wwPDB EM Validation Summary Report (i)

Dec 17, 2023 – 08:22 PM EST

PDB ID	:	1C2W
Title	:	23S RRNA STRUCTURE FITTED TO A CRYO-ELECTRON MICROSCOPIC MAP AT 7.5 ANGSTROMS RESOLUTION
Authors	:	Brimacombe, R.; Mueller, F.
Deposited on	:	1999-07-28
Resolution	:	7.50 Å(reported)
Based on initial models	:	1CSX, 1CSV

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

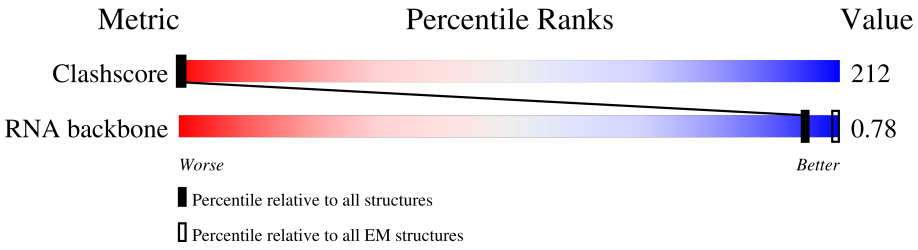
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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)	EM structures (#Entries)
Clashscore	158937	4297
