



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 02:13 AM EDT

PDB ID : 1JZZ
Title : Structural Basis for the Interaction of Antibiotics with the Peptidyl Transferase Center in Eubacteria
Authors : Schlutzen, F.; Zarivach, R.; Harms, J.; Bashan, A.; Tocilj, A.; Albrecht, R.; Yonath, A.; Franceschi, F.
Deposited on : 2001-09-17
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

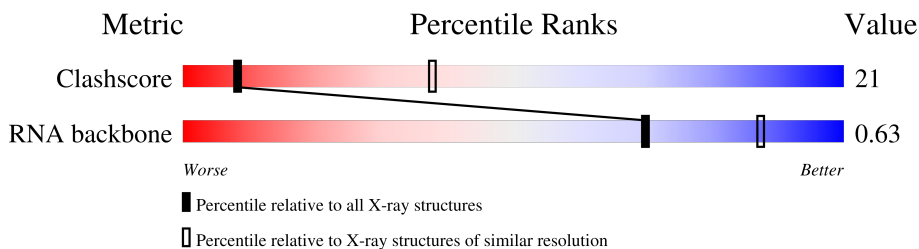
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

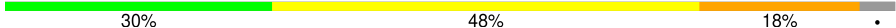
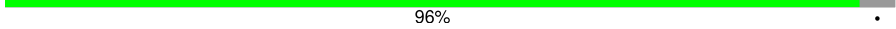
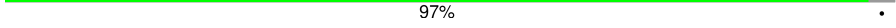
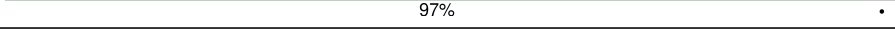
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	 30% 48% 18% .
2	K	205	 96% .
3	L	134	 97% .
4	M	60	 97% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ROX	A	2881	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59977 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2774	Total	C	N	O	P	0	0	0
			59532	26556	10982	19221	2773			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1526	U	Y	SEE REMARK 999	GB 15805042

- Molecule 2 is a protein called Ribosomal Protein L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	K	197	Total	C	0	0	197
			197	197			

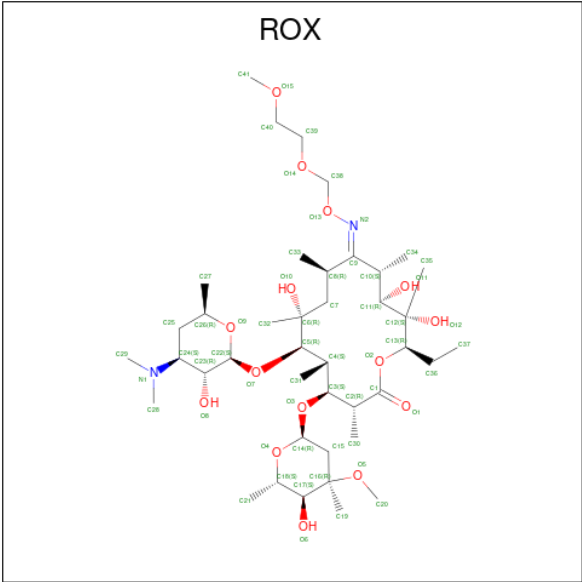
- Molecule 3 is a protein called Ribosomal Protein L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	L	130	Total	C	0	0	130
			130	130			

- Molecule 4 is a protein called Ribosomal Protein L32.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	M	58	Total	C	0	0	58
			58	58			

- Molecule 5 is ROXITHROMYCIN (three-letter code: ROX) (formula: C₄₁H₇₆N₂O₁₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			58	41	2	15		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

