wwPDB X-ray Structure Validation Summary Report (i)

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

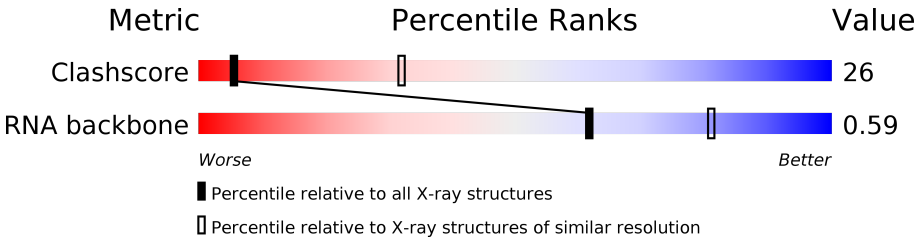
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	2	2880	24% 56% 16% .

2 Entry composition

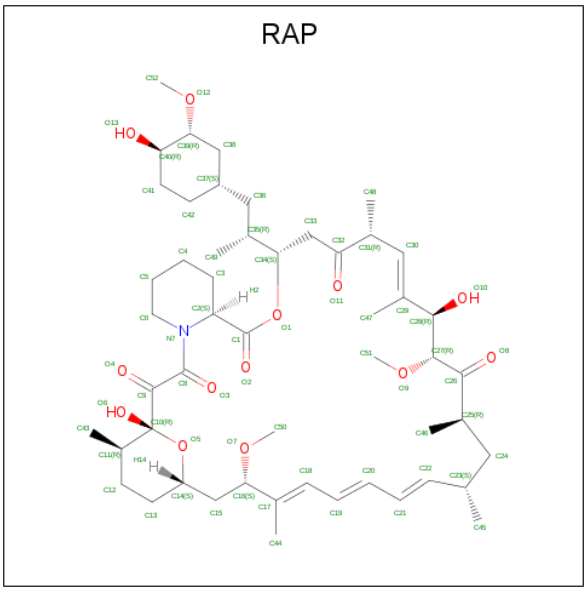
There are 2 unique types of molecules in this entry. The entry contains 59424 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_{51}H_{79}NO_{13}$).



