2 839 149		
• Molecule 27: Large rib	osomal subunit protein bL33B	
Chain 1:	79%	21%
R2 C12 18 N22 K23 K23 K23 K32 K31 K32 K41 K41 K41		
• Molecule 28: Large rib	osomal subunit protein bL34	
Chain 2:	98%	
8844 844		
• Molecule 29: Large rib	osomal subunit protein bL35	
Chain 3:	89%	11%





• Molecule 30: Large ribosomal subunit protein bL36

Chain 4:	84%	16%
MA R4 C11 C11 C12 K15 K22 K22 C37		
• Molecule 31: 16S ribosomal	RNA	
Chain a:	71% 25%	·
A5 68 69 64 64 64 64 64 64 64 64 64 65 64 65 662 662	0 0 0 0 0 0 0 0 0 0 0 0 0 0	C C C C C C C C C C C C C C C C C C C
A120 A130 C136 C136 C136 G142 G142 G142 G142 G156 G155 G155 G156 G156 G156 G156 G156	A174 A174 V185 V188 V188 C188 A190 C188 C188 C188 C188 C188 C188 C188 C18	6216 0217 0 0 0 0 0 223 0 225 0 222
0230 0233 0234 0234 0248 0265 0265 0265 0266 0266 0266 0268 0268 0268 0274 0274	A278 C279 C279 A301 A301 A328 A328 A337 C338 A337 C338 C338 C338 C338 C338 C338 C338 C	C380 A390 G396 A401 A401 C406
6412 6413 6414 6414 6414 6414 6421 6421 6421 6423 6423 6423 6423 6423 6423 6423 6423	U447 4456 4456 4456 4459 4459 4467 6468 6468 6468 0485 0485 0485 0485 0485 0485 0485 048	A499 4500 U502 4503 4503 6504 6504 6504 6514 6514 4517
4518 C519 C519 C526 C526 C526 C526 C528 C538 C538 C538 C538 C538 C538 C538 C53	4554 4555 4567 4567 16772 16578 4531 4531 4531 6586 0586 0586 0586 0587 0586 0596 0596 0596 0596 0596 0596 0596 059	U634 C640 C642 C642 A650 A650 U660 U660
6664 A673 6691 691 0694 A703 A703 A703 670 6731 6733 6731 6732 6731 6732 6731	A757 A756 A785 A788 A788 A789 A789 C793 C793 C793 C793 C793 C793 C793 C79	6826 1882 1882 1882 1882 1882 1882 1882
C C 6854 6854 6864 7869 7869 7880 7880 7881 7881 7881 7881 7883 7881 7883 7894 6911 6934 6935 6935 6937 6937 6937 6937 6937	C340 C341 C341 C341 C343 C343 C343 C343 C343	1991 1992 293 293 293 299 0198 01998 01000 01000 11001 11002 11005 11005
C1007 C1008 C1008 A A A A C C C C C C C C C C C C C C C C	с с с с с с с с с с с с с с с с с с с	U1076 C1092 C1097 C1110 C1111 A1113 A1113
G1119 C1120 C1120 C1122 C1123 C1124 C1128 G1128 G1128 G1138 G1138 G1138 C1139 C1139 C1139 C1139 C1139 C1139 C1139 C1139 C1139 C1139 C1138 C1138 C1138 C1138 C1138 C1138 C1138 C1138 C1138 C1138 C1138 C1138 C1138 C1128 C1138	U A A G G G G G G G G G G G G G G G G G	G1187 G1187 G1189 A1189 G1194 G1203 G1203 A1205 A1205 A1205
C1218 11222 11222 11222 11225 01226 11236 11236 11236 11238 11238 11238 11247 11246 11247 11250 01247 11250 01247 11250	A1256 A1256 C1265 C1266 A1267 A1267 C1269 C1269 C1269 A1271 A1290 C1283 A1292 U1292 U1292 U1296 A1298	61303 01307 01307 01308 01310 01311 01312 01313 01314 01314
61326 A1329 (1331 (1331 (1331 (1333 (1333 (1333 (1333 (1338 (1338 (1338 (1338 (1338 (1338 (1338 (1338) (1388 (1385) (1388) (1388) (1388) (1388) (1388) (1388)	U1374 U1374 G1380 A1385 A1385 C1388 U1389 U1389 U1389 U1391 U1401 U1401 U1401 U1401 C1393 C1393 C1393 C1393 C1393 C1393 C1393 C1409 C1409 C1409 C1409 C1409 C1409 C1409	G1415 1420 61429 61429 61429 6145 61451 61452 61452





