Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2021 – 09:03 am GMT

PDB ID	:	6ZDW
Title	:	Crystal structure of the ribonuclease core of R3B2
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Deposited on	:	2020-06-15
Resolution	:	1.65 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 following versions of software and data (see references ①) were used in the production of this report:

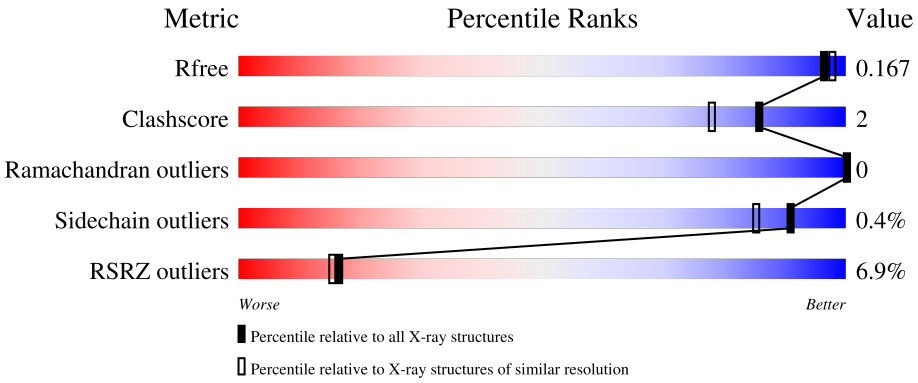
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.17.2.dev2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.2.dev2

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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	AAA	272	4% 52% 48%
1	BBB	272	4% 49% 46%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4860 atoms, of which 2332 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 protein called DRBM domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	142	Total	C	H	N	O	S	64	0	0
			2248	732	1137	181	194	4			
1	BBB	146	Total	C	H	N	O	S	64	0	0
			2366	765	1195	192	210	4			

- Molecule 2 is water.

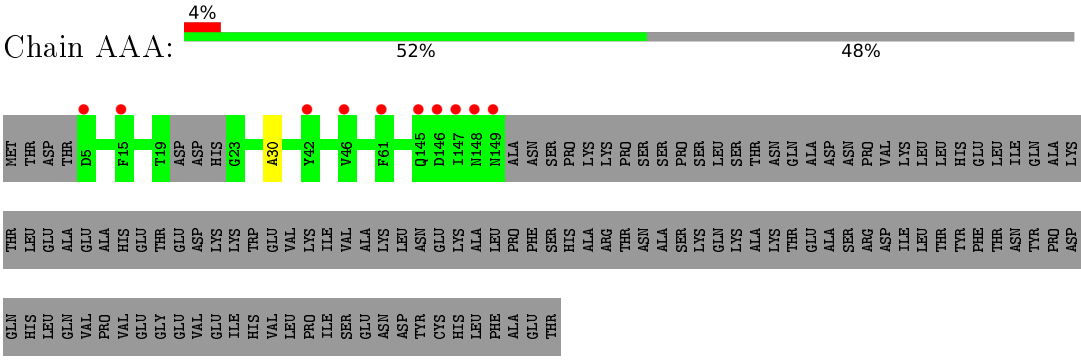
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	105	Total	O	0	0
			105	105		
2	BBB	141	Total	O	0	0
			141	141		

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.