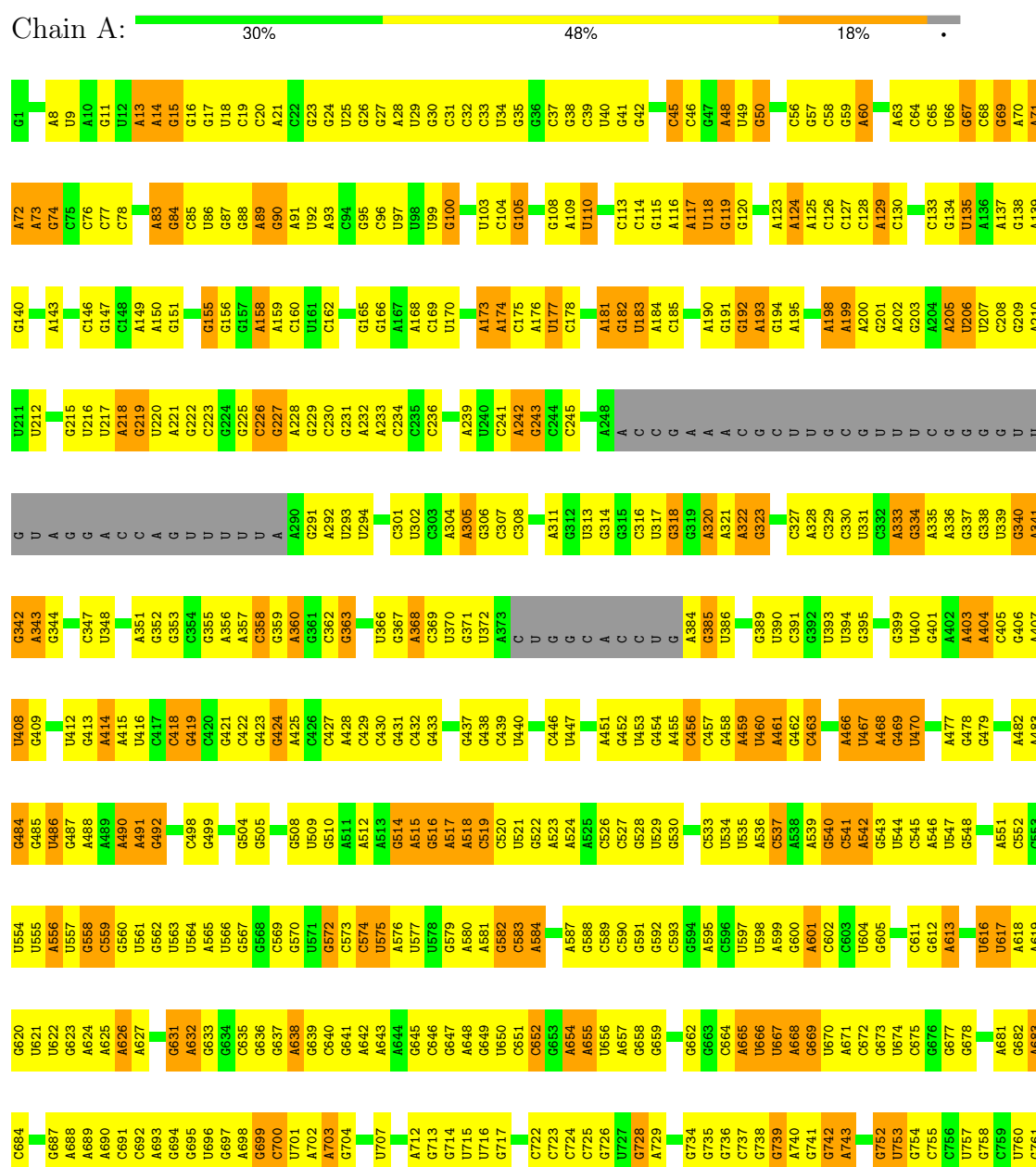
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

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.

Note EDS was not executed.

