



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:52 AM UTC

PDB ID : 5JER / pdb\_00005jer  
Title : Structure of Rotavirus NSP1 bound to IRF-3  
Authors : Zhao, B.; Li, P.  
Deposited on : 2016-04-18  
Resolution : 2.91 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

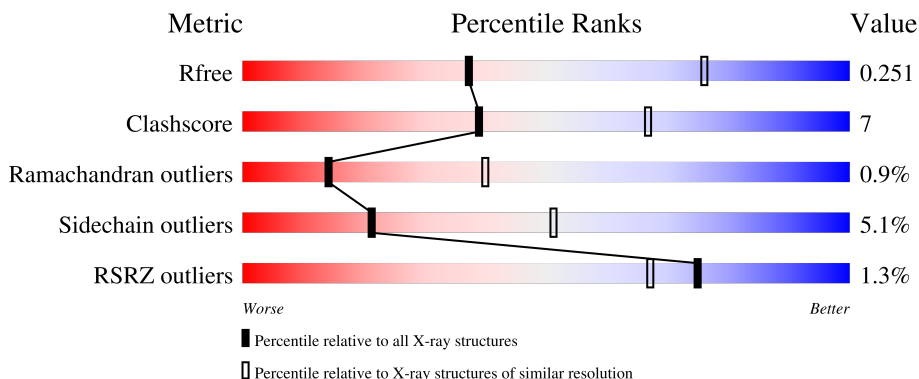
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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 of 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	B	19	32% 16% 5% 47%
1	D	19	42% 11% 47%
1	F	19	47% 5% 47%
1	H	19	26% 26% 47%
2	A	242	2% 78% 17% ..

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Mol	Chain	Length	Quality of chain
2	C	242	 <p>% 74% 20% . .</p>
2	E	242	 <p>% 76% 19% . .</p>
2	G	242	 <p>% 80% 15% . .</p>

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 7710 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 protein called Rotavirus NSP1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	B	10	82	52	11	19	0	0	0
1	D	10	82	52	11	19	0	0	0
1	F	10	82	52	11	19	0	0	0
1	H	10	82	52	11	19	0	0	0

- Molecule 2 is a protein called Interferon regulatory factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	234	1850	1179	319	342	10	6	2	0
2	C	234	1844	1176	318	340	10	0	1	0
2	E	234	1844	1176	318	340	10	0	1	0
2	G	234	1844	1176	318	340	10	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	SER	-	expression tag	UNP Q14653
A	187	GLU	-	expression tag	UNP Q14653
A	188	PHE	-	expression tag	UNP Q14653
C	186	SER	-	expression tag	UNP Q14653
C	187	GLU	-	expression tag	UNP Q14653
C	188	PHE	-	expression tag	UNP Q14653
E	186	SER	-	expression tag	UNP Q14653
E	187	GLU	-	expression tag	UNP Q14653

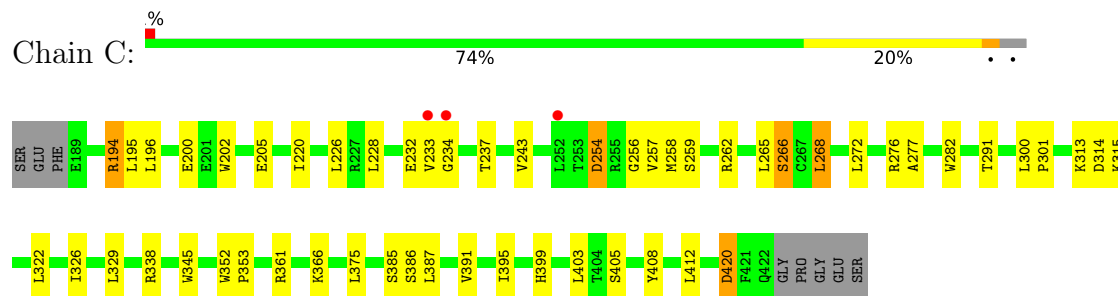
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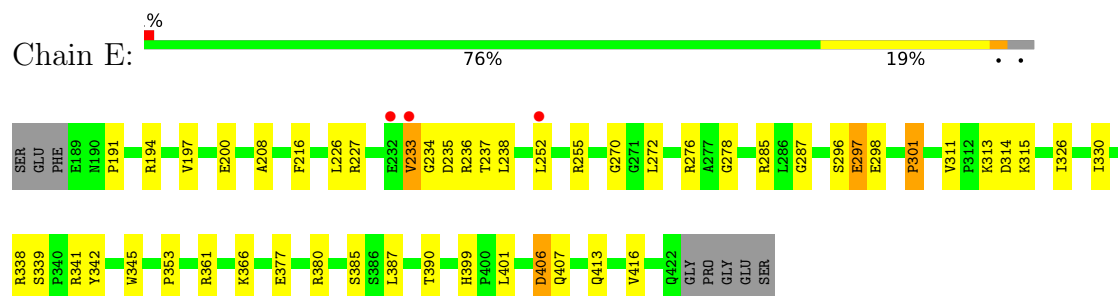
Chain	Residue	Modelled	Actual	Comment	Reference
E	188	PHE	-	expression tag	UNP Q14653
G	186	SER	-	expression tag	UNP Q14653
G	187	GLU	-	expression tag	UNP Q14653
G	188	PHE	-	expression tag	UNP Q14653