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

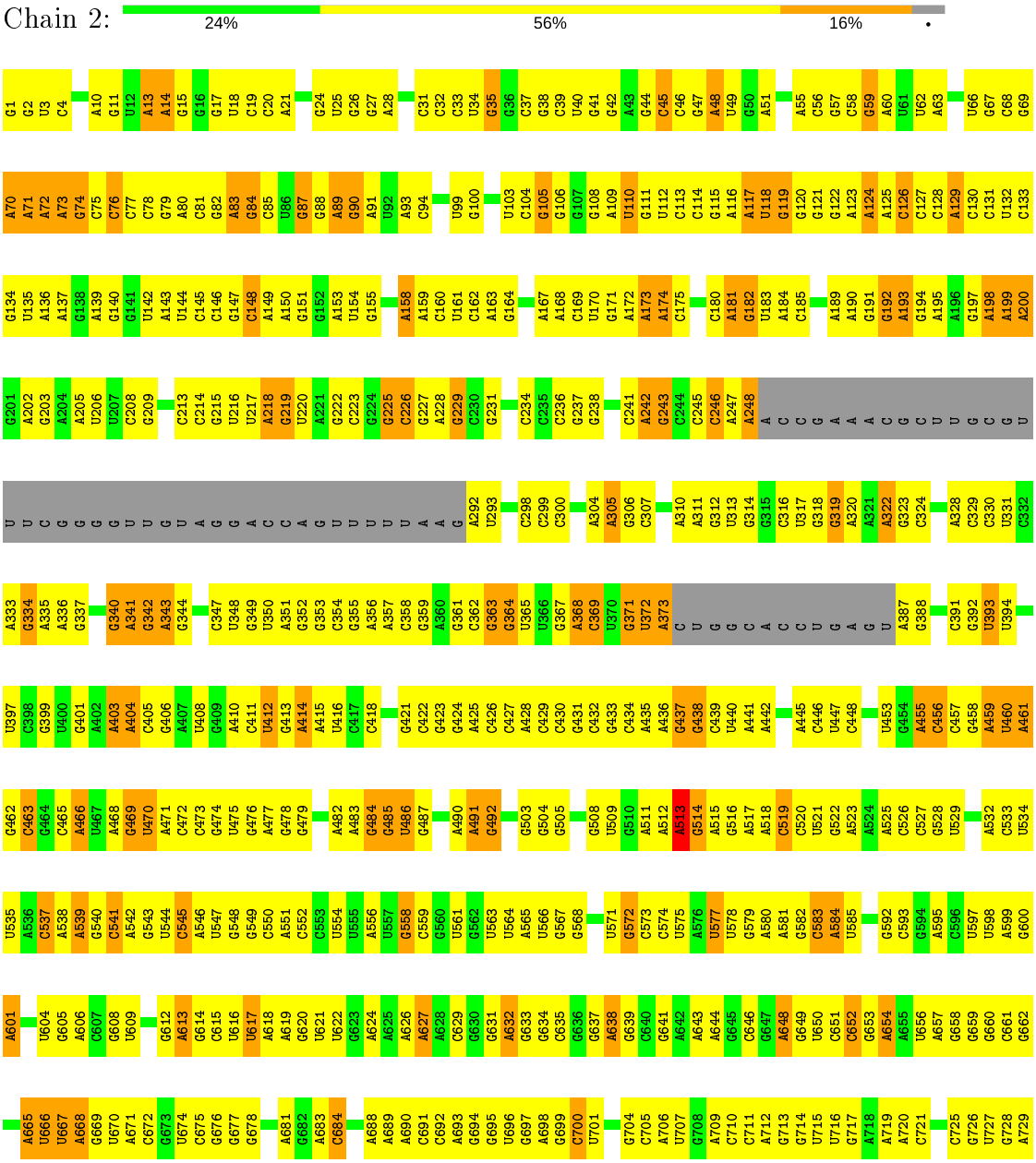
3 Residue-property plots (i)