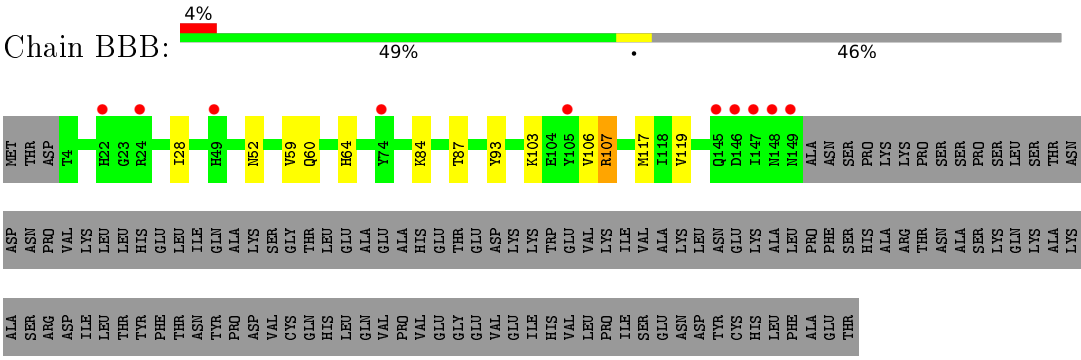
- Molecule 1: DRBM domain-containing protein

Chain AAA:



- Molecule 1: DRBM domain-containing protein

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.91Å 80.76Å 83.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.95 – 1.65 37.95 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.95-1.65) 99.8 (37.95-1.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.162 , 0.182 0.175 , 0.167	Depositor DCC
R_{free} test set	3075 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 64.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4860	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.67% 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

5.1 Standard geometry

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	AAA	0.64	0/1134	0.69	0/1538
1	BBB	0.64	0/1196	0.68	0/1623
All	All	0.64	0/2330	0.69	0/3161

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	1111	1137	1111	1	0
1	BBB	1171	1195	1182	9	0
2	AAA	105	0	0	1	0
2	BBB	141	0	0	0	0
All	All	2528	2332	2293	10	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 2.

All (10) 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:BBB:59:VAL:HG21	1:BBB:93:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:107:ARG:H	1:BBB:107:ARG:HE	1.56	0.52
1:BBB:28:ILE:C	1:BBB:28:ILE:HD12	2.31	0.51
1:BBB:52:ASN:HB3	1:BBB:117:MET:HE2	1.93	0.49
1:AAA:30:ALA:HB3	2:AAA:304:HOH:O	2.14	0.47
1:BBB:59:VAL:HG23	1:BBB:119:VAL:HG11	1.98	0.46
1:BBB:60:GLN:O	1:BBB:64:HIS:HD2	1.99	0.46
1:BBB:84:LYS:O	1:BBB:87:THR:HG23	2.18	0.44
1:BBB:103:LYS:CB	1:BBB:106:VAL:CG2	2.95	0.44
1:BBB:107:ARG:H	1:BBB:107:ARG:NE	2.13	0.43

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	
1	AAA	138/272 (51%)	137 (99%)	1 (1%)	0	100	100
1	BBB	144/272 (53%)	142 (99%)	2 (1%)	0	100	100
All	All	282/544 (52%)	279 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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
1	AAA	114/241 (47%)	114 (100%)	0	100 100
1	BBB	126/241 (52%)	125 (99%)	1 (1%)	81 70
All	All	240/482 (50%)	239 (100%)	1 (0%)	91 85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	107	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} 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	AAA	142/272 (52%)	0.27	10 (7%)	16	15	27, 41, 69, 93	0
1	BBB	146/272 (53%)	0.31	10 (6%)	17	16	28, 41, 71, 95	0
All	All	288/544 (52%)	0.29	20 (6%)	16	15	27, 41, 70, 95	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	148	ASN	4.5
1	BBB	105	TYR	4.3
1	AAA	42	TYR	4.1
1	BBB	147	ILE	4.0
1	AAA	149	ASN	3.7
1	BBB	149	ASN	3.7
1	AAA	147	ILE	3.4
1	AAA	5	ASP	3.1
1	AAA	148	ASN	2.9
1	BBB	49	HIS	2.9
1	BBB	145	GLN	2.8
1	BBB	22	HIS	2.8
1	AAA	145	GLN	2.7
1	BBB	24	ARG	2.7
1	BBB	146	ASP	2.6
1	AAA	146	ASP	2.5
1	BBB	74	TYR	2.3
1	AAA	46	VAL	2.2
1	AAA	15	PHE	2.1
1	AAA	61	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.