



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:35 AM UTC

PDB ID : 1JZZ / pdb_00001jzz
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.

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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

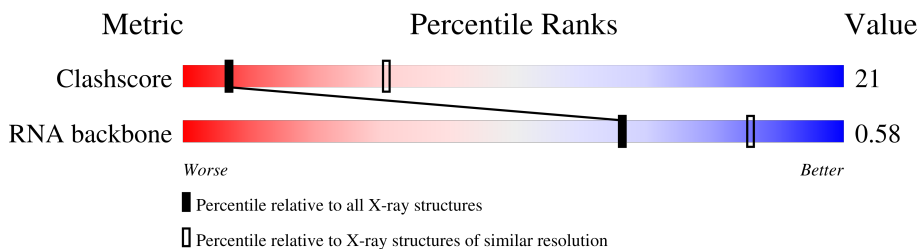
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

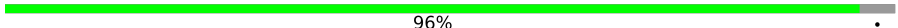
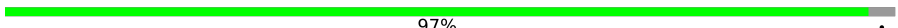
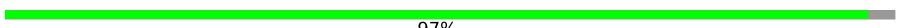
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1012 (3.94-3.66)
RNA backbone	3983	1007 (4.50-3.10)

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	 31% 48% 16% . .
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			

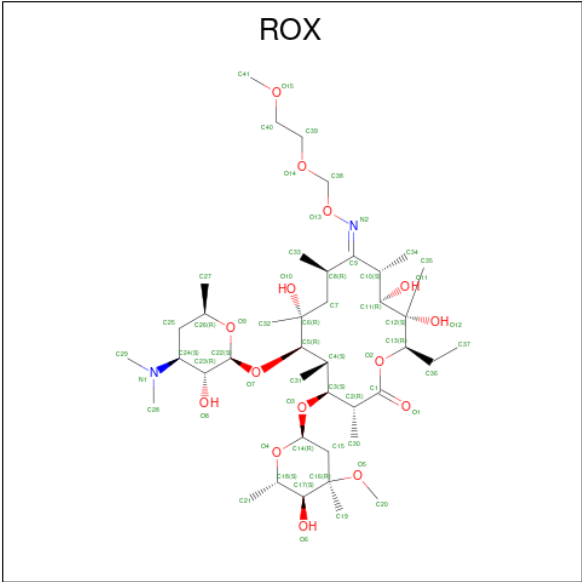
- Molecule 3 is a protein called Ribosomal Protein L22.

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

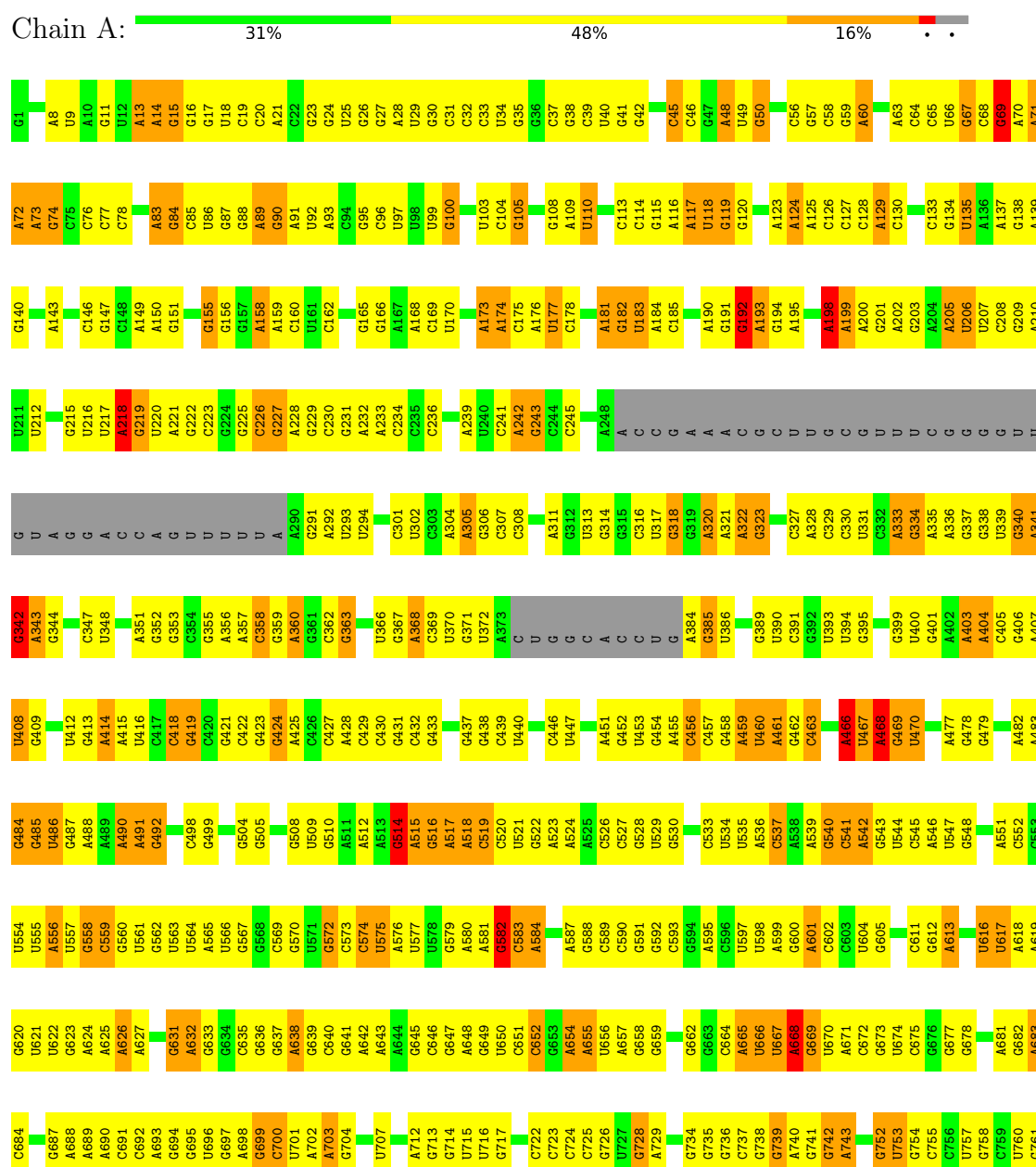
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