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	B	2904	. 32% 17% 46%

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
1	5MU	B	1915	-	-	X	-
1	5MU	B	1939	X	-	X	-
1	7MG	B	2069	-	-	X	-
1	5MU	B	2449	X	-	X	-
1	5MC	B	2498	X	-	X	-
1	7MG	B	745	-	-	X	-
1	PSU	B	746	-	-	X	-
1	5MU	B	747	-	-	X	-

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 62371 atoms, of which 23 are hydrogens and 0 are deuteriums.

In the tables below, 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.

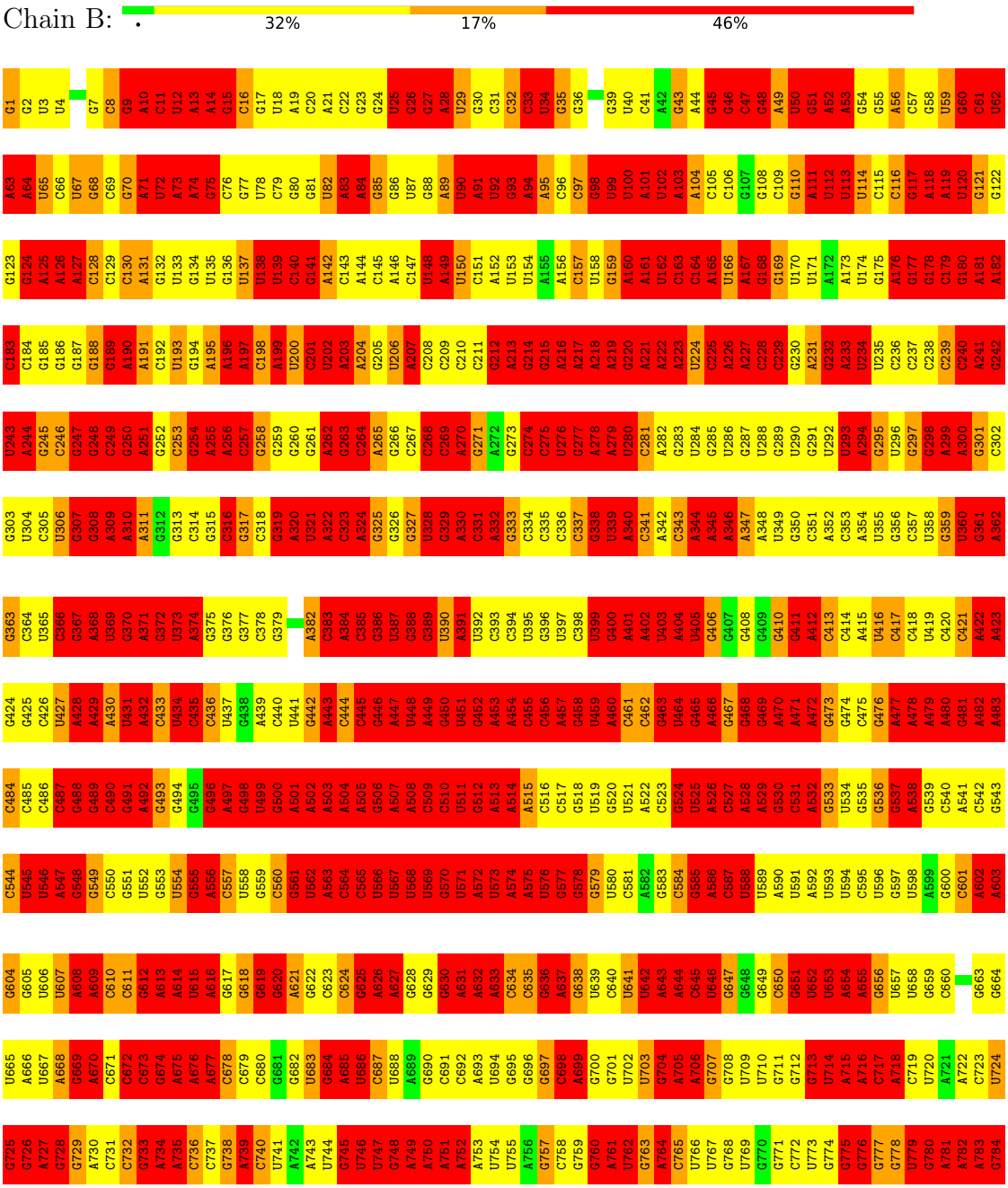
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	B	2904	62371	27819	23	11467	20158	2904	0	0

