



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:26 AM BST

PDB ID : 6KP3  
Title : STRUCTURE OF SENDAI VIRUS Y3/ALIX-BRO1 DOMAIN COMPLEX  
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Deposited on : 2019-08-14  
Resolution : 2.20 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	:	2.13
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)	:	2.13

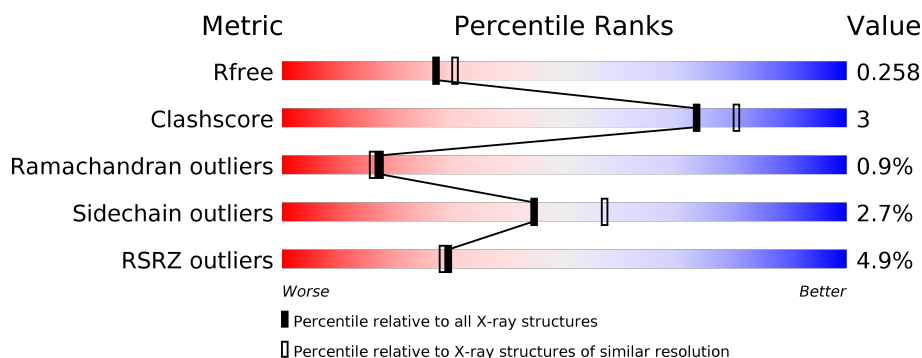
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	372	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>• •</div> </div> </div>
2	B	119	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>• • 6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3900 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 Programmed cell death 6-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2803	1792	471	529	11			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q8WUM4
A	-11	ASN	-	expression tag	UNP Q8WUM4
A	-10	HIS	-	expression tag	UNP Q8WUM4
A	-9	LYS	-	expression tag	UNP Q8WUM4
A	-8	VAL	-	expression tag	UNP Q8WUM4
A	-7	HIS	-	expression tag	UNP Q8WUM4
A	-6	HIS	-	expression tag	UNP Q8WUM4
A	-5	HIS	-	expression tag	UNP Q8WUM4
A	-4	HIS	-	expression tag	UNP Q8WUM4
A	-3	HIS	-	expression tag	UNP Q8WUM4
A	-2	HIS	-	expression tag	UNP Q8WUM4
A	-1	HIS	-	expression tag	UNP Q8WUM4
A	0	HIS	-	expression tag	UNP Q8WUM4

- Molecule 2 is a protein called C' protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	112	Total	C	N	O	S	0	0	0
			959	614	171	168	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	86	MET	-	initiating methionine	UNP Q5ECE0
B	87	ASN	-	expression tag	UNP Q5ECE0
B	88	HIS	-	expression tag	UNP Q5ECE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	89	LYS	-	expression tag	UNP Q5ECE0
B	90	VAL	-	expression tag	UNP Q5ECE0
B	91	HIS	-	expression tag	UNP Q5ECE0
B	92	HIS	-	expression tag	UNP Q5ECE0
B	93	HIS	-	expression tag	UNP Q5ECE0
B	94	HIS	-	expression tag	UNP Q5ECE0
B	95	HIS	-	expression tag	UNP Q5ECE0
B	96	HIS	-	expression tag	UNP Q5ECE0
B	97	HIS	-	expression tag	UNP Q5ECE0

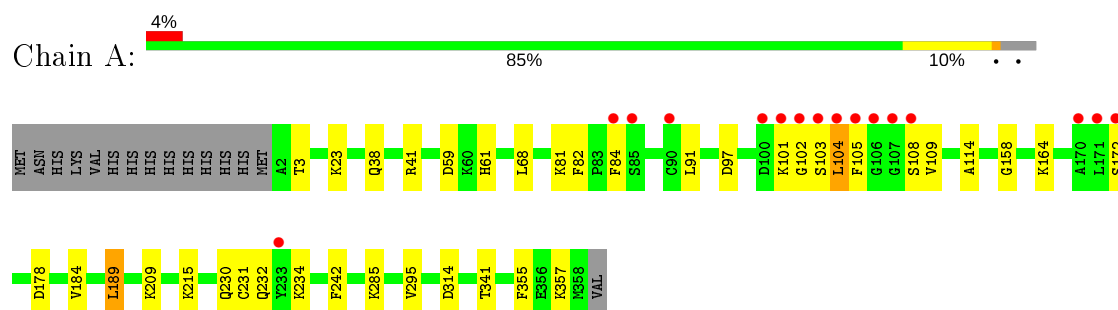
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	114	Total O 114 114	0	0
3	B	24	Total O 24 24	0	0

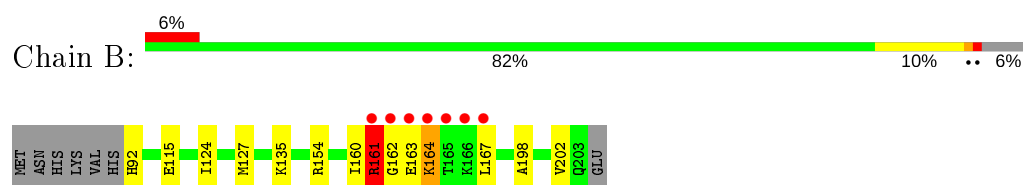
### 3 Residue-property plots

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 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: Programmed cell death 6-interacting protein



