



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:21 pm BST

PDB ID : 1OND
Title : THE CRYSTAL STRUCTURE OF THE 50S LARGE RIBOSOMAL SUB-UNIT FROM DEINOCOCCUS RADIODURANS COMPLEXED WITH TROLEANDOMYCIN MACROLIDE ANTIBIOTIC
Authors : Berisio, R.; Schlutzen, F.; Harms, J.; Bashan, A.; Auerbach, T.; Baram, D.; Yonath, A.
Deposited on : 2003-02-27
Resolution : 3.40 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)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

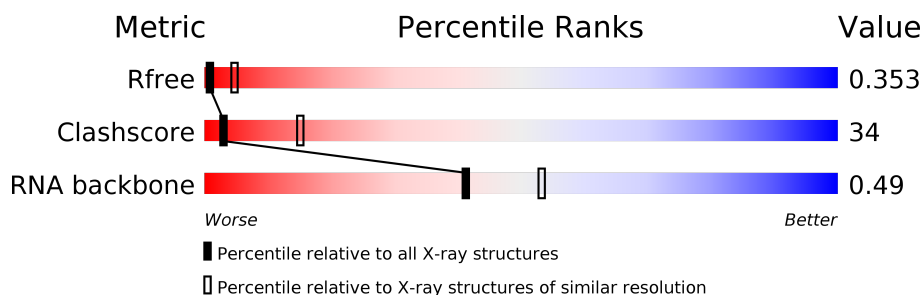
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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))
R _{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
RNA backbone	3102	1006 (3.84-2.96)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	Q	134	
3	Z	60	

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
4	TAO	0	2881	-	X	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 59581 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
1	0	2765	Total	C	N	O	P	0	0	0
			59336	26469	10944	19159	2764			

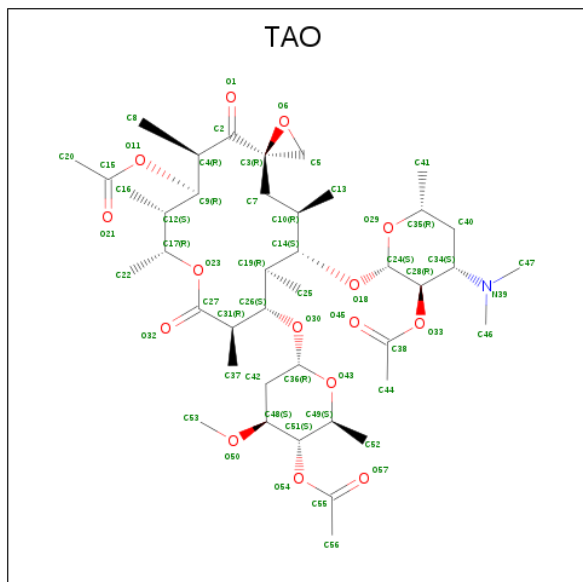
- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	Q	130	Total	C	0	0	130
			130	130			

- Molecule 3 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	Z	58	Total	C	0	0	58
			58	58			

- Molecule 4 is TROLEANDOMYCIN (three-letter code: TAO) (formula: $C_{41}H_{67}NO_{15}$).