• Molecule 1: 23S rRNA

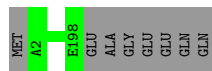


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G1749	U1680	A1607	A1538	U1474	U1402	G1334	C1264	U1112	U1045	A971	A	G831	A763
A1750	A1681	U1608	U1539	U1475	U1403	A1334	G1265	C1113	U1046	C972	C	A832	C764
U1751	A1682	C1540	C1541	U1476	A1405	G1337	A1267	G1118	U1047	U974	A	C833	C765
G1683	G1541	U1611	G1542	G1480	U1409	G1338	U1268	G1119	U1048	C975	G	A838	A766
G1684	G1543	G1612	G1544	U1481	U1410	U1339	G1269	C1120	C1049	C976	C	U839	U768
A1685	G1544	C1613	A1544	U1482	C1411	G1340	C1270	G1121	U840	U977	U	U840	G773
G1754	G1548	G1617	U1548	U1483	C1412	G1341	U1271	A1122	G841	U978	U	G841	G774
G1755	U1549	G1618	C1549	G1484	C1413	U1342	G1272	G1123	A1055	A979	A	A842	U775
G1756	G1550	G1619	C1550	U1485	C1414	C1343	G1273	U1124	U1056	C909	C	G843	U776
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C1762	C1552	C1623	C1552	C1487	C1416	G1345	A1275	A1126	A1057	A911	C	U845	A777
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A1764	A1554	A1625	A1554	C1489	A1420	C1347	U1277	G1128	A984	A912	C	C850	U784
C1765	A1555	A1626	A1555	U1490	U1421	C1348	G1278	A1129	U1060	A913	C	C851	U785
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U1770	A1560	C1632	A1560	G1497	G1427	A1353	C1283	G1137	A1068	C997	C	U856	A790
A1771	A1634	G1633	G1561	C1498	G1428	A1354	A1285	A1138	G1069	C998	C	U857	G791
C1772	G1635	G1634	G1562	U1498	A1429	G1355	U1286	U1139	U1070	A999	C	G858	G791
G1773	U1563	U1640	U1563	A1499	G1430	U1357	A1287	A1140	U1071	G1000	C	U859	A794
A1774	U1564	C1641	U1564	U1500	U1431	C1358	A1288	U1141	G1073	C1002	C	U860	A795
A1775	G1571	C1642	G1571	C1501	G1432	G1359	A1289	G1142	U1074	A1003	C	G861	A796
U1776	C1572	G1643	C1572	G1502	A1433	U1364	A1290	A1143	C1075	C1004	C	A862	A797
U1777	G1573	U1645	G1573	G1503	G1434	U1365	G1291	U1144	U1005	A930	C	G863	G798
U1778	A1574	C1646	A1574	G1504	G1435	U1366	A1292	U1145	G1006	G932	C	C864	C799
A1782	C1575	G1648	C1575	U1505	G1436	A1366	A1293	G1146	U1080	A1007	C	U865	U800
U1787	G1576	U1651	U1576	U1506	A1437	A1367	G1298	G1149	A1081	G1008	C	U866	A801
C1788	C1579	G1652	C1579	A1507	G1438	G1368	A1299	U1150	G1082	C937	C	G867	A802
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C1791	A1582	C1655	A1582	A1512	G1442	G1371	U1302	C1153	G1085	C939	C	U870	G805
C1792	U1583	U1656	A1583	U1513	G1443	U1372	A1302	A1154	C1086	G940	C	U871	A806
A1793	G1584	C1657	G1584	C1514	C1444	G1374	U1307	G1155	C1087	U941	C	G872	A807
A1794	A1585	G1660	A1585	U1515	U1446	G1377	U1308	C1160	A1088	U942	C	U873	C808
G1798	A1588	C1661	G1588	G1519	U1447	C1380	C1309	U1161	C1091	A1019	C	A874	C809
A1799	G1589	G1662	C1589	G1520	G1450	G1381	C1310	A1162	U1092	A1020	C	A875	U810
A1800	C1590	C1663	U1521	U1521	C1451	G1382	G1311	C1163	U1093	A1021	C	A876	G811
C1801	U1591	G1664	C1522	C1522	U1452	C1383	G1312	C1164	U1096	G1022	C	G877	A813
A1802	U1592	C1665	A1523	A1523	A1453	G1384	U1313	G1165	A1097	U1023	C	A878	G814
G1803	C1593	G1666	C1524	C1524	G1456	C1385	A1314	C1166	G1098	G951	C	A879	A815
A1807	U1594	C1667	A1525	A1525	C1456	A1386	G1316	A1167	A1099	A952	C	C880	U816
C1808	A1595	G1668	U1526	U1526	A1457	G1387	A1321	C1169	G1100	C1031	C	A886	G818
G1809	A1596	C1669	G1527	G1527	A1458	A1391	G1322	U1170	U1101	A1032	C	G887	C819
U1810	C1597	G1670	C1528	U1529	U1459	U1392	G1323	A1171	G1102	G1033	C	U888	U820
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G1742	U1600	C1672	G1531	U1601	G1465	C1394	U1325	G1173	G1104	G1034	C	A891	G822
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G1818	G1678	G1678	A1605	G1536	G1470	A1400	G1330	C1185	G1110	G1041	C	C	C827
													C829

