



wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 07:04 pm BST

PDB ID : 1Z58
Title : Crystal structure of a complex of the ribosome large subunit with rapamycin
Authors : Amit, M.; Berisio, R.; Baram, D.; Harms, J.; Bashan, A.; Yonath, A.
Deposited on : 2005-03-17
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.11

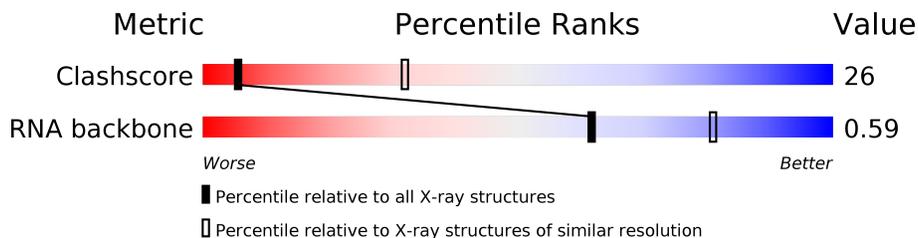
1 Overall quality at a glance

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 on 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	2	2880	

2 Entry composition i

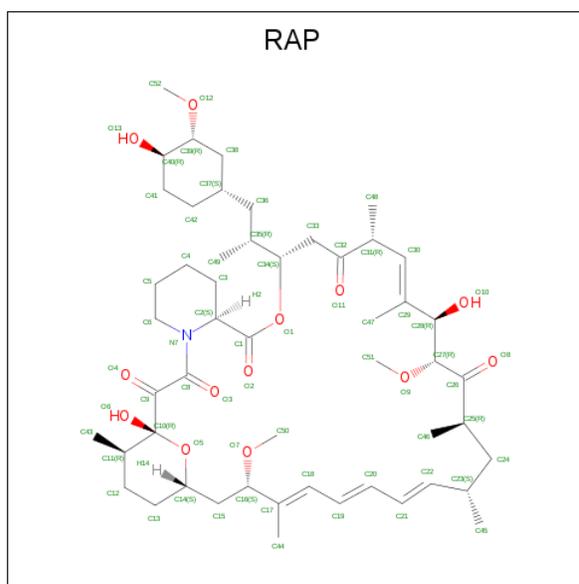
There are 2 unique types of molecules in this entry. The entry contains 59424 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	2	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is RAPAMYCIN IMMUNOSUPPRESSANT DRUG (three-letter code: RAP) (formula: C₅₁H₇₉NO₁₃).