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

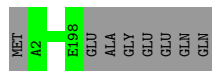


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A1751	A1682	C1540	C1404	G1337	G1286	G1189	U1112	U1045	A971	G831	A763
A1752	U1611	G1541	A1405	G1338	A1287	G1190	C1113	U1046	C972	A832	A764
A1753	G1542	G1543	U1409	G1339	U1288	G1191	U1047	U1047	C973	A833	C765
A1754	A1685	A1544	U1410	C1340	G1289	A1192	G1118	U1048	U974	A766	A767
C1614	A1686	U1544	C1411	G1341	C1271	U1194	C1120	C1049	C975	G767	U768
U1539	C1687	U1544	C1412	U1342	G1272	U1196	G1121	U1054	C976	U839	U768
C1540	U1618	U1548	C1415	C1343	G1273	U1197	A1122	U1055	U978	U840	U773
C1541	U1619	C1550	A1416	C1344	C1274	U1198	G1123	A1056	A979	G841	A774
U1539	U1551	A1486	C1417	C1345	A1275	U1199	G1124	U1056	G980	A842	U775
U1539	C1552	G1487	C1417	C1346	U1276	U1200	A1125	A1057	C981	G843	U776
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U1539	A1557	A1493	U1425	G1351	A1281	G1205	U1130	A1061	A994	U852	U786
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U1539	A1561	C1497	G1428	A1355	U1285	U1212	G1137	G1069	C998	A856	U790
U1539	G1562	G1498	A1429	G1356	U1286	U1213	A1138	G1070	A999	U857	G791
U1539	U1563	A1499	G1430	U1357	A1287	U1213	A1138	G1071	G1000	G858	U791
U1539	U1564	U1500	U1431	C1358	A1288	G1215	A1139	U1072	C927	U859	A794
U1539	U1564	U1500	U1431	G1359	A1289	G1216	A1140	U1072	C928	U860	A795
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U1539	G1572	G1503	U1434	U1365	A1291	U1217	G1142	C1074	A930	A797	U796
U1539	G1573	G1504	G1435	G1366	U1292	G1218	A1143	G1075	A931	G862	U797
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U1539	G1575	C1506	A1437	G1367	A1294	G1220	U1145	G1006	G933	C864	G799
U1539	G1576	G1507	G1438	G1368	U1295	G1221	G1146	A1080	G934	A865	U800
U1539	U1577	G1508	G1439	G1369	G1296	G1222	U1146	A1081	A1001	U866	A801
U1539	U1578	A1509	G1440	U1370	A1299	G1223	G1149	G1082	C937	G867	A802
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U1539	A1581	A1511	C1442	A1372	C1302	G1225	U1151	A1084	G1013	C804	C804
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U1539	G1584	C1514	A1445	U1375	U1307	A1227	A1154	C1087	U941	G872	A807
U1539	A1585	U1515	U1446	G1377	C1308	A1233	G1155	U1088	U942	U873	C808
U1539	U1586	U1515	U1447	U1377	C1309	A1234	U1156	C1089	U943	U874	C809
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U1539	C1590	U1521	U1452	G1382	G1312	G1241	A1162	U1092	G948	G877	G812
U1539	U1591	C1522	U1453	G1383	U1313	G1241	C1163	U1093	U1022	C878	A813
U1539	U1592	A1523	A1453	G1384	A1314	U1244	C1164	U1093	G949	A879	G814