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A2858	G2781	U2707	C2629	G2557	C2491	C2420	C2338	C2262	A2189	C2122	U2058	G1987	G1912	C1822
U2859	U2783	U2708	C2630	C2558	U2492	C2421	A2348	C2263	A2190	C2123	A2060	C1988	G1913	G1823
C2860	A2784	C2709	A2633	G2560	U2493	C2422	G2349	C2264	A2191	C2124	C2061	C1989	U1914	C1824
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G2868	G2793	A2718	G2643	A2569	C2500	U2428	C2359	C2271	U2198	G2132	G2070	U2000	U1922	
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G2874	G2797	C2723	G2646	G2573	G2503	G2433	G2362	U2274	G2201	C2139	A2073	U2003	C1925	C1836
C2875	U2798	C2724	A2653	G2574	G2504	G2434	G2363	C2275	G2202	G2140	U2075	U2005	U1927	A1840
A2877	C2799	C2725	A2654	G2575	G2505		C2364	C2276	G2203	A	G2076	G2006	G1928	
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A2810	A2810	U2734	G2665	C2590	C2518	C2445	C2373	C2293	G2213	U	U2086	G2015	G1943	
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U2822	U2822	G2741	C2671	C2595	G2524	U2455	G2379	A2298	G2225	C2157	U2092	C2023	C1948	G1879
G2823	C2823	G2742	G2672	C2596	U2525	A2456	U2380	A2299	A2226	C2158	G2093	C2024	A1949	G1880
C2824	A2744	G2743	C2673	A2600	U2526	A2457	A2381	G2300	C2227	C2159	C2094	U2024	C1950	U1881
A2825	G2745	A2745	C2674	C2601	G2527	A2458	C2382	A2301	U2228	A2159	G2095	A2025	G1951	G1882
C2826	G2756	A2756	G2675	G2602	G2528	U2459	U2385	A2306	G2229	C2160	U2096	C2026	A1952	A1853
G2827	U2757	A2757	U2677	G2603	G2529	C2459	U2386	A2307	G2234	C2161	A2097	A2032	A1953	A1854
C2828	G2758	A2758	G2678	G2604	U2530	G2460	U2387	A2308	G2235	C2162	G	G2032	A1954	C1885
A2829	U2759	U2759	U2680	G2605	U2531	G2466	A2390	A2309	U2236	U2163	A	A2034	G1955	
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G2839	U2766	U2766	C2686	G2607	U2533	G2468	G2392	A2312	G2238	A2167	A	G2039	U1965	G1890
U2840	C2767	C2767	G2687	C2608	U2534	U2469	G2393	G2313	C2239	A2168	G2103	A2040	C1966	C1891
C2842	C2768	C2768	G2688	U2613	U2544	A2476	A2394	A2314	G2240	A2169	U2105	A2041	G1970	U1894
A2843	U2769	A2770	C2689	U2615	A2545	C2477	G2395	A2315	C2241	A2170	G2106	A2042	C1971	A1895
C2844	C2770	C2770	G2690	G2616	G2546	U2478	C2396	G2316	U2242	U2171	C2109	G2043	G1972	A1896
G2845	A2771	A2771	C2691	U2617	C2547	G2479	U2397	G2317	C2243	U2172	A2109	A2044	C1973	C1897
C2846	G2772	U2772	U2692	G2620	G2548	U2479	A2405	U2318	C2244	A2175	C	A2045	G1974	U1898
G2847	G2773	G2773	G2693	G2621	G2549	C2480	A2406	G2319	A2248	U2176	C	G2048	U1975	U1900
U2848	U2774	U2774	C2694	G2622	C2550	G2481	G2407	G2324	U2251	U2177	U	C2049	G1976	A1901
C2849	U	U	A2696	G2623	C2551	A2482	G2408	A2325	A2252	U2180	C	U2051	U1978	G1905
G2852	A	A	U2697	U2624	A2552	U2483	A2409	C2326	A2253	A2181	G	G2052	C1979	U1906
			G2698	U2625	G2553	G2484	U2410	G2328	C2254	C2183	A2117	A2054	A1980	C1908

