W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2017 – 03:10 AM EDT

PDB ID	:	3CZ3
Title	:	Crystal structure of Tomato Aspermy Virus 2b in complex with siRNA
Authors	:	Ma, J.B.; Li, F.; Ding, S.W.; Patel, D.J.
Deposited on	:	unknown
Resolution	:	3.23 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
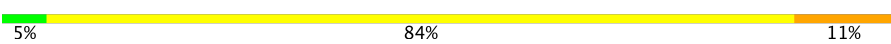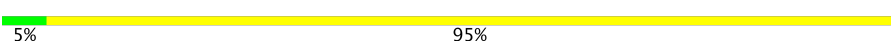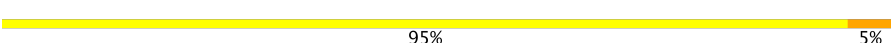*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.23 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.
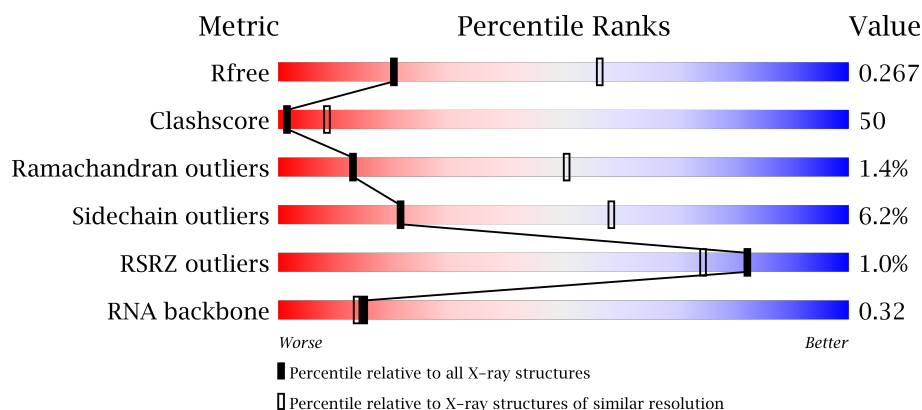
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1247 (3.28-3.20)
Clashscore	112137	1383 (3.28-3.20)
Ramachandran outliers	110173	1358 (3.28-3.20)
Sidechain outliers	110143	1357 (3.28-3.20)
RSRZ outliers	101464	1252 (3.28-3.20)
RNA backbone	2435	1068 (3.68-2.80)

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. 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	E	19	5% 79% 16%
1	G	19	5% 84% 11%
2	F	19	5% 95%
2	H	19	95% 5%

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Mol	Chain	Length	Quality of chain
3	A	70	60%　　19%　•　20%
3	B	70	.%　53%　　26%　•　20%
3	C	70	.%　56%　　19%　•　23%
3	D	70	.%　56%　　21%　•　20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5166 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 RNA (5'-R(P*CP*GP*UP*AP*CP*GP*CP*GP*GP*AP *AP*UP*AP*CP*UP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	19	Total 812	C 362	N 146	O 266	P 38	0	19	0
1	G	19	Total 812	C 362	N 146	O 266	P 38	0	19	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	19	Total 808	C 360	N 140	O 270	P 38	0	19	0
2	H	19	Total 808	C 360	N 140	O 270	P 38	0	19	0

- Molecule 3 is a protein called Protein 2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	56	Total 485	C 296	N 106	O 82	S 1	0	0	0
3	B	56	Total 485	C 296	N 106	O 82	S 1	0	0	0
3	C	54	Total 471	C 287	N 104	O 79	S 1	0	0	0
3	D	56	Total 485	C 296	N 106	O 82	S 1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q8UYT3
B	0	SER	-	EXPRESSION TAG	UNP Q8UYT3

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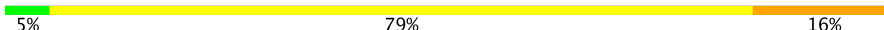
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	EXPRESSION TAG	UNP Q8UYT3
D	0	SER	-	EXPRESSION TAG	UNP Q8UYT3

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 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: RNA (5'-R(P*CP*GP*UP*AP*CP*GP*CP*GP*GP*AP*AP*UP*AP*CP*UP*U P*CP*GP*A)-3')

Chain E:
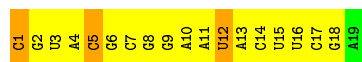
- Molecule 1: RNA (5'-R(P*CP*GP*UP*AP*CP*GP*CP*GP*GP*AP*AP*UP*AP*CP*UP*U P*CP*GP*A)-3')

