wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 12:43 AM EDT

PDB ID	:	1JBR
Title	:	Crystal Structure of the Ribotoxin Restrictocin and a 31-mer SRD RNA Inhibitor
Authors	:	Yang, X.; Gerczei, T.; Glover, L.; Correll, C.C.
Deposited on	:	2001-06-06
Resolution	:	2.15 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

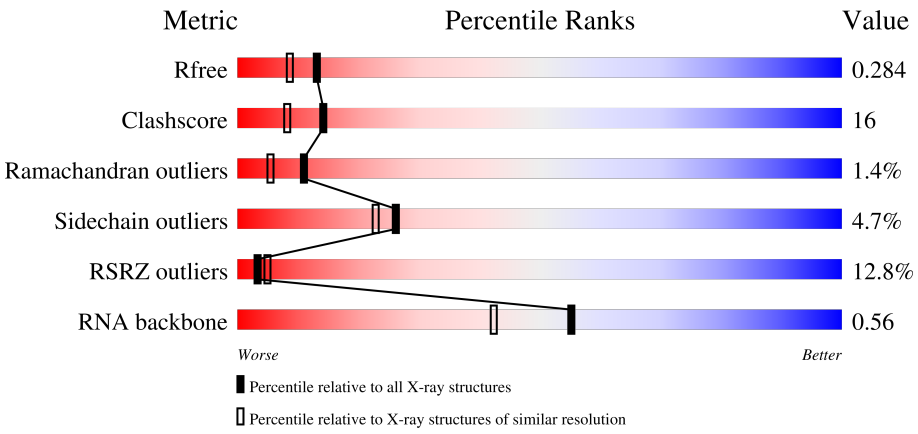
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.15 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))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)
RNA backbone	3102	1060 (2.60-1.72)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	18	61% 22% 11% 6%
2	F	13	46% 46% 8%
3	D	31	3% 65% 29% • •
4	A	149	12% 81% 18% •

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Mol	Chain	Length	Quality of chain
4	B	149	18% 60% 35% 5%

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	A23	C	17	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3883 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 5'-R(*GP*CP*GP*CP*UP*CP*CP*UP*CP*AP*GP*UP*AP*CP*GP*AP*GP*(A23))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	18	383	171	69	125	18	0	0	0

- Molecule 2 is a RNA chain called 5'-R(*GP*GP*AP*AP*CP*CP*GP*GP*AP*GP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	13	281	126	57	86	12	0	0	0

- Molecule 3 is a RNA chain called 31-mer SRD RNA analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	31	664	297	126	211	30	0	0	0

- Molecule 4 is a protein called Restrictocin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	149	1191	748	217	221	5	0	0	0
4	B	149	1191	748	217	221	5	0	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
5	C	1	1	1	0	0
5	F	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
5	D	3	3	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	C	20	20	20	0	0
			Total	O		
6	F	21	21	21	0	0
			Total	O		
6	D	39	39	39	0	0
			Total	O		
6	A	54	54	54	0	0
			Total	O		
6	B	34	34	34	0	0

3 Residue-property plots (i)

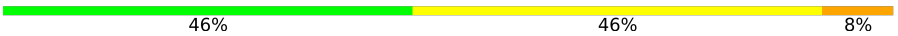
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

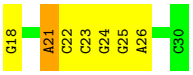
• Molecule 1: 5'-R(*GP*CP*GP*CP*UP*CP*CP*UP*CP*AP*GP*UP*AP*CP*GP*AP*GP*(A23))-3'

Chain C:

• Molecule 2: 5'-R(*GP*GP*AP*AP*CP*CP*GP*GP*AP*GP*CP*GP*C)-3'

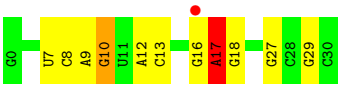
Chain F:





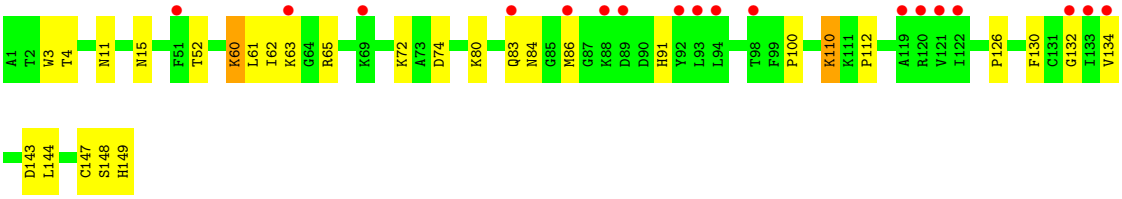
• Molecule 3: 31-mer SRD RNA analog

Chain D:



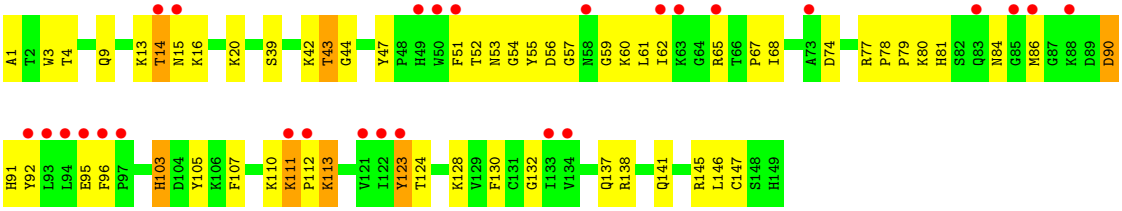
• Molecule 4: Restrictocin

Chain A:



• Molecule 4: Restrictocin

Chain B:


A1 T2 W3 T4 Q9 K13 T14 N15 K16 K20 S39 K42 T43 G44 Y47 P48 H49 W50 F51 T52 N53 G54 Y55 D56 G57 N58 G59 K60 L61 I62 K63 G64 R65 T66 P67 I68 A73 D74 R77 P78 P79 K80 H81 S82 Q83 N84 G85 M86 G87 K88 D89 D90
H91 Y92 L93 L94 E95 F96 P97 H103 D104 Y105 K106 F107 K110 K111 P112 K113 V121 I122 Y123 T124 K128 V129 F130 C131 G132 I133 V134 Q137 R138 Q141 R145 L146 C147 S148 H149

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.40Å 109.70Å 40.00Å 90.00° 97.80° 90.00°	Depositor
Resolution (Å)	19.96 – 2.15 19.95 – 2.15	Depositor EDS
% Data completeness (in resolution range)	88.4 (19.96-2.15) 88.5 (19.95-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.15Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.290 0.222 , 0.284	Depositor DCC
R_{free} test set	2437 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3883	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A23, K

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	C	0.45	0/399	0.83	0/620
2	F	0.39	0/315	0.69	0/491
3	D	0.49	1/743 (0.1%)	0.80	2/1158 (0.2%)
4	A	0.39	0/1229	0.64	0/1660
4	B	0.37	0/1229	0.64	0/1660
All	All	0.41	1/3915 (0.0%)	0.70	2/5589 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	17	A	O3'-P	-5.13	1.54	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	17	A	O4'-C1'-C2'	5.71	112.74	107.60
3	D	17	A	C4'-C3'-C2'	5.18	107.78	102.60

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	C	383	0	195	20	0
2	F	281	0	145	7	0
3	D	664	0	340	4	0
4	A	1191	0	1133	29	0
4	B	1191	0	1133	56	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
5	F	1	0	0	0	0
6	A	54	0	0	5	0
6	B	34	0	0	4	0
6	C	20	0	0	2	0
6	D	39	0	0	0	0
6	F	21	0	0	1	0
All	All	3883	0	2946	104	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 16.

The worst 5 of 104 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:C:15:A:H4'	1:C:16:G:H5'	1.05	1.05
4:B:62:ILE:HG23	4:B:65:ARG:HG3	1.47	0.97
1:C:17:A23:H2	4:A:52:THR:H	1.40	0.87
1:C:15:A:C4'	1:C:16:G:H5'	1.99	0.84
1:C:16:G:N7	4:A:65:ARG:CZ	2.46	0.78

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
4	B	147/149 (99%)	136 (92%)	7 (5%)	4 (3%)	5	1
All	All	294/298 (99%)	275 (94%)	15 (5%)	4 (1%)	11	5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	15	ASN
4	B	43	THR
4	B	14	THR
4	B	111	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	128/128 (100%)	122 (95%)	6 (5%)	26	23
4	B	128/128 (100%)	122 (95%)	6 (5%)	26	23
All	All	256/256 (100%)	244 (95%)	12 (5%)	26	23

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	103	HIS
4	B	113	LYS
4	B	141	GLN
4	B	123	TYR
4	A	110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	9	GLN
4	B	84	ASN

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Mol	Chain	Res	Type
4	B	141	GLN
4	B	137	GLN
4	A	127	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	17/18 (94%)	3 (17%)	0
2	F	12/13 (92%)	2 (16%)	0
3	D	30/31 (96%)	7 (23%)	1 (3%)
All	All	59/62 (95%)	12 (20%)	1 (1%)

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	10	G
1	C	16	G
1	C	17	A23
2	F	21	A
2	F	26	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	17	A

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

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
1	A23	C	17	1	19,28,29	0.80	0	19,43,46	1.53	4 (21%)

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	A23	C	17	1	-	2/3/35/36	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	17	A23	O2'-C2'-C3'	3.37	111.27	105.08
1	C	17	A23	C5-C6-N6	2.26	123.78	120.35
1	C	17	A23	C1'-N9-C4	-2.21	122.76	126.64
1	C	17	A23	C5'-C4'-C3'	2.04	121.17	114.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	17	A23	O4'-C4'-C5'-O5'
1	C	17	A23	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	17	A23	13	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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)

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	C	17/18 (94%)	-0.43	0 100 100	30, 44, 74, 106	0
2	F	13/13 (100%)	-0.63	0 100 100	40, 46, 57, 57	0
3	D	31/31 (100%)	-0.56	1 (3%) 47 56	40, 50, 63, 91	0
4	A	149/149 (100%)	0.63	18 (12%) 4 6	23, 43, 69, 73	0
4	B	149/149 (100%)	1.00	27 (18%) 1 1	28, 50, 79, 86	0
All	All	359/360 (99%)	0.59	46 (12%) 3 5	23, 47, 74, 106	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	93	LEU	5.0
4	B	122	ILE	5.0
4	B	111	LYS	4.8
4	A	122	ILE	4.6
4	A	133	ILE	4.2

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

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. 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	A23	C	17	25/26	0.76	0.26	98,102,107,108	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	K	D	205	1/1	0.93	0.14	65,65,65,65	0
5	K	D	204	1/1	0.94	0.09	53,53,53,53	0
5	K	F	203	1/1	0.98	0.07	44,44,44,44	0
5	K	D	201	1/1	0.98	0.08	50,50,50,50	0
5	K	C	202	1/1	0.99	0.07	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.