W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2020 – 10:20 AM EDT

PDB ID	:	6D3P
Title	:	Crystal structure of an exoribonuclease-resistant RNA from Sweet clover necrotic mosaic virus (SCNMV)
Authors	:	Steckelberg, A.-L.; Akiyama, B.M.; Costantino, D.A.; Sit, T.L.; Nix, J.C.; Kieft, J.S.
Deposited on	:	2018-04-16
Resolution	:	2.90 Å(reported)

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

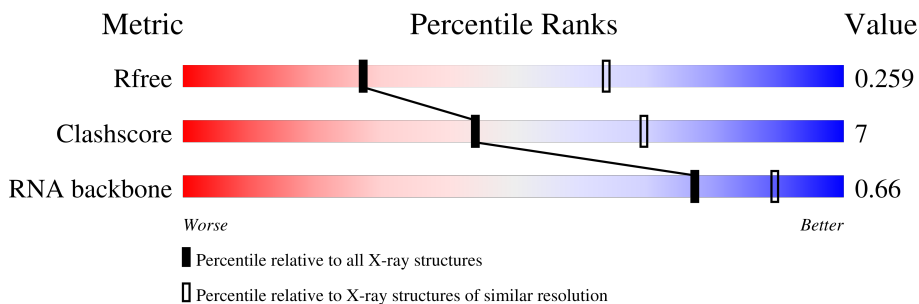|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 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		0.259
Clashscore		7
RNA backbone		0.66

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 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%

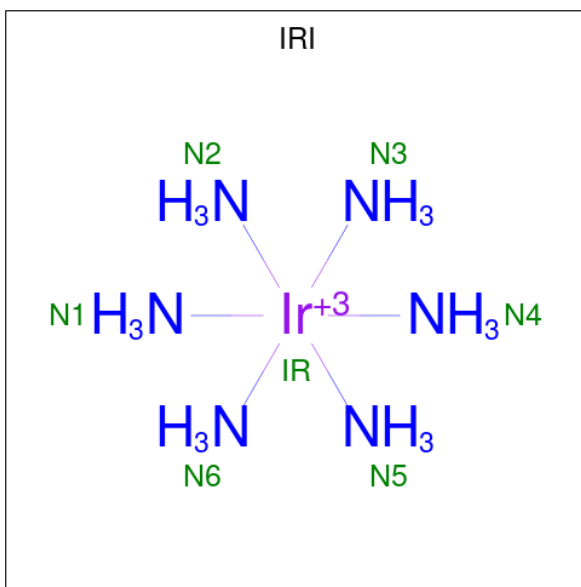| Mol	Chain	Length	Quality of chain
1	A	45	67% 31% •

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 1036 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 (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	45	Total	C	N	O	P	0	0	0
			966	431	180	310	45			

- Molecule 2 is IRIDIUM HEXAMMINE ION (three-letter code: IRI) (formula: $H_{18}IrN_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Ir	N	0	0
			7	1	6		
2	A	1	Total	Ir	N	0	0
			7	1	6		
2	A	1	Total	Ir	N	0	0
			7	1	6		
2	A	1	Total	Ir	N	0	0
			7	1	6		
2	A	1	Total	Ir	N	0	0
			7	1	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Ir	N	0	0
			7	1	6		
2	A	1	Total	Ir	N	0	0
			7	1	6		
2	A	1	Total	Ir	N	0	0
			7	1	6		
2	A	1	Total	Ir	N	0	0
			7	1	6		
2	A	1	Total	Ir	N	0	0
			7	1	6		

3 Residue-property plots ⓘ

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.

• Molecule 1: RNA (45-MER)

Chain A:

67%   31%   •

G1 G2 G3 C10 U15 G18 A19 G23 A26 G27 A28 G29 A30 G31 G32 C39 C43 U44 C45

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	83.40Å 83.40Å 94.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.45 – 2.90 39.46 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.45-2.90) 88.2 (39.46-2.55)	Depositor EDS
R_{merge}	0.59	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.23 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.241 , 0.259 0.242 , 0.259	Depositor DCC
R_{free} test set	641 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 55.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	1036	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.15	0/1081	0.68	0/1684

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	A	966	0	489	10	0
2	A	70	0	0	8	0
All	All	1036	0	489	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 7.

The worst 5 of 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:A:2:G:N7	2:A:102:IRI:N2	2.42	0.67
1:A:30:A:OP1	2:A:104:IRI:N3	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:G:OP1	2:A:102:IRI:N3	2.36	0.59
1:A:29:G:OP1	2:A:104:IRI:N5	2.35	0.58
1:A:32:G:N7	2:A:107:IRI:N1	2.56	0.53

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2   Protein sidechains ⓘ

There are no protein molecules in this entry.

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	44/45 (97%)	6 (13%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	C
1	A	26	A
1	A	28	A
1	A	29	G
1	A	39	C

There are no RNA pucker outliers to report.

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

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

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5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands 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	#$|Z| > 2$
2	IRI	A	101	-	0,6,6	0.00	-	-		
2	IRI	A	105	-	0,6,6	0.00	-	-		
2	IRI	A	102	-	0,6,6	0.00	-	-		
2	IRI	A	106	-	0,6,6	0.00	-	-		
2	IRI	A	108	-	0,6,6	0.00	-	-		
2	IRI	A	110	-	0,6,6	0.00	-	-		
2	IRI	A	103	-	0,6,6	0.00	-	-		
2	IRI	A	107	-	0,6,6	0.00	-	-		
2	IRI	A	109	-	0,6,6	0.00	-	-		
2	IRI	A	104	-	0,6,6	0.00	-	-		

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.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	IRI	1	0
2	A	102	IRI	3	0
2	A	107	IRI	1	0
2	A	109	IRI	1	0
2	A	104	IRI	2	0

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.