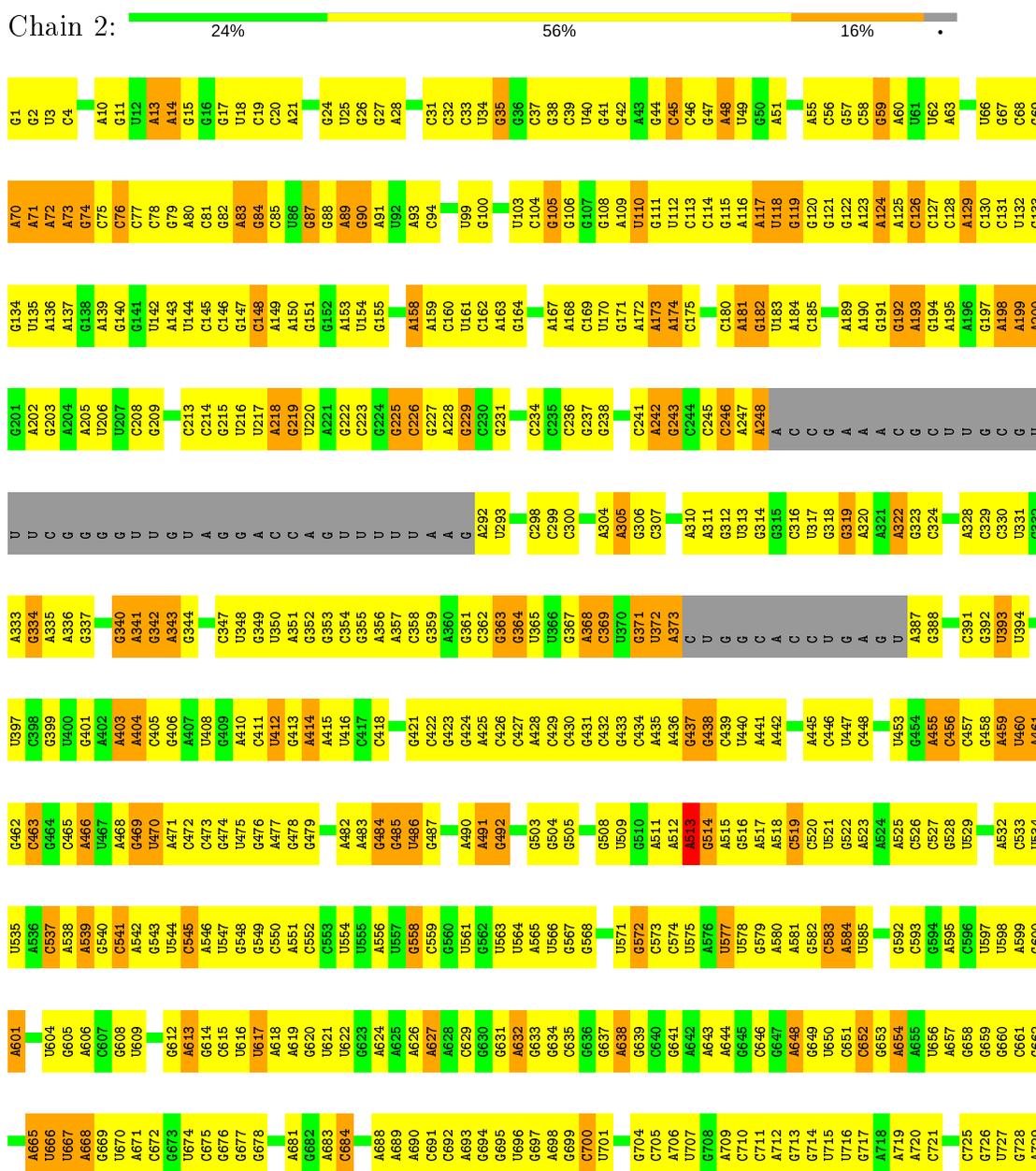
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	2	1	65	51	1	13	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 RIBOSOMAL RNA



C1677	C1678	U1679	A1681	A1682	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	A1690	A1691	A1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	C1700	C1701	U1705	A1706	A1707	A1708	A1709	A1710	A1711	A1712	A1713	A1714	A1715	A1716	A1717	G1720	G1721	G1722	G1723	G1724	G1725	C1726	A1727	A1728	A1729	G1730	G1731	U1732	G1737	U1738	G1742	G1743	G1744	C1745						
U1808	G1609	A1610	U1611	A1612	A1613	A1614	C1615	C1616	C1617	A1618	A1619	A1620	C1621	G1622	C1623	A1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632	A1633	A1634	A1635	G1636	G1637	A1638	A1639	A1640	A1641	A1642	A1643	A1644	A1645	A1646	A1647	A1648	U1651	G1652	A1653	A1654	C1655	U1656	A1657	U1658	U1659	U1660	U1661	U1662	A1663	A1664	A1665	A1666	G1670	A1671	A1672	C1673	C1674	A1675	U1676
A1538	U1539	C1540	G1541	A1542	A1543	A1544	A1545	C1546	C1547	A1548	A1549	A1550	A1551	C1552	G1557	C1558	G1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	U1600	U1601	U1602	A1603	A1604	A1605	A1606	A1607	
U1473	A1474	U1475	A1476	A1477	A1478	A1479	A1480	A1481	U1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	U1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	U1521	C1522	A1523	C1524	A1525	U1526	A1527	C1528	C1529	U1530	A1531	A1532	A1533	A1534	U1537	
U1409	U1410	C1411	A1412	U1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	G1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	C1472			
G1341	U1342	C1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	U1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	U1392	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1407	A1408						
A1278	G1279	U1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	U1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1321	A1322	A1323	A1324	U1325	A1326	A1327	A1328	A1329	G1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340						
C1210	A1211	U1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1233	A1234	C1235	A1236	G1243	U1244	A1245	A1246	U1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	U1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277							
A1139	A1140	U1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1160	A1161	A1162	A1163	A1166	A1167	A1168	A1169	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1186	A1187	A1188	A1189	A1190	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207							
C996	C997	A998	A999	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1014	A1015	A1018	A1019	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1064	A1065	A1066									
G932	G933	G934	G935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995						
U868	C869	C870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	C882	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931		
A806	A807	C808	C809	C810	A811	A812	A813	A814	A815	A816	A817	A818	A819	U820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	U837	A838	A839	U840	A841	A842	A843	A844	A845	A846	A847	A848	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868					
G736	C737	G738	G739	A740	A741	A742	A743	A746	A747	A754	C755	C756	C757	C758	C759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U772	A773	A774	U775	U776	U777	U778	U779	U780	U781	U782	U785	U786	A787	U788	U789	A790	A791	A796	A797	U798	C799	U800	A801	A802	A803	A804	A805											