- Molecule 2: C' protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.33 Å 102.65 Å 103.63 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.31 – 2.20 45.27 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.31-2.20) 100.0 (45.27-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.205 , 0.262 0.210 , 0.258	Depositor DCC
$R_{free}$ test set	1486 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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	0.68	0/2856	0.82	0/3854
2	B	0.67	0/981	0.79	0/1320
All	All	0.68	0/3837	0.82	0/5174

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	SER	Peptide

### 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	2803	0	2828	16	2
2	B	959	0	973	9	2
3	A	114	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	0	1	0
All	All	3900	0	3801	25	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 3.

All (25) 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:B:154:ARG:HB3	2:B:154:ARG:HH11	1.55	0.71
2:B:164:LYS:HA	2:B:167:LEU:HD23	1.73	0.70
2:B:160:ILE:O	2:B:162:GLY:N	2.32	0.63
1:A:91:LEU:O	1:A:114:ALA:HA	2.02	0.60
1:A:81:LYS:HE3	1:A:355:PHE:O	2.02	0.59
1:A:104:LEU:CD2	1:A:109:VAL:HG21	2.37	0.54
2:B:154:ARG:NH1	2:B:154:ARG:HB3	2.21	0.54
1:A:3:THR:HG22	1:A:295:VAL:HG12	1.91	0.53
2:B:163:GLU:O	2:B:164:LYS:HB2	2.10	0.51
1:A:164:LYS:HB2	1:A:184:VAL:HG23	1.91	0.51
2:B:163:GLU:N	2:B:163:GLU:OE2	2.45	0.50
2:B:92:HIS:N	3:B:302:HOH:O	2.45	0.49
2:B:124:ILE:O	2:B:127:MET:HG2	2.13	0.48
1:A:82:PHE:HB2	1:A:84:PHE:CE2	2.48	0.48
1:A:59:ASP:HB2	1:A:61:HIS:ND1	2.29	0.48
1:A:81:LYS:CE	1:A:355:PHE:O	2.63	0.47
1:A:38:GLN:HE22	1:A:357:LYS:HD3	1.80	0.47
1:A:104:LEU:HD22	1:A:109:VAL:HG21	1.99	0.45
1:A:103:SER:O	1:A:104:LEU:CB	2.65	0.44
1:A:97:ASP:HA	1:A:178:ASP:OD2	2.19	0.42
1:A:101:LYS:HG2	1:A:102:GLY:N	2.34	0.42
2:B:198:ALA:O	2:B:202:VAL:HG12	2.19	0.42
1:A:158:GLY:HA3	1:A:341:THR:O	2.19	0.41
1:A:232:GLN:HG2	1:A:242:PHE:HE2	1.85	0.41
1:A:189:LEU:HD12	1:A:230:GLN:OE1	2.21	0.41

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)
1:A:105:PHE:CZ	2:B:115:GLU:OE1[3_655]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:OD1	2:B:161:ARG:NH2[2_555]	2.18	0.02

## 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	A	355/372 (95%)	344 (97%)	9 (2%)	2 (1%)	25	26
2	B	110/119 (92%)	106 (96%)	2 (2%)	2 (2%)	8	5
All	All	465/491 (95%)	450 (97%)	11 (2%)	4 (1%)	17	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	161	ARG
2	B	164	LYS
1	A	104	LEU
1	A	172	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	A	299/314 (95%)	290 (97%)	9 (3%)	41	53
2	B	105/112 (94%)	103 (98%)	2 (2%)	57	71
All	All	404/426 (95%)	393 (97%)	11 (3%)	44	57

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	41	ARG
1	A	68	LEU
1	A	189	LEU
1	A	209	LYS
1	A	215	LYS
1	A	231	CYS
1	A	234	LYS
1	A	285	LYS
2	B	135	LYS
2	B	161	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	230	GLN

### 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<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	357/372 (95%)	0.25	16 (4%) 33 32	33, 52, 102, 177	0
2	B	112/119 (94%)	0.33	7 (6%) 20 19	38, 54, 123, 155	0
All	All	469/491 (95%)	0.27	23 (4%) 29 28	33, 52, 108, 177	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	PHE	14.0
1	A	106	GLY	11.1
1	A	107	GLY	10.8
1	A	233	TYR	6.5
1	A	102	GLY	6.2
2	B	166	LYS	5.4
1	A	108	SER	5.0
2	B	165	THR	4.6
2	B	163	GLU	4.1
2	B	167	LEU	4.0
1	A	101	LYS	3.7
1	A	103	SER	3.4
2	B	161	ARG	3.0
1	A	90	CYS	3.0
1	A	104	LEU	3.0
1	A	172	SER	2.8
2	B	164	LYS	2.8
1	A	170	ALA	2.5
1	A	85	SER	2.3
2	B	162	GLY	2.3
1	A	100	ASP	2.2
1	A	84	PHE	2.1
1	A	171	LEU	2.1

## 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 monosaccharides 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.