Chain G:
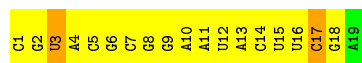
- Molecule 2: RNA (5'-R(P*UP*CP*GP*AP*AP*GP*UP*AP*UP*UP*CP*CP*GP*CP*GP*U P*AP*CP*G)-3')

Chain F:
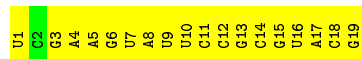
- Molecule 2: RNA (5'-R(P*UP*CP*GP*AP*AP*GP*UP*AP*UP*UP*CP*CP*GP*CP*GP*U P*AP*CP*G)-3')

Chain H:

- Molecule 3: Protein 2b

Chain A:

- Molecule 3: Protein 2b

Chain B:

53% 26% • 20%

SER MET ALA S3 I6 P7 L8 H9 E10 I11 I12 R13 K14 L15 E16 R17 M18 K21 K22 H29 R33 R46 L49 A52 R53 E56 L57 S58 ALA ILE ASN SER ASP ASN SER ASP GLU GLY

● Molecule 3: Protein 2b

Chain C:

56% 19% • 23%

SER MET ALA SER ILE E5 I6 P7 L8 H9 E10 I11 I12 R13 E16 K22 Q25 R33 K34 S40 E43 V55 S58 ALA ILE ASN SER ASP ASN SER ASP GLU GLY

● Molecule 3: Protein 2b

Chain D:

56% 21% • 20%

SER MET ALA S3 I4 E5 I6 I11 L15 M18 A24 R28 R33 K34 S40 E43 W50 R53 Q54 V55 E56 L57 S58 ALA ILE ASN SER ASP ASN SER SER ASP GLU GLY
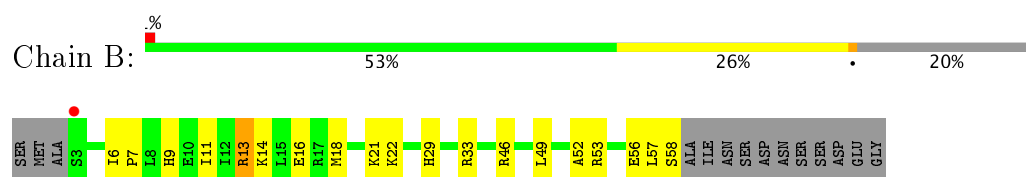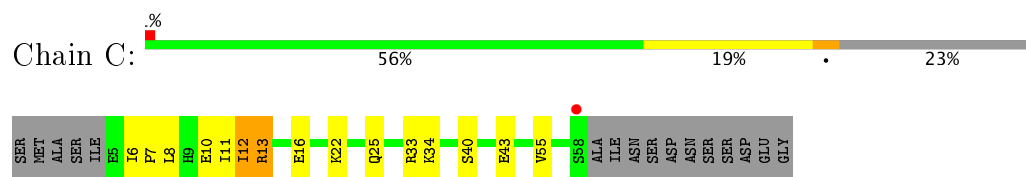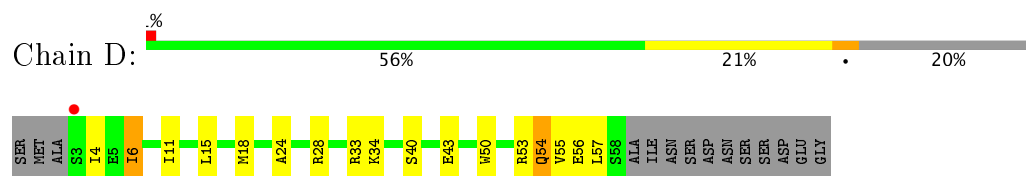
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	120.90Å 165.67Å 35.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.23 34.17 – 3.23	Depositor EDS
% Data completeness (in resolution range)	65.0 (50.00-3.23) 65.1 (34.17-3.23)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$<I/\sigma(I)>$ [1]	3.33 (at 3.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.274 0.219 , 0.267	Depositor DCC
R_{free} test set	755 reflections (10.56%)	DCC
Wilson B-factor (Å²)	118.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.21 , 37.8	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	5166	wwPDB-VP
Average B, all atoms (Å²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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)