C2747	G2811
C2748	A2812
A2749	G2813
G2750	
C2751	A2817
C2752	G2818
C2753	G2819
C2754	C2820
A2755	G2821
A2756	U2822
G2757	G2823
A2758	C2824
U2759	A2825
G2760	C2826
A2761	G2827
G2762	C2828
	A2829
	U2830
	A2831
C2765	U2836
U2766	G2837
C2767	U2838
C2768	U2839
A2769	G2840
C2770	U2841
C2771	U2842
U2772	A2843
G2773	G2844
U2774	C2845
U	
U	
A	
U2778	G2846
C2779	G2847
A2780	A2848
G2781	C2849
G2782	
U2783	G2854
A2784	
A2785	A2858
G2786	U2859
A2787	C2860
C2788	A2861
U2789	G2862
C2790	U2863
C2791	C2864
C2792	G2865
G2793	A2866
G2794	G2867
A2795	G2868
A2796	U2869
G2797	C2870
C2800	A2874
A2801	C2875
	C2876
G2805	A2877
G2806	C
U2807	U
U2808	C
A2809	
A2810	

4 Data and refinement statistics

Xtrriage (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	168.50Å 404.00Å 689.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.80)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.368	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	59424	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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: RAP

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	2	0.15	0/66467	0.63	1/103673 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	513	A	C2'-C3'-O3'	6.09	123.44	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	2	59359	0	29917	2275	0
2	2	65	0	79	20	0
All	All	59424	0	29996	2275	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 26.

The worst 5 of 2275 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)
1:2:1773:C:H41	2:2:2881:RAP:C15	1.42	1.32
1:2:1773:C:N4	2:2:2881:RAP:H151	1.54	1.20
1:2:700:C:H42	1:2:800:U:H4'	1.11	1.15
1:2:1663:C:H5'	1:2:1664:G:H5''	1.32	1.08
1:2:940:G:H3'	1:2:941:U:H5''	1.36	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	2757/2880 (95%)	529 (19%)	65 (2%)

5 of 529 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	14	A
1	2	35	G
1	2	45	C
1	2	48	A
1	2	49	U

5 of 65 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1325	U
1	2	1632	A
1	2	2633	A
1	2	1345	G
1	2	1410	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
2	RAP	2	2881	-	65,68,68	1.88	13 (20%)	73,96,96	1.45	8 (10%)

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
2	RAP	2	2881	-	-	3/81/124/124	0/3/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2881	RAP	C8-C9	-8.41	1.42	1.53
2	2	2881	RAP	C40-C39	4.46	1.60	1.52
2	2	2881	RAP	O1-C1	3.86	1.43	1.34
2	2	2881	RAP	O1-C34	-3.40	1.40	1.46
2	2	2881	RAP	C44-C17	2.99	1.56	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2881	RAP	O1-C1-C2	4.99	121.78	110.78
2	2	2881	RAP	C34-O1-C1	4.47	124.60	117.89
2	2	2881	RAP	C9-C8-N7	3.91	123.72	119.25
2	2	2881	RAP	O1-C1-O2	-3.05	118.24	123.94
2	2	2881	RAP	C3-C2-N7	-2.91	106.49	110.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