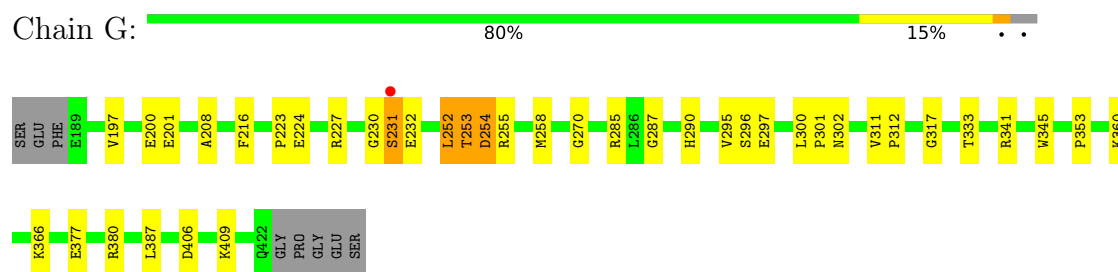
- Molecule 2: Interferon regulatory factor 3



- Molecule 2: Interferon regulatory factor 3



- Molecule 2: Interferon regulatory factor 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.77Å 107.92Å 135.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.94 – 2.91 47.94 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.94-2.91) 94.8 (47.94-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.210 , 0.250 0.210 , 0.251	Depositor DCC
$R_{free}$ test set	2000 reflections (8.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtrriage
Anisotropy	0.164	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.49% 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	B	0.34	0/82	0.80	0/109
1	D	0.28	0/82	0.72	0/109
1	F	0.29	0/82	0.59	0/109
1	H	0.40	0/82	0.68	0/109
2	A	0.26	0/1903	0.69	0/2593
2	C	0.25	0/1897	0.67	1/2585 (0.0%)
2	E	0.26	0/1897	0.68	0/2585
2	G	0.26	0/1897	0.69	0/2585
All	All	0.26	0/7922	0.68	1/10784 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	232	GLU	N-CA-C	-6.22	105.97	112.93

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	B	82	0	75	1	0
1	D	82	0	75	1	0
1	F	82	0	75	0	0
1	H	82	0	75	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1850	0	1794	22	0
2	C	1844	0	1790	29	0
2	E	1844	0	1790	26	0
2	G	1844	0	1790	25	0
All	All	7710	0	7464	103	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 103 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:B:482:GLU:OE2	2:A:360:LYS:NZ	1.95	1.00
2:C:194:ARG:NH1	2:C:200:GLU:OE2	1.94	1.00
2:A:194:ARG:NH1	2:A:397:ASN:O	2.02	0.92
2:A:377:GLU:OE1	2:A:380:ARG:NH1	2.08	0.87
2:G:377:GLU:OE1	2:G:380:ARG:NH1	2.08	0.85

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	B	8/19 (42%)	7 (88%)	1 (12%)	0	100	100
1	D	8/19 (42%)	7 (88%)	1 (12%)	0	100	100
1	F	8/19 (42%)	8 (100%)	0	0	100	100
1	H	8/19 (42%)	7 (88%)	1 (12%)	0	100	100
2	A	234/242 (97%)	216 (92%)	14 (6%)	4 (2%)	7	24
2	C	233/242 (96%)	216 (93%)	17 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	233/242 (96%)	217 (93%)	13 (6%)	3 (1%)	9	30
2	G	233/242 (96%)	215 (92%)	16 (7%)	2 (1%)	14	40
All	All	965/1044 (92%)	893 (92%)	63 (6%)	9 (1%)	14	40

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	254	ASP
2	A	248	PRO
2	A	385	SER
2	E	236	ARG
2	G	231	SER

### 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	B	10/19 (53%)	6 (60%)	4 (40%)	0	0
1	D	10/19 (53%)	10 (100%)	0	100	100
1	F	10/19 (53%)	9 (90%)	1 (10%)	7	23
1	H	10/19 (53%)	9 (90%)	1 (10%)	7	23
2	A	201/205 (98%)	192 (96%)	9 (4%)	24	56
2	C	200/205 (98%)	188 (94%)	12 (6%)	17	45
2	E	200/205 (98%)	191 (96%)	9 (4%)	24	56
2	G	200/205 (98%)	193 (96%)	7 (4%)	32	64
All	All	841/896 (94%)	798 (95%)	43 (5%)	21	51

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	233	VAL
2	E	407	GLN

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Mol	Chain	Res	Type
2	E	297	GLU
2	E	390	THR
2	G	231	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	217	GLN
2	C	389	ASN
2	E	263	HIS
2	E	407	GLN
2	G	389	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 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 oligosaccharides 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, 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	B	10/19 (52%)	0.11	0 100 100	46, 54, 85, 89	0
1	D	10/19 (52%)	0.27	0 100 100	43, 52, 80, 92	0
1	F	10/19 (52%)	0.42	0 100 100	48, 61, 99, 113	0
1	H	10/19 (52%)	0.61	0 100 100	48, 58, 85, 94	0
2	A	234/242 (96%)	0.01	6 (2%) 57 47	16, 44, 77, 100	2 (0%)
2	C	234/242 (96%)	0.02	3 (1%) 75 67	16, 46, 78, 99	1 (0%)
2	E	234/242 (96%)	-0.03	3 (1%) 75 67	16, 45, 79, 99	1 (0%)
2	G	234/242 (96%)	-0.03	1 (0%) 88 85	15, 43, 73, 83	1 (0%)
All	All	976/1044 (93%)	0.01	13 (1%) 75 67	15, 45, 78, 113	5 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	233	VAL	3.3
2	A	233	VAL	3.1
2	A	384	ALA	3.1
2	C	252	LEU	2.7
2	G	231	SER	2.5

### 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 oligosaccharides 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.