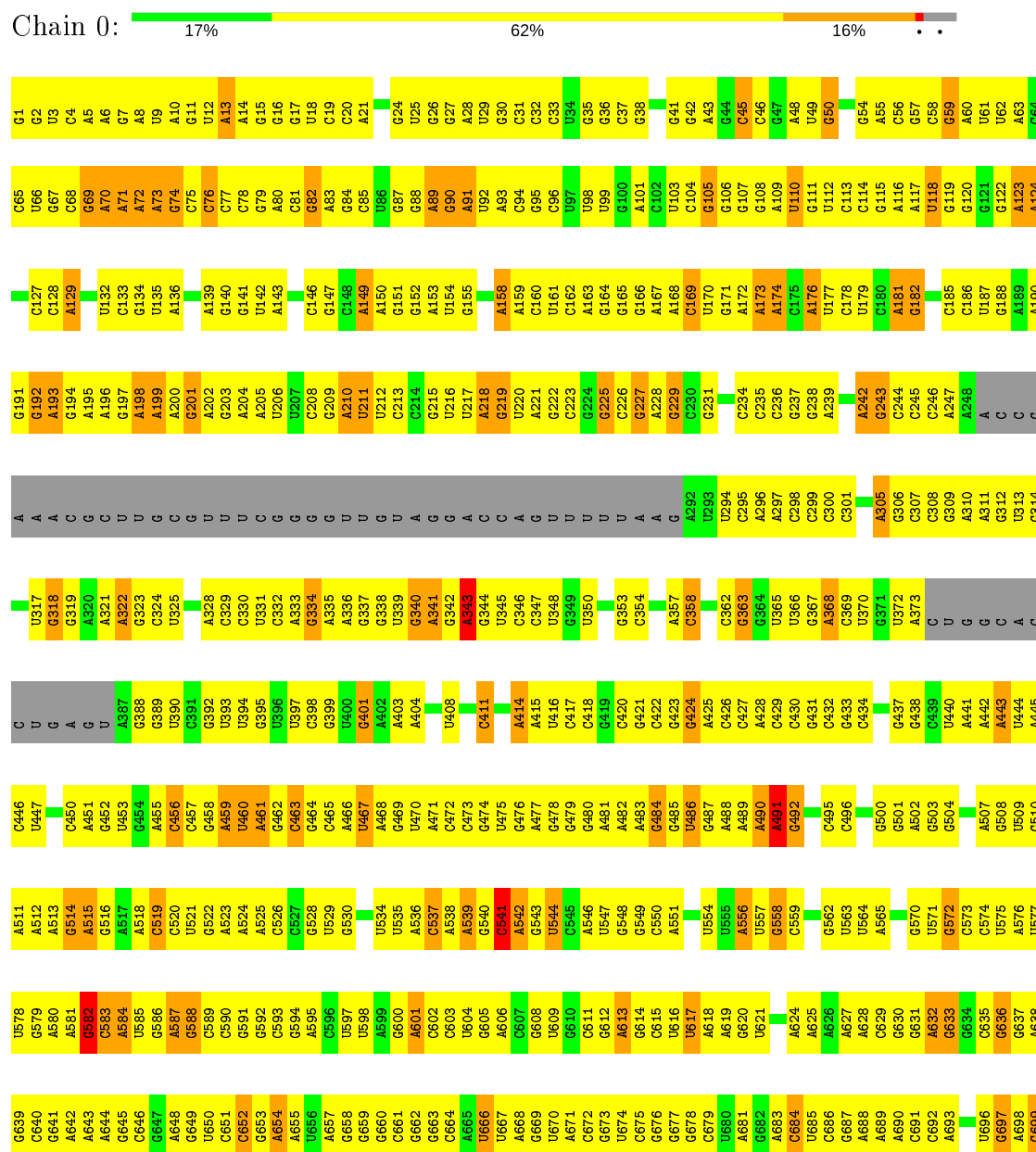


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	0	1	Total	C	N	O	0	0
			57	41	1	15		

3 Residue-property plots

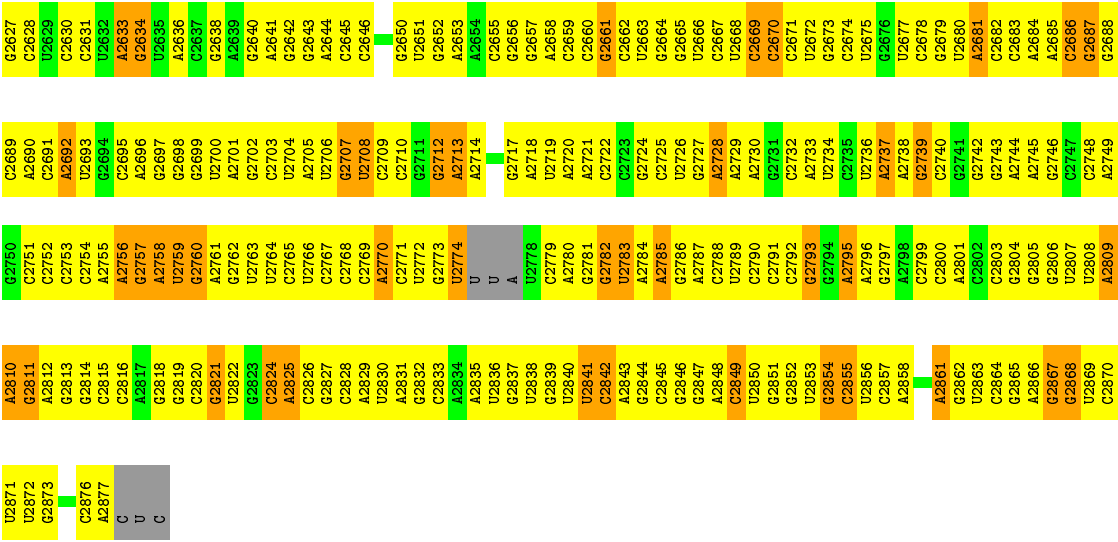
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