MET T2 D54 L60 G68 R121 M132

 \bullet Molecule 39: Small ribosomal subunit protein uS9

Chain i: 95% · ·



• Molecule 40: Small ribosomal subunit protein uS10

Chain j:							89%	6%	5%
MET ALA LYS GLN LYS LYS I6	L10	E23	K30 R31	L92	D97	L102			

• Molecule 41: Small ribosomal subunit protein uS11

Chain k:	84%	·	12%
MET ALA ALA ALA CLVS CLN VAL LVS ARG ARG ARG LVS LVS LVS LVS	N18 E37 E68 E68 R126 N126 VAL		

 \bullet Molecule 42: Small ribosomal subunit protein uS12

Chain l:	85%	5% • 9%
NET GLY LAU LYS SER SER SER ARG ARG ARG ARG HTTR HTS HTTR HTS	K64 867 867 867 869 1139 1132 1133 1133 1133 1133 1133 113	

 \bullet Molecule 43: Small ribosomal subunit protein uS13

 Chain m:
 91%
 5%

 Image: Second sec

96%

Chain o:



. .



• Molecule 46: Small ribosomal subunit protein bS16

Chain p:	93%			•••
MET A2 R32 K51 K88	LYS			
• Molecule	e 47: Small ribosomal subunit protein uS17			
Chain q:	83%		9%	8%
MET SER GLU ARG D6 D20	K31 K31 K34 K34 K34 K34 K34 K34 K34 K34 K34 K34			
• Molecule	e 48: Small ribosomal subunit protein bS18			
Chain r:	75%	5%	20%	_
MET ALA GLY GLY PRO ARG ARG GLY GLY	ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG			
• Molecule	e 49: Small ribosomal subunit protein uS19			
Chain s:	70% 6%	0	24%	_
MET CYS GLY LEU LEU HLS ALA	ASN LYS LYS CLY CLY CLY CLN MIG MIG MIG MIG MIG MIG MIG MIG MIG MIG			
• Molecule	e 50: Small ribosomal subunit protein bS20			
Chain t:	94%			•••
MET A2 840 870 172				



4 Experimental information (i)

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 $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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 Chai		Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.53	0/69148	0.80	1/107836~(0.0%)	
2	В	0.36	0/2733	0.72	0/4257	
3	С	0.65	0/2125	0.87	0/2853	
4	D	0.71	0/1651	0.83	0/2215	
5	Е	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	Н	0.51	0/1165	0.71	0/1570	
9	Ι	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	М	0.59	0/900	0.77	0/1205	
14	Ν	0.59	0/901	0.76	0/1209	
15	0	0.44	0/954	0.64	0/1264	
16	Р	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	Т	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	Х	0.51	0/451	0.63	0/606	
25	Y	0.37	0/361	0.67	0/500	
26	Ζ	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	$\overline{0/299}$	0.91	0/393	
31	a	0.25	0/35498	0.84	0/55345	
32	b	0.26	0/1829	0.53	0/2455	



Mal	Chain	Bond lengths		Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
33	с	0.24	0/1618	0.50	0/2173	
34	d	0.25	0/1646	0.50	0/2211	
35	е	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	1	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	0	0.24	0/735	0.53	0/982	
46	р	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	$Observed(^{o})$	$Ideal(^{o})$
1	А	1555	G	C3'-C2'-C1'	-5.30	97.26	101.50
16	Р	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 (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	Perce	ntiles
3	С	272/274~(99%)	245~(90%)	26 (10%)	1 (0%)	30	63
4	D	213/215~(99%)	200 (94%)	13~(6%)	0	100	100
5	Ε	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	Н	143/145~(99%)	131 (92%)	12 (8%)	0	100	100
9	Ι	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	М	117/119~(98%)	107 (92%)	10 (8%)	0	100	100
14	Ν	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
15	Ο	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
16	Р	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	Т	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	Х	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	Perce	ntiles
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	с	200/217~(92%)	190 (95%)	10 (5%)	0	100	100
34	d	197/200~(98%)	187 (95%)	10 (5%)	0	100	100
35	е	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	1	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	0	85/89~(96%)	82 (96%)	3 (4%)	0	100	100
46	р	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

Continued from previous page...

