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PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2014 – 07:18 PM GMT

PDB ID : 2JLT
Title : CRYSTAL STRUCTURE OF AN RNA KISSING COMPLEX
Authors : Diprimo, C.; Fribourg, S.
Deposited on : 2008-09-15
Resolution : 2.90 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Rfree		0.229
Clashscore		0
RSRZ outliers		0
RNA backbone		0.55

Worse   Better

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
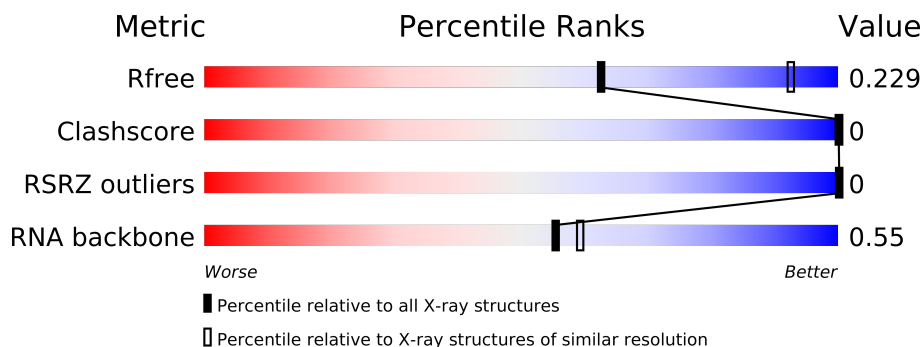
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	18	
2	B	16	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 725 atoms, of which 0 are hydrogen and 0 are deuterium.

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 R06.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	18	Total	Br	C	N	O	P	0	0	0
			382	1	171	70	123	17			

- Molecule 2 is a RNA chain called TAR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	16	Total	Br	C	N	O	P	0	0	0
			343	1	153	64	110	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: R06

Chain A:
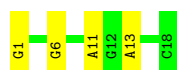
• Molecule 2: TAR

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	85.00Å 85.00Å 85.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.08 – 2.90 23.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (60.08-2.90) 99.9 (23.57-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.187 , 0.227 0.186 , 0.229	Depositor DCC
R_{free} test set	216 reflections (4.79%)	DCC
Wilson B-factor (Å^2)	73.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 5.4	EDS
Estimated twinning fraction	0.107 for l,-k,h	Xtriage
L-test for twinning	$< |L| > = 0.45, < L^2 > = 0.29$	Xtriage
Outliers	0 of 4726 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	725	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5BU

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	0.81	0/403	1.36	2/627 (0.3%)
2	B	0.75	0/360	1.24	0/561
All	All	0.78	0/763	1.31	2/1188 (0.2%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	11	A	O4'-C1'-N9	5.97	112.98	108.20
1	A	1	G	C5-C6-N1	5.47	114.24	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	382	0	197	0	0
2	B	343	0	175	0	0
All	All	725	0	372	0	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3　Torsion angles

5.3.1　Protein backbone ⓘ

There are no protein chains in this entry.

5.3.2　Protein sidechains ⓘ

There are no protein chains in this entry.

5.3.3　RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	17/18 (94%)	2 (11%)	0
2	B	15/16 (93%)	1 (6%)	0
All	All	32/34 (94%)	3 (9%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	13	A
2	B	6	C

There are no RNA pucker outliers to report.

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

2 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	5BU	A	3	1	20,22,23	1.25	2 (10%)	25,32,35	1.98	4 (16%)
2	5BU	B	14	2	20,22,23	1.01	1 (5%)	25,32,35	1.33	2 (8%)

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	5BU	A	3	1	-	0/6/25/26	0/2/2/2
2	5BU	B	14	2	-	0/6/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	5BU	C2-N1	2.41	1.41	1.38
1	A	3	5BU	O4'-C1'	2.10	1.44	1.41
2	B	14	5BU	C2-N1	2.07	1.40	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	5BU	C6-N1-C2	-7.31	120.33	122.41
1	A	3	5BU	C2-N1-C1'	4.73	121.17	118.21
2	B	14	5BU	C6-N1-C2	-3.76	121.34	122.41
2	B	14	5BU	C2-N1-C1'	3.58	120.45	118.21
1	A	3	5BU	C5-C6-N1	2.39	121.25	119.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5   Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6   Ligand geometry ⓘ

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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	18/18 (100%)	0.32	0	100	100	15, 27, 30, 31	0
2	B	16/16 (100%)	0.47	0	100	100	16, 26, 35, 36	0
All	All	34/34 (100%)	0.39	0	100	100	15, 27, 31, 36	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	5BU	A	3	21/22	0.16	-0.75	22,28,29,31	1
2	5BU	B	14	21/22	0.14	-1.22	26,29,32,35	1

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

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6.5 Other polymers (i)

There are no such residues in this entry.