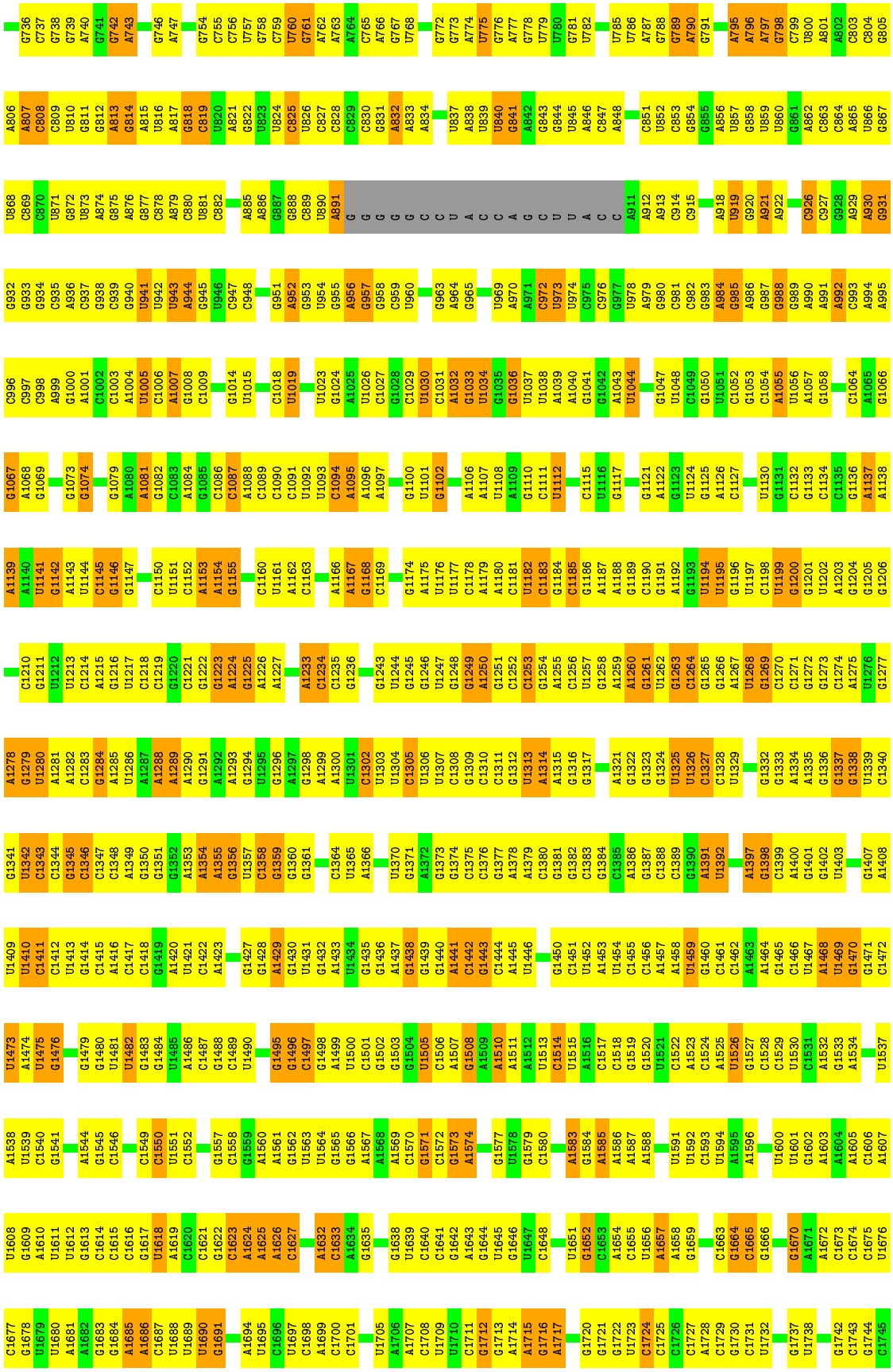
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

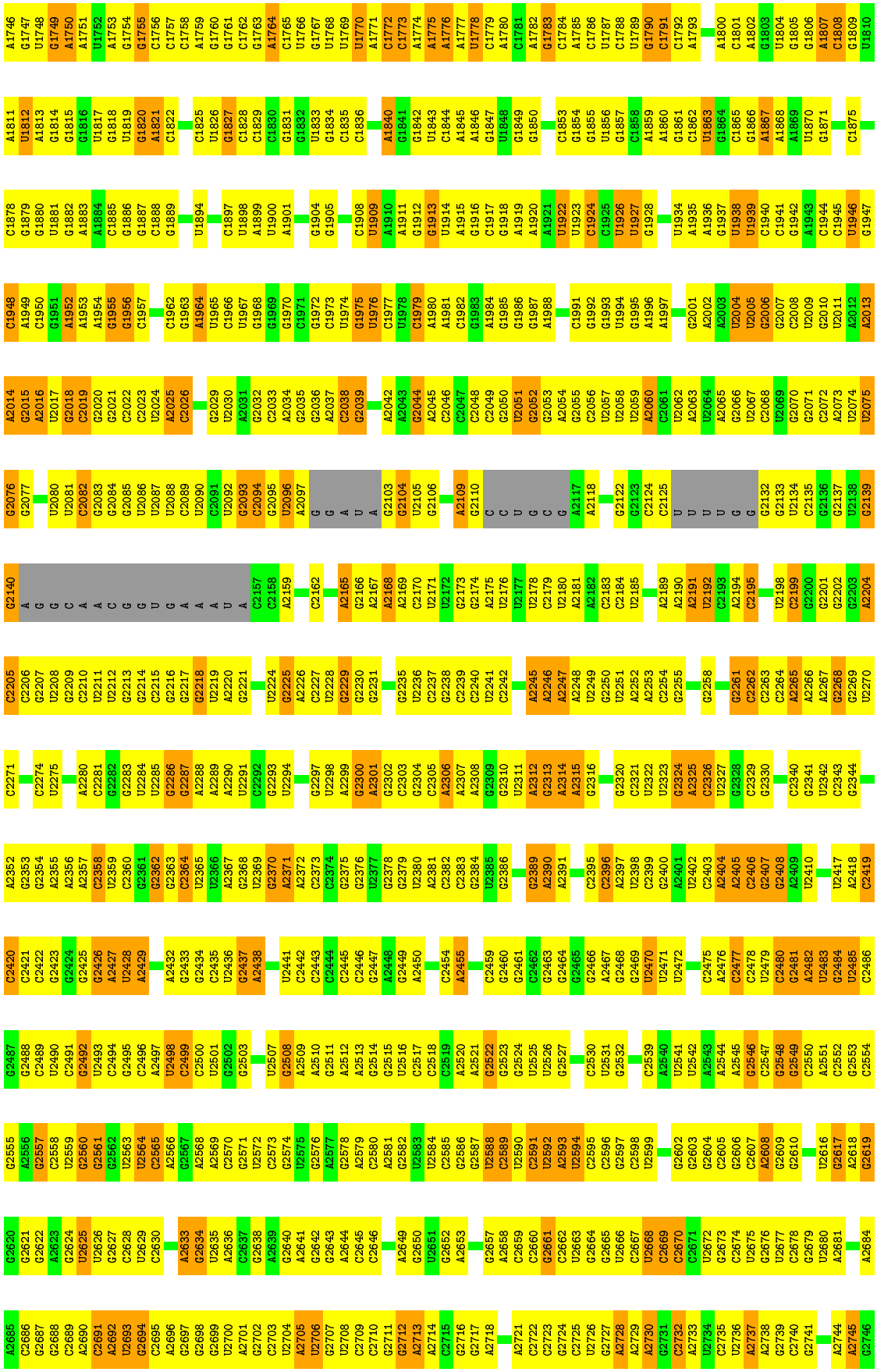
Note EDS was not executed.