U1539	C1593	C1524	C1456	C1385	A1315	G1245	G1165	A1096	G950	C880	A815
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U1539	A1595	U1526	A1458	G1387	A1321	G1250	A1167	A1099	A953	A856	A817
U1539	A1596	G1527	U1459	U1392	G1322	G1251	G1168	U1099	U954	G887	G818
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G2867	U2783	U2708	A2633	U2559	C2420	A2348	C2263	C2124	A2060	C1989	G1913	G1823
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G2869	G2794	U2719	U2644	C2567	U2428	U2358	C2271	G2132	U2070	U2000	A1921	G1831
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G2805	G2805	A2729	G2660	C2576	U2440	U2368	U2209	A	U2081	G2010	G1931	G1854
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G2815	G2815	C2740	G2670	U2586	A2450	G2378	U2229	A	C2091	U2092	G1947	C1877
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G2823	G2823	G2742	U2672	U2588	A2455	U2380	A2226	C2157	U2093	C2023	A1949	G1879
G2824	G2824	G2743	C2673	U2589	U2456	G2381	C2227	C2158	C2094	C2024	G1950	G1880
A2825	A2825	A2744	U2674	C2590	A2457	C2382	U2228	A2159	G2095	A2025	U1881	U1881
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G2827	G2827	A2766	U2676	C2592	C2459	U2384	G2229	C2161	A2097	G	A1883	A1883
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U2840	U2840	A2761	C2686	C2597	U2470	C2392	G2239	A2167	G2103	G2039	U1965	G1890
U2841	U2841	G2762	G2687	U2598	U2471	C2393	C2240	A2168	G2104	A2040	C1966	C1891
C2842	C2842	G2763	C2688	G2599	U2472	C2394	U2241	A2169	U2105	A2041	G1970	U1894
A2843	A2843	U2764	A2690	U2600	G2475	C2395	C2242	C2170	G	G2042	C1971	A1895
G2844	G2844	C2770	C2691	U2601	C2476	C2396	C2243	U2171	A2109	A2043	G1972	A1896
G2845	G2845	U2771	U2692	U2602	C2477	C2397	C2244	U2172	G	G2044	C1973	C1897
G2846	G2846	U2772	U2693	G2603	C2478	C2398	A2245	A2175	C	A2045	U1974	U1898
G2847	G2847	G2773	G2694	C2604	U2479	U2399	A2246	U2176	U	C2048	G1975	A1899
A2848	A2848	U2774	C2695	U2605	C2480	U2399	A2247	U2177	C	C2049	U1976	U1900
C2849	C2849	U	A2696	U2606	G2481	C2399	A2248	U2178	U	G2050	C1977	A1901
G	G	U	G2697	U2607	A2482	G2407	U2251	U2180	C	U2051	U1978	G
G	G	A	U2698	C2608	A2483	G2408	U2252	A2181	G	G2052	C1979	G1905
G2852	G2852	U2778	G2699	U2609	G2484	U2410	A2253	A2182	A2117	G2053	A1980	U1906
U2853	U2853	C2779	U2699	U2610	G2485	U2411	C2254	C2183	A2118	A2054	C1907	C1907
G2854	G2854	G2779	U2699	U2611	U2486	U2412	G2255	U2184	A2119	G2055	U1908	U1908
G2855	G2855	A2780	C2699	U2612	C2487	U2413	G2256	U2185	U2121	C2056	G1985	G1985
										U2057	G1986	A1910

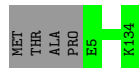
- Molecule 2: Ribosomal Protein L4

Chain K:  96% .