• Molecule 1: 23S RIBOSOMAL RNA

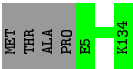


A1603	C1540	U1473	U1409	C1346	A1285	G1222	A1154	A1088	C1018	G955	G	C825	A763	C700
A1604	G1541	A1474	U1410	C1347	U1286	G1223	G1155	C1089	U1019	A956	G	U826	A764	U701
A1605	G1542	U1475	C1411	C1348	A1287	A1224	G	C1090	A1020	C958	G	C827	C765	A702
	G1543	G1476	C1412	A1349	A1288	G1225	C1160	C1091	A1021	G958	C	C828	A766	A703
U1608	A1544	C1477	G	G1350	A1289	A1226	U1161	U1092	A1022	C959	C	C829	C767	G704
G1610	G1545	U1478	C1418	G1351	A1290	G1228	A1162	G	U1023	U960	U	C830	C768	C705
G1611	C1546	G1479	G1419	G1352	G1291	G1229	C1163	A1095	G1024	C963	A	C831	C769	A706
U1612	U1547	G1480	A1420	A1353	A1292	C1230	C1164	A1096	A1025	C962	C	A832	U770	U707
G1613	U1548	U1481	U1421	A1354	A1293	C1231	G1165	A1097	A1026	G963	C	A833	C771	G708
C1614	C1549	U1482	C1422	A1355	G1294	A1231	A1166	G1098	C1027	G964	A	U834	A772	A709
C1615	C1550	G1483	A1423	G1356	U1295	U1232	A1167	U1099	G1028	G965	A	U835	G773	C710
C1616	U1551	G1484	U1424	U1357	G1296	A1233	C1168	G1100	C1029	C966	C	G836	A774	C711
G1617	G1552	U1485	G1425	C1358	A1297	C1234	G1169	U1101	U1030	C967	U	U837	U775	A712
U1618	G	A1486	U1426	G1359	G1298	C1235	U1170	G1102	C1031	U968	U	A838	U776	G713
G1619	G1553	C1487	G1427	G	A1299	A1238	U1171	C1103	A1032	A970	A	U839	G777	G714
A1620	A1554	G1488	G1428	A1362	A1300	G	A1172	G1104	G1033	A971	C	U840	U778	U715
C1621	A1556	C1489	A1429	C1363	U1301	G1241	G1173	U1105	U1034	C972	C	G841	G716	U716
G1622	G1557	U1490	G1430	C1364	C1302	A1242	G1174	A1106	G1035	U973	A911	A842	U717	G717
C1623	A1491	U1431	U1431	U1365	U1303	G1243	A1175	A1107	G1036	U974	A912	G843	A718	A718
A1624	A1492	G1432	A1432	A1366	U1304	G1244	G	G1110	U1037	C975	A913	G844	A719	A720
A1625	A1493	G1433	U1434	A1367	U1305	G1245	C1178	C1111	U1038	C976	C914	G845	A721	A721
G1626	G1494	G1435	G1435	G1368	U1306	G1246	A1179	C1112	A1039	G977	C915	U846	U785	C721
C1627	G1495	G1436	U1370	G1369	U1307	G1247	A1180	C1113	A1040	U978	U916	C847	U786	C722
U1628	U1563	G1496	A1437	G1371	C1308	G1248	C1181	A1114	G1041	A979	U917	A848	A787	C723
G1629	U1564	G	A1438	G1372	C1310	G1249	C1182	C1115	U1044	C980	A918	G788	G788	G726
A1630	A1569	C1501	G1439	G1373	C1311	A1250	C1183	C1116	G1045	C981	U919	U852	G789	G727
C1631	C1570	G1502	G1440	G1374	G1312	G1251	G1184	U1117	U1046	C982	G920	C853	A790	U727
A1632	G1503	C1514	G1441	C1375	G1313	C1252	C1185	G1118	A921	C983	A922	G854	A791	G728
C1633	C1572	G1504	C1442	G1376	U1314	G1253	G	G1121	G1053	A985	A923	U857	U792	G732