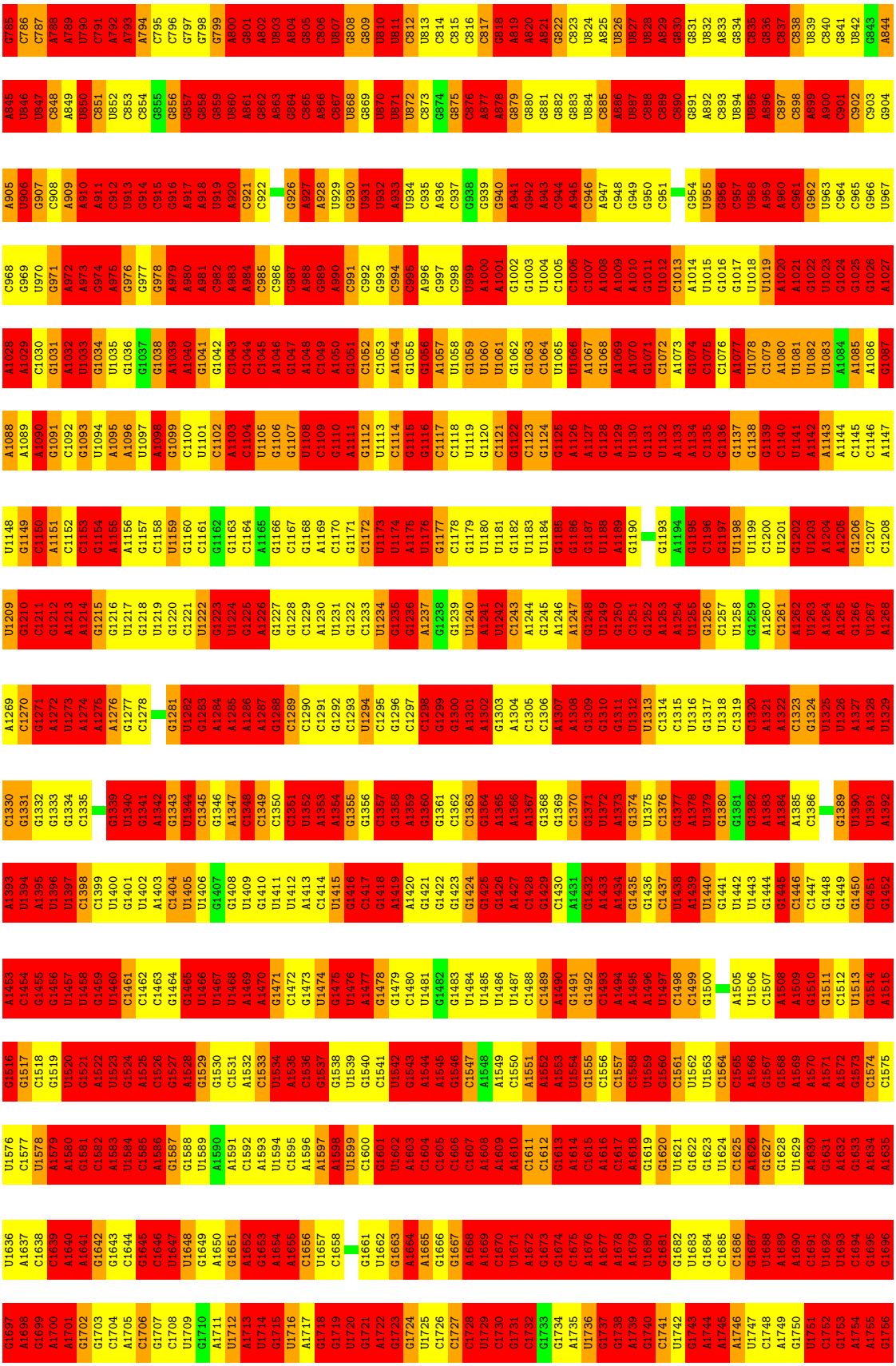
3 Residue-property plots (i)