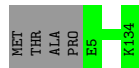
- Molecule 2: Ribosomal Protein L4

Chain K:  96% .



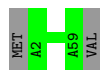
- Molecule 3: Ribosomal Protein L22

Chain L:  97% .



- Molecule 4: Ribosomal Protein L32

Chain M:  97% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.40 Å 410.70 Å 694.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.209 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59977	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

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: ROX, 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	A	0.23	0/66661	0.66	2/103976 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	777	A	C2'-C3'-O3'	5.48	122.47	113.70
1	A	1746	A	C2'-C3'-O3'	5.31	122.19	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59532	0	30004	1878	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	58	0	76	22	0
6	A	2	0	0	0	0
All	All	59977	0	30080	1896	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 21.

The worst 5 of 1896 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1747:G:H4'	1:A:1749:G:H1'	1.31	1.13
1:A:940:G:H3'	1:A:941:U:H5''	1.35	1.09
1:A:367:G:H2'	1:A:368:A:H5''	1.34	1.08
1:A:1199:U:H3'	1:A:1200:G:H5''	1.35	1.07
5:A:2881:ROX:H211	5:A:2881:ROX:H71	1.36	1.06

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2765/2880 (96%)	557 (20%)	142 (5%)

5 of 557 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	23	G
1	A	45	C

5 of 142 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2404	A
1	A	2437	G
1	A	2615	U
1	A	929	A
1	A	925	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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$
5	ROX	A	2881	-	60,60,60	1.60	12 (20%)	87,89,89	3.42	48 (55%)

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	ROX	A	2881	-	-	12/80/115/115	1/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	ROX	C7-C8	4.91	1.60	1.54
5	A	2881	ROX	C7-C6	3.45	1.60	1.54
5	A	2881	ROX	O2-C13	-3.34	1.40	1.46
5	A	2881	ROX	C35-C12	3.21	1.58	1.52
5	A	2881	ROX	C10-C9	-3.20	1.50	1.53

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	ROX	C8-C9-N2	-9.35	119.32	126.21
5	A	2881	ROX	C34-C10-C9	-7.99	101.01	110.58
5	A	2881	ROX	O3-C3-C4	7.39	116.94	108.23
5	A	2881	ROX	C19-C16-C17	6.95	124.86	111.19
5	A	2881	ROX	C33-C8-C7	6.94	122.80	109.88

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	ROX	C17-C16-O5-C20
5	A	2881	ROX	O4-C14-O3-C3
5	A	2881	ROX	C1-C2-C3-O3
5	A	2881	ROX	O13-C38-O14-C39
5	A	2881	ROX	C6-C7-C8-C33

All (1) ring outliers are listed below:

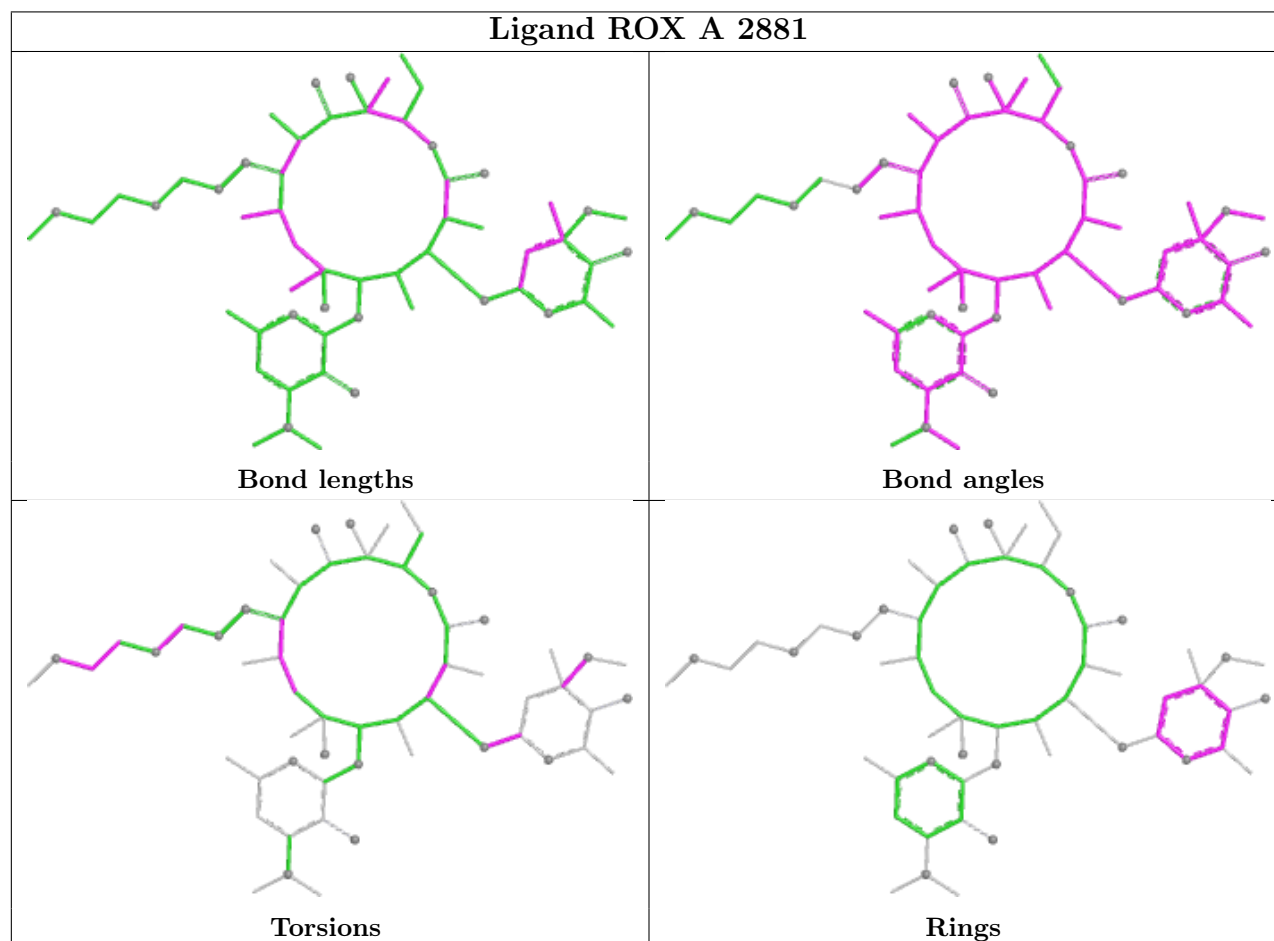
Mol	Chain	Res	Type	Atoms
5	A	2881	ROX	C14-C15-C16-C17-C18-O4

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	ROX	22	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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.