G1634	A1573	U1505	G1443	G1377	A1315	G1254	A1188	A1122	C1054	A986	C924	G858	A794	G733
A1635	A1574	G	A1444	A1378	G1316	G1255	C1189	G1122	A1055	C987	U925	U859	A795	G734
G1636	G1575	U1509	A1445	A1379	C1317	C1256	G1191	A1123	U1056	A990	C927	U860	A796	G735
G1637	G1577	G	U1446	C1380	A1318	U1257	A1192	G1124	A1057	A991	C928	G861	A797	G736
G1638	G1578	A1512	U1447	G1381	C1319	G1258	G1193	G1125	G1058	A992	C929	G864	C798	C737
A1639	U1578	U1513	A1448	G1382	A1320	A1259	U1194	A1126	G1062	C993	A929	C864	G738	G738
C1640	G1579	C1514	C1449	C1383	A1321	A1260	U1195	U1130	C1063	C993	A930	U865	U800	G739
C1641	C1580	U1515	G1450	G1384	G1322	G1261	G1196	G1131	A1064	A994	C931	U866	A801	A740
G1642	C1581	A1516	U1451	C1385	G1323	U1262	U1197	C1132	C1065	A995	G932	G867	A802	G741
A1643	A1582	C1517	U1452	A1386	G1324	G1263	C1198	G1133	G1066	C996	G933	U868	C803	G742
G1644	A1583	C1518	A1453	G1387	U1325	C1264	U1199	C1134	G1067	G	G	C869	C804	A743
U1645	G1584	U1454	U1454	C1388	U1326	G1265	G1200	G1135	G1068	A999	A956	U871	G805	C744
A1646	A1585	C1455	C1455	C1389	G1327	G1266	G1201	G1136	A1069	G1000	C937	G872	A806	C745
G1647	A1586	G1456	G1456	G1390	C1328	A1267	U1202	G1137	G1069	A1001	G938	U873	A807	G746
C1648	A1587	A1457	A1458	A1391	U1329	U1268	A1203	A1137	C1002	C1002	C939	G874	U810	A747
A1649	A1588	C1524	U1459	G1393	G	G1269	G1204	A1138	U1072	C1003	G940	A874	A748	A748
U1650	G1589	G1527	G1460	G	G1332	C1270	G1205	A1139	G1073	A1004	U941	G875	G811	C749
G1651	C1590	U1528	C1461	G1396	C1333	G1271	G1206	A1140	G1074	U1005	U942	A876	G812	C750
C1652	U1591	C1529	G1462	C1398	A1334	G1272	U1141	G1141	C1075	C1006	U943	G877	A813	G751
A1654	C1593	U1530	A1463	C1399	G1335	G1273	G1207	G1142	U1076	A1007	A944	C878	G814	G752
C1655	C1594	C1531	A1464	G1400	G1336	C1274	U1212	C1145	U1077	G1008	G945	A879	A815	U753
U1656	A1595	A1532	G1465	G1401	G1337	A1275	U1213	G1146	A1078	C1009	U946	U816	U816	G754
A1657	A1596	G1533	C1466	G1402	G1338	U1276	C1214	G1147	G1079	U1010	C947	A886	A817	C755
G1658	G1597	A1534	U1467	U1403	U1339	G1277	A1215	G1147	A1080	A1011	C948	G887	G818	C756
C1659	C1598	A1535	A1468	C1404	G1341	A1278	G1216	G1148	A1081	G1012	G949	G888	C819	U757
G1660	G1599	G1536	U1469	A1405	C1342	G1279	U1217	C1149	G1082	G1013	G950	C889	U820	G758
C1662	U1600	U1537	G1470	A1406	U1280	U1280	C1218	C1150	C1083	G1014	G951	U890	A821	C759
G1663	C1601	G1407	C1344	A1406	A1281	G	C1219	C1151	C1086	U1015	A952	G	G822	U760
A1664	G1602	C1472	G1345	A1408	G1284	G	C1221	A1153	C1087	C1017	U954	G	U824	A762