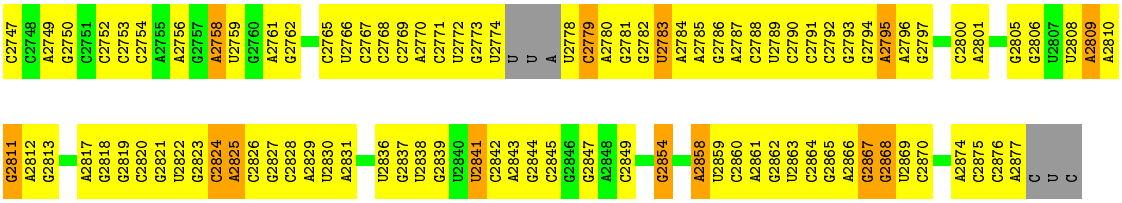
- Molecule 1: 23S RIBOSOMAL RNA

Chain 2:








C2747 G2748 A2749 G2750 G2751 C2752 C2753 C2754 A2755 A2756 G2757 A2758 U2759 G2760 A2761 G2762
C2765 U2766 C2767 C2768 C2769 A2770 C2771 U2772 G2773 U2774 U U A U2778 C2779 A2780 G2781 G2782 U2783 A2784 A2785 G2786 A2787 C2788 U2789 C2790 C2791 C2792 G2793 G2794 A2795 A2796 G2797
C2800 A2801
G2805 G2806 U2807 U2808 A2809 A2810
G2811 A2812 G2813
A2817 G2818 G2819 C2820 G2821 U2822 G2823 C2824 A2825 C2826 G2827 C2828 A2829 U2830 A2831
U2836 G2837 U2838 G2839 U2840 U2841 C2842 A2843 G2844 C2845 G2846 G2847 A2848 C2849
G2854
A2858 U2859 C2860 A2861 G2862 U2863 C2864 G2865 A2866 G2867 G2868 U2869 C2870
A2874 C2875 C2876 A2877 C U C

4 Data and refinement statistics (i)

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	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.	Xtriage
Total number of atoms	59424	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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