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Р	51	PRO
9	Ι	98	ILE
6	F	139	PRO
16	Р	50	ALA
42	1	132	THR



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
3	\mathbf{C}	220/221~(100%)	202~(92%)	18 (8%)	9	34
4	D	173/173~(100%)	151 (87%)	22 (13%)	3	19
5	Ε	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	Н	122/123~(99%)	114 (93%)	8 (7%)	14	42
9	Ι	100/100~(100%)	85 (85%)	15 (15%)	2	15
10	J	109/112~(97%)	97~(89%)	12 (11%)	5	25
11	Κ	108/114 (95%)	90 (83%)	18 (17%)	2	11
12	L	96/101~(95%)	92 (96%)	4 (4%)	25	54
13	М	86/95~(90%)	69 (80%)	17 (20%)	1	7
14	Ν	93/100~(93%)	74 (80%)	19 (20%)	1	6
15	О	96/96~(100%)	87 (91%)	9 (9%)	7	30
16	Р	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	Т	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	Х	52/52~(100%)	47 (90%)	5 (10%)	7	29
25	Y	21/56~(38%)	19 (90%)	2 (10%)	7	30
26	Ζ	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	Perce	entiles
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	с	164/175~(94%)	158 (96%)	6 (4%)	29	58
34	d	174/175~(99%)	169 (97%)	5 (3%)	37	63
35	е	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	1	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	О	79/81~(98%)	77 (98%)	2 (2%)	42	66
46	р	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

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



Mol	Chain	Res	Type
14	Ν	43	GLN
49	s	22	GLN
20	Т	88	HIS
41	k	119	ASN
33	с	88	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	А	2878/2921~(98%)	941 (32%)	78~(2%)
2	В	114/115~(99%)	45 (39%)	4(3%)
31	а	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	\mathbf{Res}	Type
1	А	5	А
1	А	13	А
1	А	18	С
1	А	19	G
1	А	23	G

5 of 82 RNA pucker outliers are listed below:

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

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

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.



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
	туре	Chain	Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
1	2MA	А	2530	52,1	17,25,26	1.07	0	17,37,40	1.29	3 (17%)
1	2MG	А	2472	1	18,26,27	1.19	1 (5%)	16,38,41	1.17	2 (12%)
1	5MU	А	792	1	19,22,23	1.48	5 (26%)	28,32,35	2.24	8 (28%)
1	OMG	А	2278	1	18,26,27	1.08	1 (5%)	19,38,41	1.22	3 (15%)
1	5MU	А	1966	1	19,22,23	1.66	5 (26%)	28,32,35	2.33	8 (28%)

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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	А	2530	52,1	-	0/3/25/26	0/3/3/3
1	2MG	А	2472	1	-	0/5/27/28	0/3/3/3
1	$5 \mathrm{MU}$	А	792	1	-	0/7/25/26	0/2/2/2
1	OMG	А	2278	1	-	1/5/27/28	0/3/3/3
1	5MU	А	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	А	2472	2MG	C6-N1	-3.61	1.32	1.37
1	А	792	5MU	C4-N3	-3.27	1.32	1.38
1	А	1966	5MU	C4-N3	-3.22	1.32	1.38
1	А	2278	OMG	C6-N1	-3.16	1.33	1.37
1	А	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		$Observed(^{o})$	$Ideal(^{o})$
1	А	1966	5MU	N3-C2-N1	5.91	122.73	114.89
1	А	1966	5MU	C5-C4-N3	5.42	119.94	115.31
1	А	792	5MU	N3-C2-N1	5.30	121.93	114.89
1	А	1966	5MU	C4-N3-C2	-5.20	120.62	127.35
1	А	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	\mathbf{Res}	Type	Atoms
1	А	2278	OMG	C1'-C2'-O2'-CM2

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	Turno	Chain	Dog	Tiple	B	ond leng	ths	Bond angles		
	Ullaili	nes	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
51	A1D6G	А	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	А	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	А	3000	A1D6G	C65-N64	8.53	1.45	1.33
51	А	3000	A1D6G	C11-N13	7.12	1.49	1.34
51	А	3000	A1D6G	O10-C11	4.94	1.43	1.35
51	А	3000	A1D6G	C22-C21	4.64	1.55	1.44
51	А	3000	A1D6G	O67-C65	4.63	1.43	1.36



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

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

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

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





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.