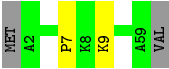




• Molecule 2: 50S ribosomal protein L22



• Molecule 3: 50S ribosomal protein L32



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.25Å 411.09Å 695.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40 20.02 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.40) 88.0 (20.02-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.310 0.352 , 0.353	Depositor DCC
R_{free} test set	14435 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	59581	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: TAO

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	0	0.83	17/66440 (0.0%)	0.75	34/103628 (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	0	0	47

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	1549	C	N1-C2	11.30	1.51	1.40
1	0	1549	C	N3-C4	9.79	1.40	1.33
1	0	929	A	N1-C2	8.60	1.42	1.34
1	0	1149	G	C6-O6	-8.38	1.16	1.24
1	0	1549	C	C2-O2	7.25	1.30	1.24

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2590	U	P-O3'-C3'	-9.16	108.70	119.70
1	0	633	G	N3-C2-N2	7.30	125.01	119.90
1	0	2591	C	OP1-P-OP2	-6.77	109.45	119.60
1	0	2428	U	N1-C1'-C2'	6.61	122.60	114.00
1	0	459	A	N9-C1'-C2'	6.53	122.49	114.00

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	211	U	Sidechain
1	0	343	A	Sidechain
1	0	470	U	Sidechain
1	0	491	A	Sidechain
1	0	82	G	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	0	59336	0	29907	3024	0
2	Q	130	0	0	0	0
3	Z	58	0	0	4	0
4	0	57	0	67	22	0
All	All	59581	0	29974	3039	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 34.

The worst 5 of 3039 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)
4:0:2881:TAO:C31	4:0:2881:TAO:C26	1.82	1.56
4:0:2881:TAO:C24	4:0:2881:TAO:O18	1.65	1.41
1:0:2058:U:H1'	1:0:2576:G:H21	1.09	1.17
1:0:1458:A:H3'	1:0:1459:U:C5'	1.74	1.17
1:0:2548:G:H2'	1:0:2549:G:H5''	1.17	1.15

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	0	2755/2880 (95%)	523 (18%)	52 (1%)

5 of 523 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1338	G
1	0	1651	U
1	0	2592	U
1	0	1354	A
1	0	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
4	TAO	0	2881	-	59,60,60	4.30	35 (59%)	77,89,89	4.28	48 (62%)

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
4	TAO	0	2881	-	-	45/77/113/113	1/4/4/4

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	0	2881	TAO	C31-C26	11.80	1.82	1.55
4	0	2881	TAO	O11-C9	10.13	1.60	1.44
4	0	2881	TAO	O11-C15	9.06	1.55	1.35
4	0	2881	TAO	C31-C27	8.79	1.71	1.51
4	0	2881	TAO	O18-C24	8.52	1.65	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	0	2881	TAO	O23-C27-C31	11.74	137.34	111.56
4	0	2881	TAO	C16-C12-C17	-11.23	97.66	112.18
4	0	2881	TAO	C26-C31-C27	11.18	132.86	110.01
4	0	2881	TAO	O18-C14-C19	9.77	119.99	108.22
4	0	2881	TAO	C16-C12-C9	-8.26	96.58	111.40

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	0	2881	TAO	C56-C55-O54-C51
4	0	2881	TAO	C31-C26-O30-C36
4	0	2881	TAO	C19-C26-O30-C36
4	0	2881	TAO	C31-C27-O23-C17