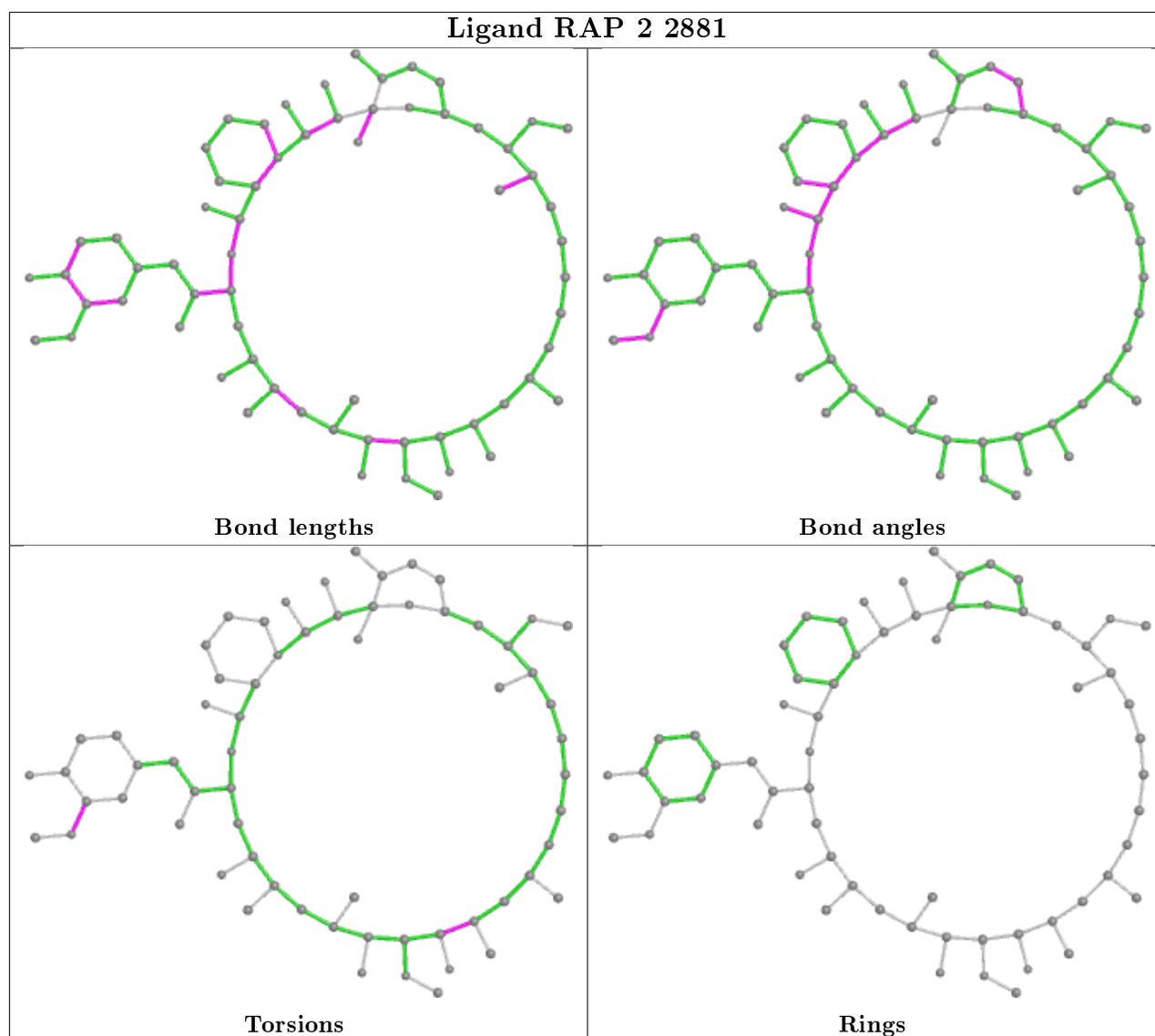
Mol	Chain	Res	Type	Atoms
2	2	2881	RAP	C46-C25-C26-O8
2	2	2881	RAP	C40-C39-O12-C52
2	2	2881	RAP	C24-C25-C26-O8

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	2881	RAP	20	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.