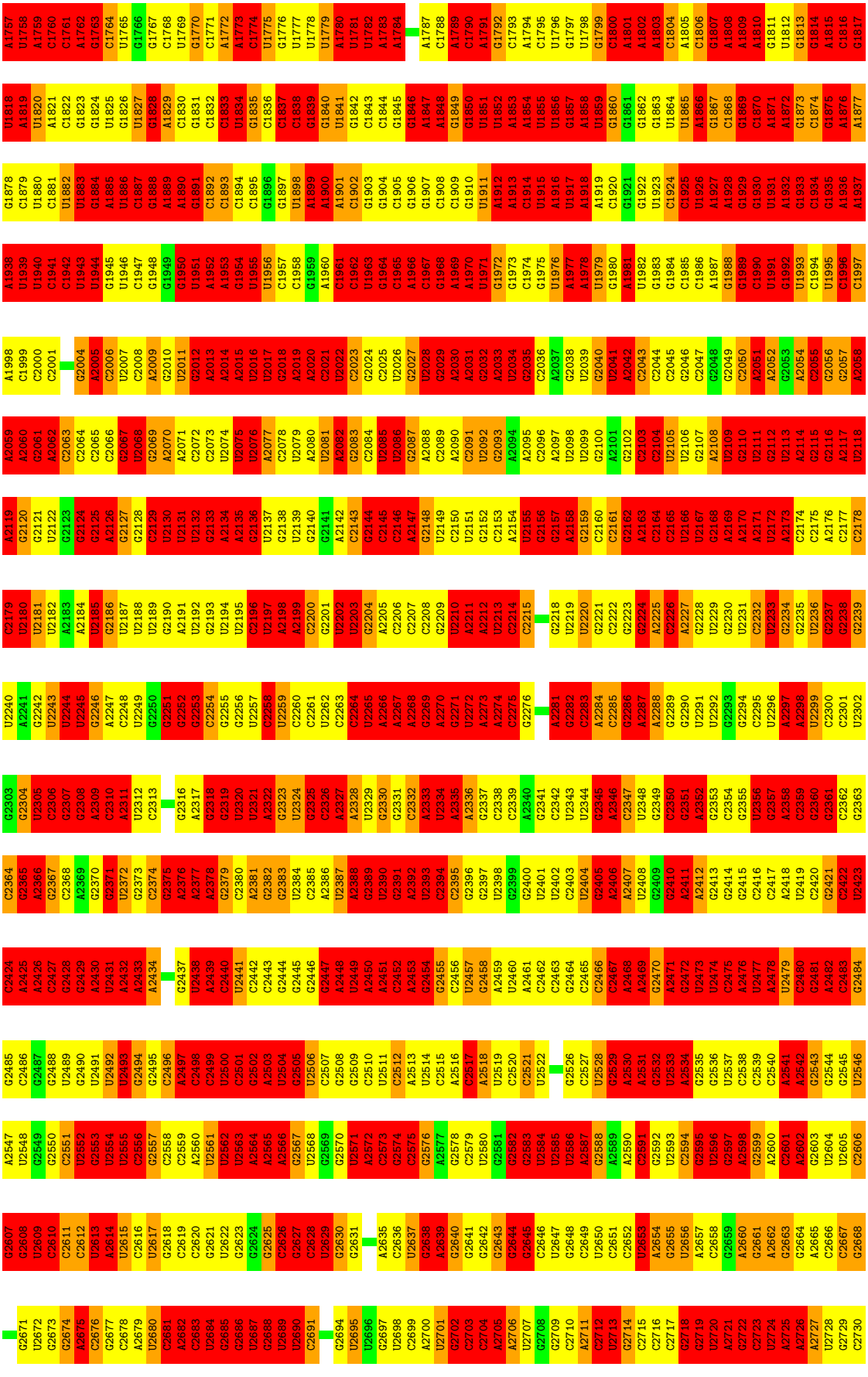
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