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Mol	Chain	Res	Type	Atoms
4	0	2881	TAO	O32-C27-O23-C17

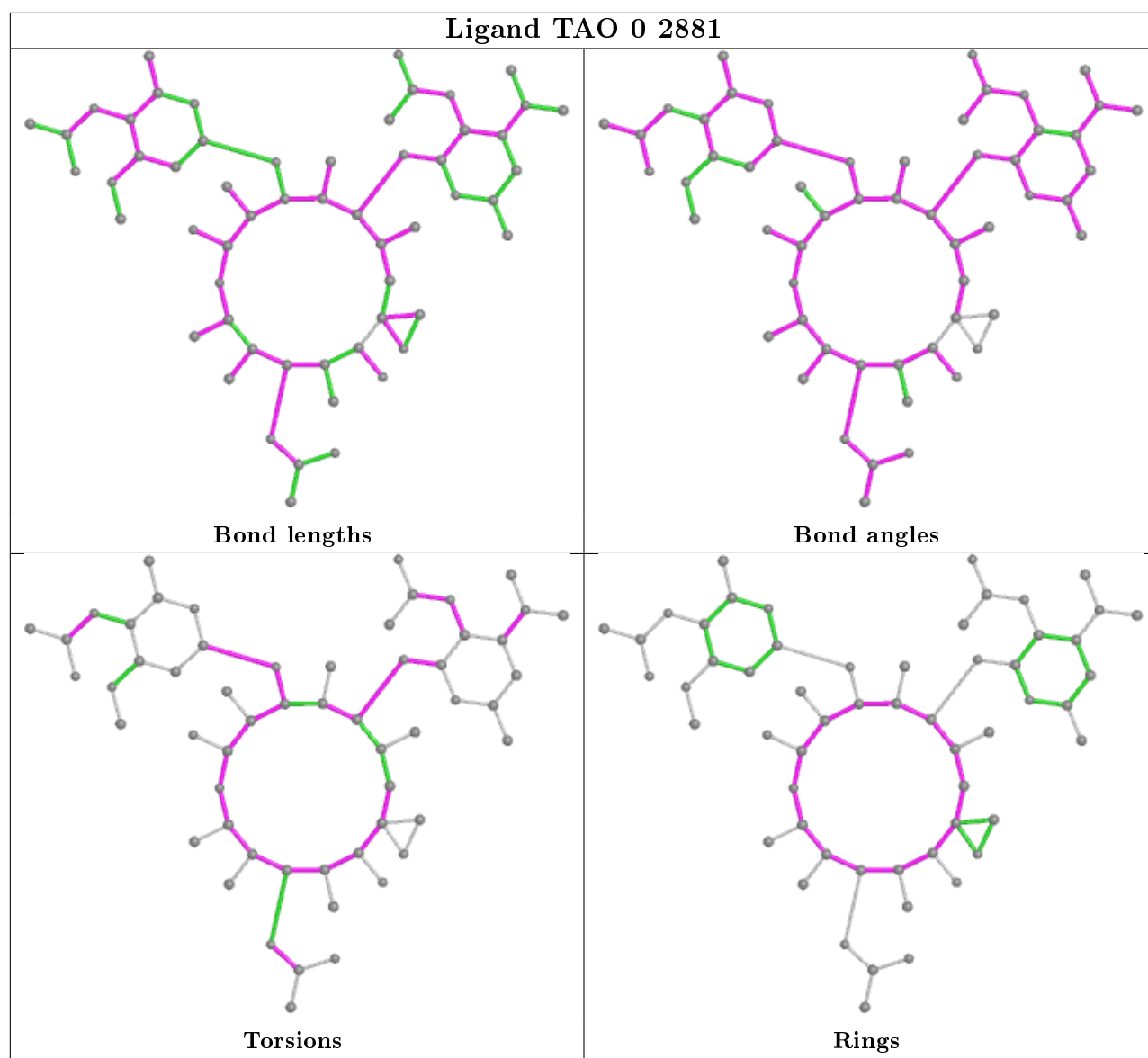
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	0	2881	TAO	C10-C12-C14-C17-C19-C2-C26-C27-C3-C31-C4-C7-C9-O23

