



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7UCR
Title : Joint X-ray/neutron structure of the Sarcin-Ricin loop RNA
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Deposited on : 2022-03-17
Resolution : 1.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.29

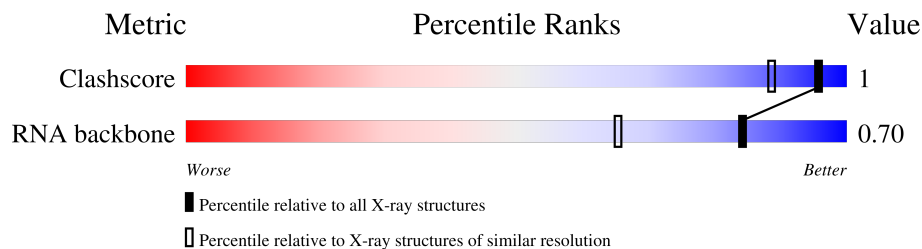
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 1.00 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	1117 (1.06-0.94)
RNA backbone	3102	1000 (2.34-0.62)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	27	 67% 30%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1278 atoms, of which 304 are hydrogens and 265 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 Sarcin-Ricin loop RNA.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	P			
1	A	27	1033	280	105	304	116	200	28	34	27	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	D	O		
3	A	80	240	160	80	0	0

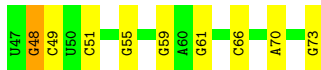
3 Residue-property plots [i](#)

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.

Note EDS failed to run properly.

- Molecule 1: Sarcin-Ricin loop RNA

Chain A:  67% 30%



4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	29.50Å 29.50Å 76.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.05 – 1.00	Depositor
% Data completeness (in resolution range)	99.4 (16.05-1.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.00Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.178 , 0.197	Depositor
Wilson B-factor (Å ²)	8.4	Xtrriage
Anisotropy	0.063	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.072 for h,-k,-l	Xtrriage
Total number of atoms	1278	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.71% 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: SO4, DOD

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	1.33	2/1340 (0.1%)	1.66	32/2088 (1.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61[A]	G	P-OP1	7.92	1.62	1.49
1	A	61[B]	G	P-OP1	7.92	1.62	1.49

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61[A]	G	O5'-P-OP2	-14.03	93.08	105.70
1	A	61[B]	G	O5'-P-OP2	-14.03	93.08	105.70
1	A	73[A]	G	N3-C4-C5	7.74	132.47	128.60
1	A	73[B]	G	N3-C4-C5	7.74	132.47	128.60
1	A	48[A]	G	N3-C4-N9	-6.94	121.83	126.00
1	A	48[B]	G	N3-C4-N9	-6.94	121.83	126.00
1	A	59[A]	G	N9-C1'-C2'	-6.05	105.34	112.00
1	A	59[B]	G	N9-C1'-C2'	-6.05	105.34	112.00
1	A	73[A]	G	C4-C5-N7	5.99	113.19	110.80
1	A	73[B]	G	C4-C5-N7	5.99	113.19	110.80
1	A	70[A]	A	C5-C6-N1	5.74	120.57	117.70
1	A	70[B]	A	C5-C6-N1	5.74	120.57	117.70
1	A	70[A]	A	C2-N3-C4	5.70	113.45	110.60
1	A	70[B]	A	C2-N3-C4	5.70	113.45	110.60
1	A	73[A]	G	N9-C4-C5	-5.62	103.15	105.40
1	A	73[B]	G	N9-C4-C5	-5.62	103.15	105.40
1	A	55[A]	G	C5'-C4'-C3'	-5.59	107.06	116.00
1	A	55[B]	G	C5'-C4'-C3'	-5.59	107.06	116.00
1	A	73[A]	G	C8-N9-C4	5.43	108.57	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73[B]	G	C8-N9-C4	5.43	108.57	106.40
1	A	55[A]	G	O5'-P-OP1	5.42	117.20	110.70
1	A	55[B]	G	O5'-P-OP1	5.42	117.20	110.70
1	A	51[A]	C	C2-N3-C4	5.42	122.61	119.90
1	A	51[B]	C	C2-N3-C4	5.42	122.61	119.90
1	A	48[A]	G	C5-C6-O6	5.31	131.79	128.60
1	A	48[B]	G	C5-C6-O6	5.31	131.79	128.60
1	A	55[A]	G	O5'-P-OP2	-5.25	100.98	105.70
1	A	55[B]	G	O5'-P-OP2	-5.25	100.98	105.70
1	A	48[A]	G	C8-N9-C4	-5.09	104.36	106.40
1	A	48[B]	G	C8-N9-C4	-5.09	104.36	106.40
1	A	73[A]	G	C4-C5-C6	-5.01	115.79	118.80
1	A	73[B]	G	C4-C5-C6	-5.01	115.79	118.80

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	729	304	52	1	1
2	A	5	0	0	0	1
3	A	240	0	0	0	1
All	All	974	304	52	1	2

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 1.

All (1) 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:48[A]:G:H2'	1:A:49[A]:C:O4'	1.85	0.72

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:211:DOD:D1	3:A:226:DOD:D1[1_655]	1.32	0.88
1:A:66[A]:C:H42	2:A:101:SO4:O3[1_455]	1.57	0.03

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	A	0/27	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 monosaccharides 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	SO4	A	101	-	4,4,4	0.19	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	SO4	0	1

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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.