



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:46 am BST

PDB ID : 6BJG  
Title : CIRV p19 mutant T111H in complex with siRNA  
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Deposited on : 2017-11-06  
Resolution : 2.29 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

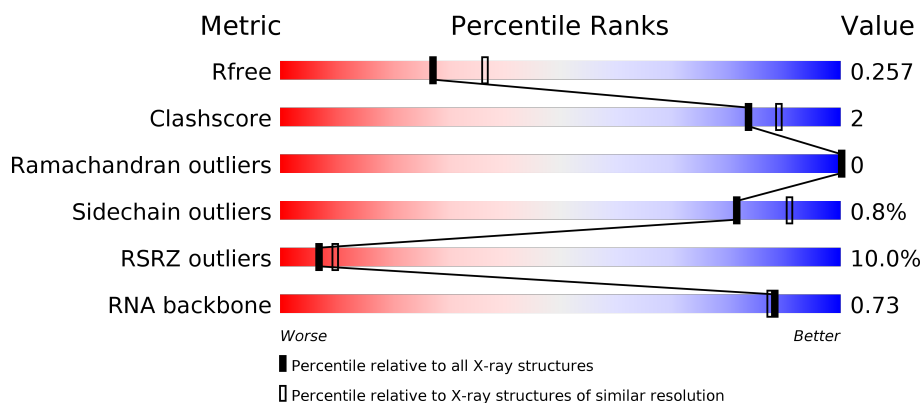
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	172	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>6%</div> <div>17%</div> </div> </div>
1	B	172	<div> <div>9%</div> <div> <div></div> <div>81%</div> <div>•</div> <div>15%</div> </div> </div>
2	C	21	<div> <div>14%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>10%</div> </div> </div>
3	D	21	<div> <div>10%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5797 atoms, of which 2479 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 RNA silencing suppressor p19.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	143	Total	C	H	N	O	S	0	0	0
			2172	712	1030	210	216	4			
1	B	146	Total	C	H	N	O	S	0	0	0
			2205	726	1040	214	221	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	HIS	THR	engineered mutation	UNP Q66104
B	111	HIS	THR	engineered mutation	UNP Q66104

- 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\*GP\*UP\*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	21	Total	C	H	N	O	P	4	0	0
			648	198	204	74	151	21			

- Molecule 3 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\*AP\*UP\*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	21	Total	C	H	N	O	P	3	0	0
			651	199	205	77	149	21			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	48	Total	O	0	0
			48	48		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	21	Total	O	0	0
			21	21		
4	D	16	Total	O	0	0
			16	16		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.39 Å 46.93 Å 54.62 Å 109.33° 111.12° 96.61°	Depositor
Resolution (Å)	34.83 – 2.29 34.83 – 2.29	Depositor EDS
% Data completeness (in resolution range)	87.6 (34.83-2.29) 87.6 (34.83-2.29)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.11 (at 2.29 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.212 , 0.257 0.214 , 0.257	Depositor DCC
$R_{free}$ test set	794 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5797	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	A	0.24	0/1168	0.42	0/1574
1	B	0.35	1/1192 (0.1%)	0.52	2/1608 (0.1%)
2	C	0.50	1/494 (0.2%)	0.68	0/765
3	D	0.50	1/497 (0.2%)	0.66	0/770
All	All	0.37	3/3351 (0.1%)	0.55	2/4717 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	U	OP3-P	-10.52	1.48	1.61
3	D	1	C	OP3-P	-10.46	1.48	1.61
1	B	44	LEU	C-N	-8.88	1.13	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	TYR	O-C-N	7.35	134.46	122.70
1	B	45	TYR	CA-C-N	-5.54	105.02	117.20

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	A	1142	1030	1092	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1165	1040	1113	3	0
2	C	444	204	225	4	2
3	D	446	205	226	0	0
4	A	36	0	0	0	0
4	B	48	0	0	2	0
4	C	21	0	0	1	0
4	D	16	0	0	0	0
All	All	3318	2479	2656	14	2

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 (14) 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)
2:C:20:U:O2'	2:C:21:U:O5'	2.04	0.75
1:B:47:ASP:O	4:B:201:HOH:O	2.06	0.73
2:C:21:U:O3'	4:C:101:HOH:O	2.08	0.70
2:C:20:U:HO2'	2:C:21:U:P	2.19	0.66
1:B:5:ILE:HB	1:B:102:PHE:HA	1.78	0.65
1:A:48:GLU:O	1:A:49:THR:OG1	2.16	0.57
1:A:44:LEU:O	1:A:48:GLU:HG2	2.07	0.55
1:B:111:HIS:NE2	4:B:202:HOH:O	2.33	0.54
1:A:3:ARG:HG3	1:A:5:ILE:HD12	1.90	0.53
1:A:1:MET:N	1:A:3:ARG:H	2.11	0.49
2:C:20:U:O2	2:C:21:U:H4'	2.15	0.46
1:A:5:ILE:HG23	1:A:102:PHE:HA	1.99	0.44
1:A:1:MET:H2	1:A:3:ARG:H	1.67	0.43
1:A:20:ASP:N	1:A:21:GLY:HA2	2.34	0.42

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:C:O2'	2:C:20:U:O4[1_544]	1.96	0.24
2:C:2:C:HO2'	2:C:20:U:O4[1_544]	1.46	0.14



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	A	139/172 (81%)	135 (97%)	4 (3%)	0	100	100
1	B	142/172 (83%)	136 (96%)	6 (4%)	0	100	100
All	All	281/344 (82%)	271 (96%)	10 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
1	A	120/147 (82%)	118 (98%)	2 (2%)	60	76
1	B	123/147 (84%)	123 (100%)	0	100	100
All	All	243/294 (83%)	241 (99%)	2 (1%)	81	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	55	ASN

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

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	20/21 (95%)	2 (10%)	0
3	D	20/21 (95%)	2 (10%)	0
All	All	40/42 (95%)	4 (10%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	20	U
2	C	21	U
3	D	20	U
3	D	21	U

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	44:LEU	C	45:TYR	N	1.13

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	143/172 (83%)	0.49	12 (8%) 11 15	19, 35, 81, 169	0
1	B	146/172 (84%)	0.50	16 (10%) 5 7	18, 32, 85, 112	0
2	C	21/21 (100%)	0.95	3 (14%) 2 3	28, 42, 82, 104	0
3	D	21/21 (100%)	0.46	2 (9%) 8 11	28, 48, 73, 107	0
All	All	331/386 (85%)	0.52	33 (9%) 7 10	18, 37, 90, 169	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ILE	7.5
1	B	4	ALA	5.2
1	B	2	GLU	5.2
1	A	49	THR	5.0
1	B	5	ILE	5.0
2	C	21	U	4.3
1	A	4	ALA	3.8
2	C	20	U	3.8
1	B	148	THR	3.6
1	A	81	ALA	3.5
1	A	1	MET	3.4
1	B	149	PRO	3.3
1	B	3	ARG	3.2
3	D	20	U	3.2
2	C	17	A	3.1
1	B	1	MET	3.0
3	D	21	U	2.9
1	B	47	ASP	2.9
1	B	48	GLU	2.9
1	B	49	THR	2.8
1	A	2	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	55	ASN	2.6
1	A	54	ASP	2.6
1	A	39	TRP	2.5
1	B	53	GLN	2.4
1	A	20	ASP	2.3
1	B	21	GLY	2.2
1	B	54	ASP	2.1
1	B	45	TYR	2.1
1	A	105	ALA	2.1
1	A	80	GLU	2.0
1	B	9	ASP	2.0
1	B	113	SER	2.0

## 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.