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	E	0.87	2/906 (0.2%)	1.39	10/1404 (0.7%)
1	G	0.85	2/906 (0.2%)	1.18	6/1404 (0.4%)
2	F	0.83	2/900 (0.2%)	1.64	4/1394 (0.3%)
2	H	0.83	2/900 (0.2%)	1.29	4/1394 (0.3%)
3	A	0.45	0/492	0.61	0/651
3	B	0.42	0/492	0.56	0/651
3	C	0.44	0/478	0.58	0/632
3	D	0.42	0/492	0.53	0/651
All	All	0.73	8/5566 (0.1%)	1.19	24/8181 (0.3%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1[A]	C	OP3-P	-10.98	1.48	1.61
1	G	1[B]	C	OP3-P	-10.98	1.48	1.61
1	E	1[A]	C	OP3-P	-10.57	1.48	1.61
1	E	1[B]	C	OP3-P	-10.57	1.48	1.61
2	H	1[A]	U	OP3-P	-10.43	1.48	1.61

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1[A]	U	OP1-P-OP2	-22.71	85.53	119.60
2	F	1[B]	U	OP1-P-OP2	-22.71	85.53	119.60
2	F	1[A]	U	O5'-P-OP2	-14.92	92.27	105.70
2	F	1[B]	U	O5'-P-OP2	-14.92	92.27	105.70
1	E	5[A]	C	O3'-P-O5'	-10.87	83.34	104.00

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	E	812	0	346	143	0
1	G	812	0	343	127	0
2	F	808	0	342	118	0
2	H	808	0	346	74	0
3	A	485	0	508	9	0
3	B	485	0	508	14	0
3	C	471	0	492	14	0
3	D	485	0	508	13	0
All	All	5166	0	3393	422	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 50.

The worst 5 of 422 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:E:5[A]:C:O2'	1:E:6[A]:G:H5'	1.22	1.28
1:G:6[A]:G:O2'	1:G:7[A]:C:H5'	1.26	1.26
2:H:17[A]:A:O2'	2:H:18[A]:C:H5'	1.40	1.20
1:E:15[A]:U:O2'	1:E:16[A]:U:C5'	1.91	1.18
2:F:5[A]:A:O2'	2:F:6[A]:G:H5'	1.41	1.18

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	
3	A	54/70 (77%)	47 (87%)	6 (11%)	1 (2%)	9	44
3	B	54/70 (77%)	46 (85%)	8 (15%)	0	100	100
3	C	52/70 (74%)	45 (86%)	6 (12%)	1 (2%)	9	44
3	D	54/70 (77%)	50 (93%)	3 (6%)	1 (2%)	9	44
All	All	214/280 (76%)	188 (88%)	23 (11%)	3 (1%)	13	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	12	ILE
3	D	56	GLU
3	A	45	ARG

5.3.2 Protein sidechains ⓘ

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	
3	A	53/64 (83%)	50 (94%)	3 (6%)	24	62
3	B	53/64 (83%)	47 (89%)	6 (11%)	7	29
3	C	51/64 (80%)	50 (98%)	1 (2%)	60	84
3	D	53/64 (83%)	50 (94%)	3 (6%)	24	62
All	All	210/256 (82%)	197 (94%)	13 (6%)	21	58

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	18	MET
3	B	22	LYS
3	D	4	ILE
3	B	13	ARG
3	C	13	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	32	ASN
3	B	9	HIS
3	B	25	GLN
3	C	25	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	0/19	-	-
1	G	0/19	-	-
2	F	0/19	-	-
2	H	0/19	-	-
All	All	0/76	-	-

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 carbohydrates 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)

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	E	19/19 (100%)	-0.97	0	100	100	85, 99, 126, 127	0
1	G	19/19 (100%)	-0.90	0	100	100	86, 101, 122, 125	0
2	F	19/19 (100%)	-0.98	0	100	100	88, 95, 121, 128	0
2	H	19/19 (100%)	-0.90	0	100	100	84, 94, 129, 135	0
3	A	56/70 (80%)	-0.29	0	100	100	99, 107, 155, 158	0
3	B	56/70 (80%)	-0.32	1 (1%)	69	58	100, 107, 132, 133	0
3	C	54/70 (77%)	-0.20	1 (1%)	67	55	101, 109, 157, 160	0
3	D	56/70 (80%)	-0.46	1 (1%)	69	58	99, 108, 125, 130	0
All	All	298/356 (83%)	-0.48	3 (1%)	82	74	84, 107, 146, 160	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	3	SER	5.2
3	B	3	SER	3.8
3	C	58	SER	3.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.