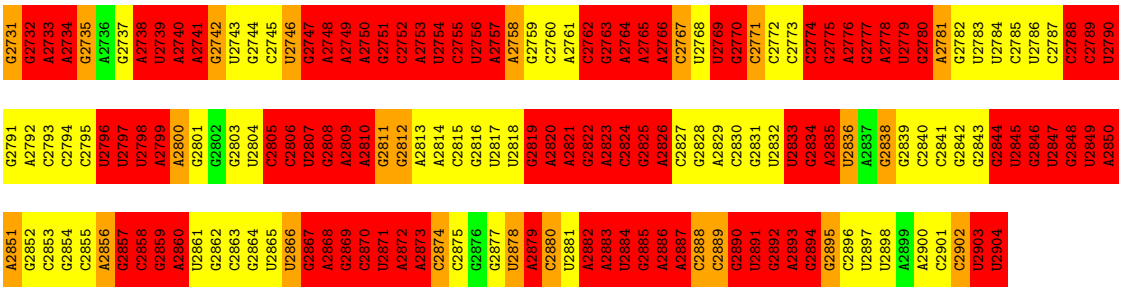
- Molecule 1: 23S RIBOSOMAL RNA

Chain B:








G2731 G2732 A2733 A2734 G2735 A2736 G2737 A2738 U2739 A2740 A2741 G2742 U2743 G2744 C2745 U2746 G2747 A2748 A2749 A2750 G2751 C2752 A2753 U2754 C2755 U2756 A2757 A2758 G2759 C2760 A2761 C2762 G2763 A2764 A2765 A2766 C2767 U2768 U2769 G2770 C2771 C2772 C2773 C2774 G2775 A2776 G2777 A2778 U2779 G2780 A2781 G2782 U2783 U2784 C2785 U2786 C2787 C2788 C2789 U2790
G2791 A2792 C2793 C2794 C2795 U2796 U2797 U2798 A2799 A2800 G2801 G2802 G2803 U2804 C2805 C2806 U2807 G2808 A2809 A2810 G2811 G2812 A2813 A2814 C2815 G2816 U2817 U2818 G2819 A2820 A2821 G2822 A2823 C2824 G2825 A2826 C2827 G2828 A2829 C2830 G2831 U2832 U2833 G2834 A2835 U2836 A2837 G2838 G2839 C2840 C2841 G2842 G2843 G2844 U2845 G2846 U2847 G2848 U2849 A2850
A2851 G2852 C2853 G2854 C2855 A2856 G2857 C2858 G2859 A2860 U2861 G2862 C2863 G2864 U2865 U2866 G2867 A2868 G2869 C2870 U2871 A2872 A2873 C2874 C2875 G2876 G2877 U2878 A2879 C2880 U2881 A2882 A2883 U2884 G2885 A2886 A2887 C2888 C2889 G2890 U2891 G2892 A2893 G2894 G2895 C2896 U2897 U2898 A2899 A2900 C2901 C2902 U2903 U2904

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 7.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-7.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	ERNA-3D	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	62371	wwPDB-VP
Average B, all atoms (Å^2)	0.0	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: 5MC, PSU, 7MG, 5MU, 1MA

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	B	5.79	6577/69489 (9.5%)	3.05	5861/108346 (5.4%)

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	B	466	117

The worst 5 of 6577 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	U	P-O5'	65.66	2.25	1.59
1	B	2848	G	C1'-N9	60.36	2.39	1.48
1	B	75	G	P-O5'	53.62	2.13	1.59
1	B	2322	A	P-O5'	53.13	2.12	1.59
1	B	429	A	C3'-O3'	52.73	2.15	1.42

The worst 5 of 5861 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	120	U	O5'-P-OP2	-42.40	59.83	110.70
1	B	1103	A	O5'-P-OP2	-38.71	64.25	110.70
1	B	239	C	P-O3'-C3'	-37.22	75.03	119.70
1	B	913	U	P-O5'-C5'	35.58	177.83	120.90
1	B	2849	U	P-O5'-C5'	35.58	177.83	120.90

5 of 466 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	10	A	C4’
1	B	12	U	C4’
1	B	15	G	C4’
1	B	27	G	C3’,C4’
1	B	28	A	C4’

5 of 117 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	10	A	Sidechain
1	B	14	A	Sidechain
1	B	52	A	Sidechain
1	B	53	A	Sidechain
1	B	64	A	Sidechain

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	B	62348	23	31477	19819	0
All	All	62348	23	31477	19819	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 212.

The worst 5 of 19819 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:B:69:C:H4’	1:B:85:G:C4’	1.23	1.68
1:B:318:C:H5’	1:B:319:G:C8	1.24	1.68
1:B:1853:A:C5’	1:B:1853:A:H4’	1.23	1.68
1:B:1627:G:H1’	1:B:1641:A:C8	1.27	1.67
1:B:901:C:H5’	1:B:902:C:C5	1.19	1.66

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein molecules in this entry.

5.3.2 Protein sidechains

There are no protein molecules in this entry.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	2880/2904 (99%)	1502 (52%)	1148 (39%)

5 of 1502 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	9	G
1	B	10	A
1	B	11	C
1	B	12	U
1	B	13	A

5 of 1148 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	2326	C
1	B	2894	G
1	B	2394	C
1	B	2325	G
1	B	2639	A