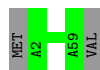
- Molecule 3: Ribosomal Protein L22

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: MG, ROX

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	0.27	0/66661	0.59	55/103976 (0.1%)

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	A	C2'-C3'-O3'	7.65	120.97	109.50
1	A	2608	A	C2'-C3'-O3'	7.33	120.50	109.50
1	A	1715	A	C2'-C3'-O3'	7.32	120.48	109.50
1	A	813	A	C2'-C3'-O3'	7.23	120.34	109.50
1	A	2693	U	C2'-C3'-O3'	7.06	120.08	109.50

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	1874	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	59977	0	30080	1892	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 1892 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

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Mol	Chain	Res	Type
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 oligosaccharides 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:

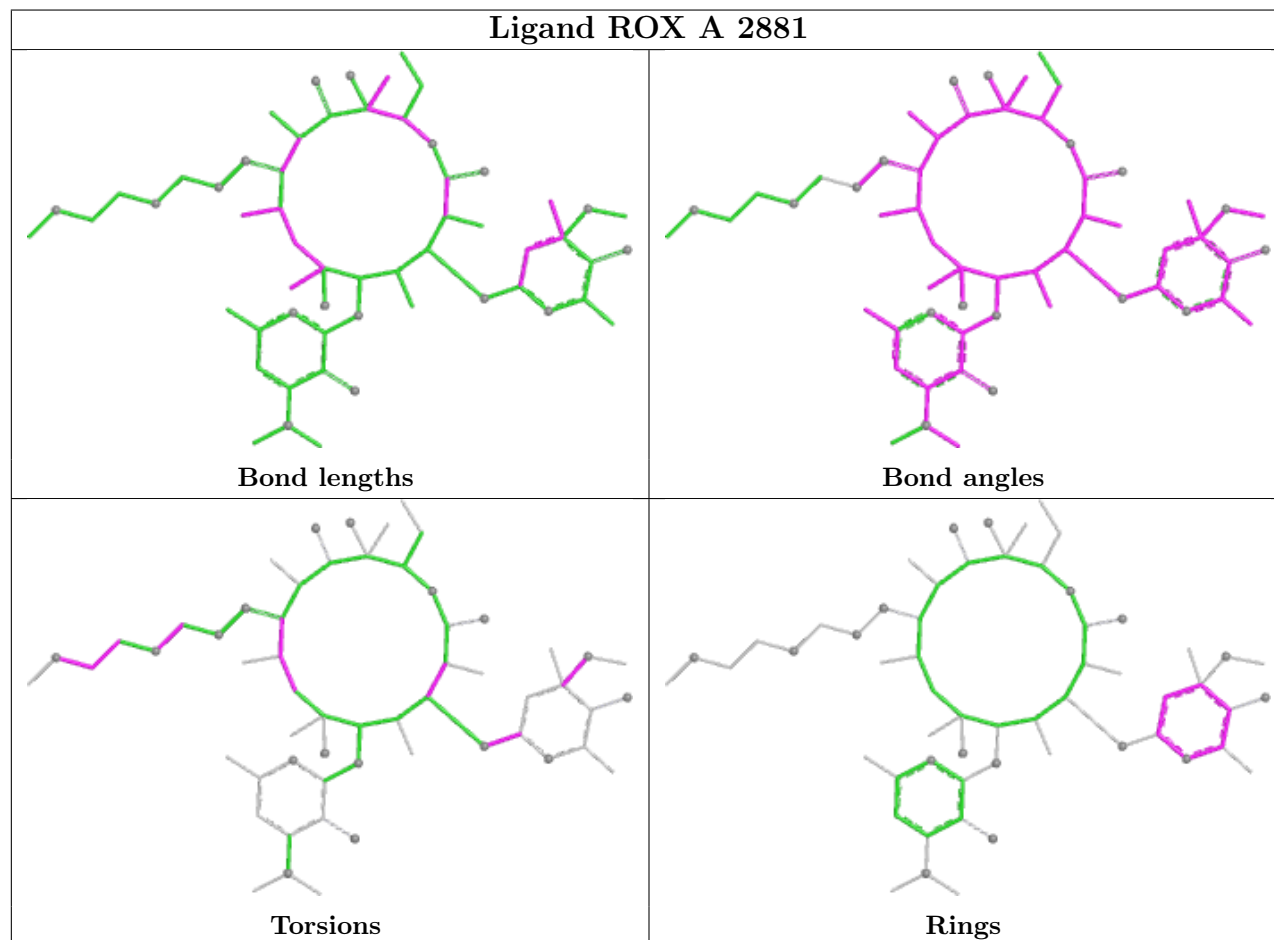
Mol	Chain	Res	Type	Atoms
5	A	2881	ROX	C14-C15-C16-C17-C18-O4

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.