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	0	2881	TAO	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

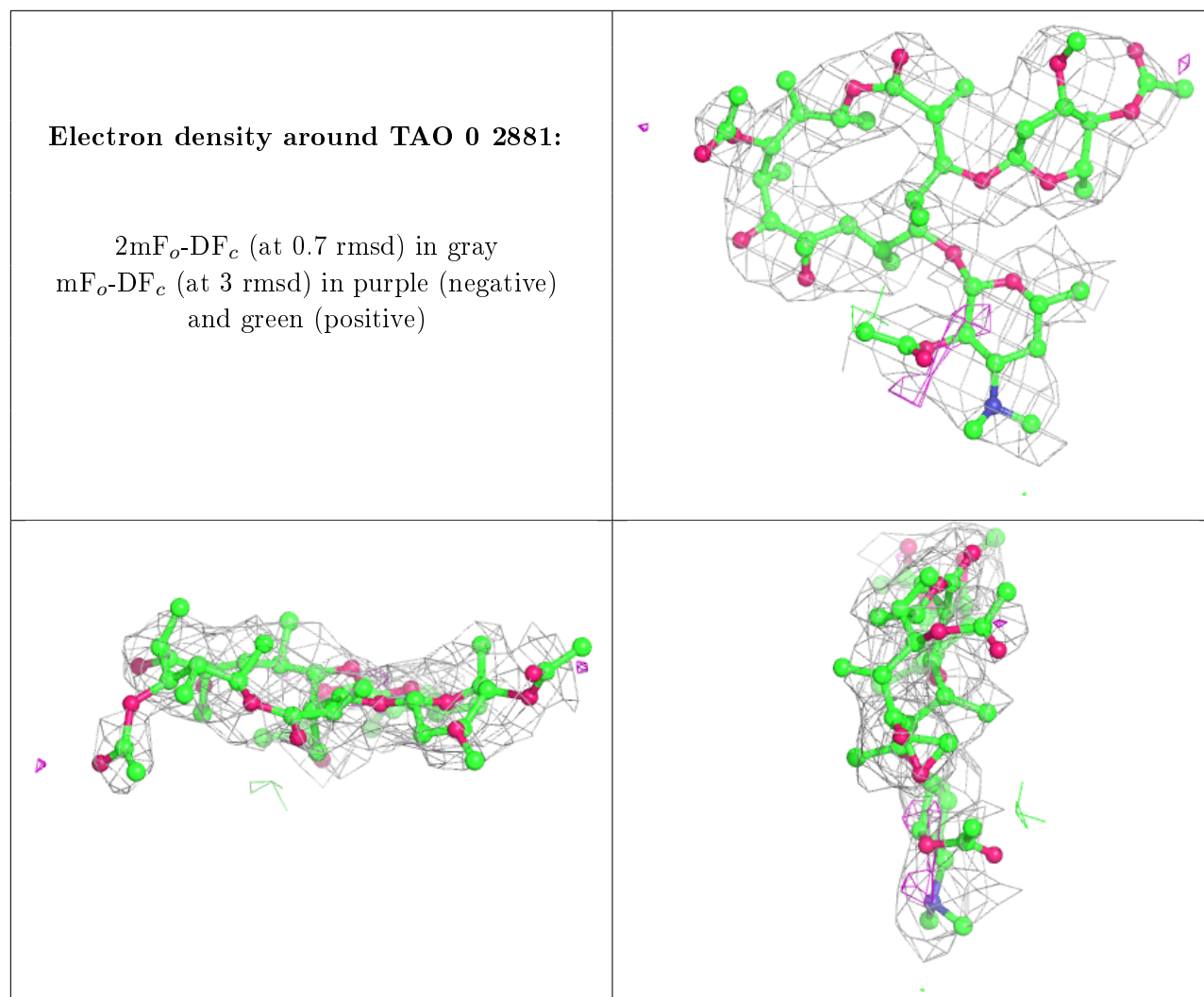
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.