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

13 non-standard protein/DNA/RNA residues are 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	$\#\|Z\|>2$
1	5MC	B	2498	1	18,22,23	3.29	4 (22%)	26,32,35	2.68	7 (26%)
1	5MU	B	747	1	19,22,23	0.65	1 (5%)	28,32,35	1.14	4 (14%)
1	1MA	B	2030	1	16,25,26	1.97	6 (37%)	18,37,40	1.65	5 (27%)
1	PSU	B	1917	1	18,21,22	0.68	0	22,30,33	0.81	0
1	7MG	B	2251	1	22,26,27	7.73	5 (22%)	29,39,42	1.76	3 (10%)
1	7MG	B	745	1	22,26,27	7.53	6 (27%)	29,39,42	2.49	5 (17%)
1	PSU	B	1911	1	18,21,22	0.59	0	22,30,33	0.75	0
1	1MA	B	1618	1	16,25,26	2.09	6 (37%)	18,37,40	1.56	5 (27%)
1	5MU	B	1915	1	19,22,23	0.45	0	28,32,35	1.40	3 (10%)
1	PSU	B	746	1	18,21,22	0.89	0	22,30,33	1.37	2 (9%)
1	5MU	B	2449	1	19,22,23	2.53	3 (15%)	28,32,35	2.21	5 (17%)
1	5MU	B	1939	1	19,22,23	0.99	2 (10%)	28,32,35	1.77	5 (17%)
1	7MG	B	2069	1	22,26,27	3.17	2 (9%)	29,39,42	1.67	2 (6%)

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
1	5MC	B	2498	1	1/1/5/5	2/7/25/26	0/2/2/2
1	5MU	B	747	1	-	2/7/25/26	0/2/2/2
1	1MA	B	2030	1	-	3/3/25/26	0/3/3/3
1	PSU	B	1917	1	-	1/7/25/26	0/2/2/2
1	7MG	B	2251	1	-	2/7/37/38	0/3/3/3
1	7MG	B	745	1	-	2/7/37/38	0/3/3/3
1	PSU	B	1911	1	-	0/7/25/26	0/2/2/2
1	1MA	B	1618	1	-	2/3/25/26	0/3/3/3
1	5MU	B	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	B	746	1	-	1/7/25/26	0/2/2/2
1	5MU	B	2449	1	1/1/5/5	6/7/25/26	0/2/2/2
1	5MU	B	1939	1	2/2/5/5	2/7/25/26	0/2/2/2
1	7MG	B	2069	1	-	0/7/37/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2251	7MG	C1'-N9	32.23	2.06	1.46
1	B	745	7MG	C1'-N9	31.10	2.04	1.46
1	B	2251	7MG	C8-N9	-14.54	1.37	1.46
1	B	2069	7MG	C8-N9	-14.06	1.38	1.46
1	B	745	7MG	C8-N9	-13.55	1.38	1.46

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2449	5MU	O4'-C4'-C5'	-8.06	82.84	109.37
1	B	2498	5MC	C1'-N1-C6	7.80	134.11	121.12
1	B	2069	7MG	N9-C8-N7	7.43	114.01	103.38
1	B	745	7MG	N9-C8-N7	7.35	113.90	103.38
1	B	2251	7MG	N9-C8-N7	7.34	113.88	103.38

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	1939	5MU	C3'
1	B	1939	5MU	C4'
1	B	2449	5MU	C4'
1	B	2498	5MC	C4'

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1939	5MU	C3'-C4'-C5'-O5'
1	B	2030	1MA	O4'-C4'-C5'-O5'
1	B	2030	1MA	C3'-C4'-C5'-O5'
1	B	2449	5MU	C3'-C4'-C5'-O5'
1	B	2449	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 161 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	2498	5MC	18	0
1	B	747	5MU	26	0
1	B	2030	1MA	4	0
1	B	1917	PSU	6	0
1	B	2251	7MG	1	0
1	B	745	7MG	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1911	PSU	1	0
1	B	1618	1MA	1	0
1	B	1915	5MU	10	0
1	B	746	PSU	22	0
1	B	2449	5MU	14	0
1	B	1939	5MU	41	0
1	B	2069	7MG	14	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1566

The worst 5 of 1566 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	75:G	O3'	76:C	P	2.66
1	B	2023:C	O3'	2024:G	P	2.65
1	B	87:U	O3'	88:G	P	2.57
1	B	1004:U	O3'	1005:C	P	2.55
1	B	2652:C	O3'	2653:U	P	2.55