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(^{o})	Ideal(^{o})
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

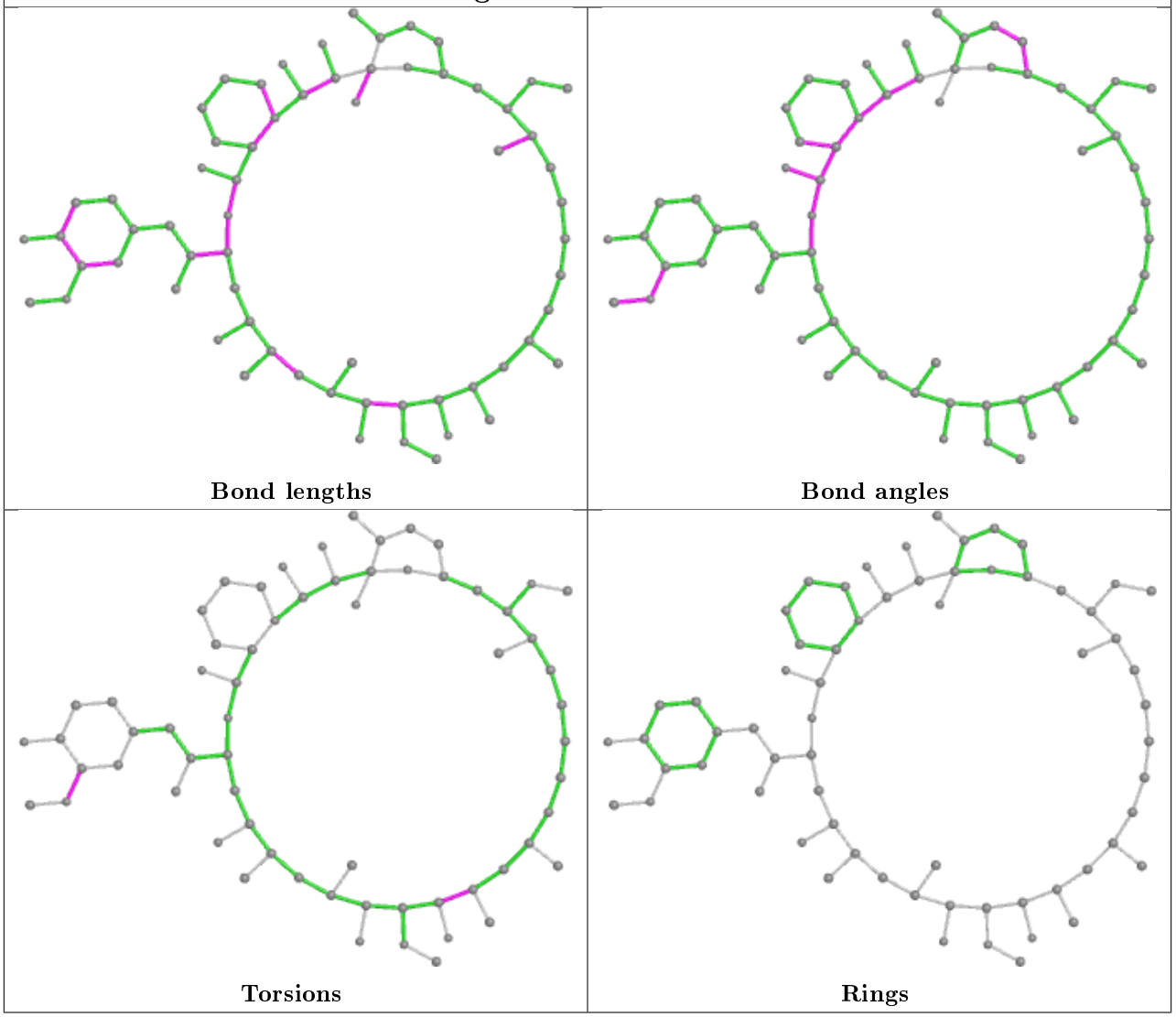
There are no ring outliers.

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 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.

Ligand RAP 2 2881



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.