

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 23, 2020 - 06:00 am BST

PDB ID	:	1JVN
$\operatorname{Title}$	:	CRYSTAL STRUCTURE OF IMIDAZOLE GLYCEROL PHOSPHATE SYN-
		THASE: A TUNNEL THROUGH A (BETA/ALPHA)8 BARREL JOINS
		TWO ACTIVE SITES
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Deposited on		
Resolution	:	2.10 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 https://www.wwpdb.org/validation/2017/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:

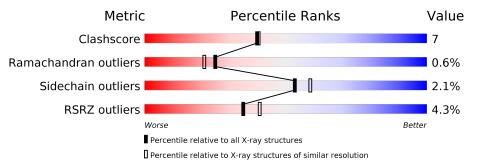
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647(2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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% 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	А	555	81%	15%	·
1	В	555	4%	15%	••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	143	А	83	-	-	Х	-
4	POP	В	999	-	-	Х	-



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8818 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 BIFUNCTIONAL HISTIDINE BIOSYNTHESIS PROTEIN HISHF.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	537	Total	С	Ν	0	S	0	0	0
		007	4185	2659	699	812	15	0		
1	В	537	Total	С	Ν	Ο	S	0	0	0
	D	007	4185	2659	699	812	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

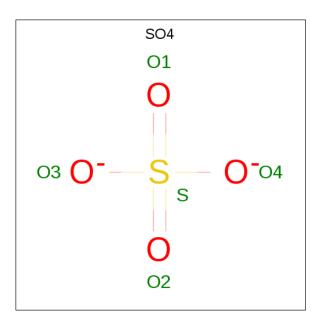
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P33734
А	-2	SER	-	EXPRESSION TAG	UNP P33734
А	-1	HIS	-	EXPRESSION TAG	UNP P33734
А	83	143	CYS	MODIFIED RESIDUE	UNP P33734
В	-3	GLY	-	EXPRESSION TAG	UNP P33734
В	-2	SER	-	EXPRESSION TAG	UNP P33734
В	-1	HIS	-	EXPRESSION TAG	UNP P33734
В	83	143	CYS	MODIFIED RESIDUE	UNP P33734

• Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Ni 1 1	0	0
2	А	1	Total Ni 1 1	0	0

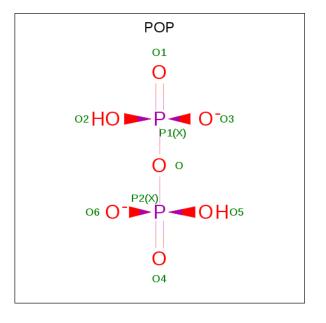
• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $H_2O_7P_2$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	В	1	Total 9	0 7	Р 2	0	0

• Molecule 5 is water.

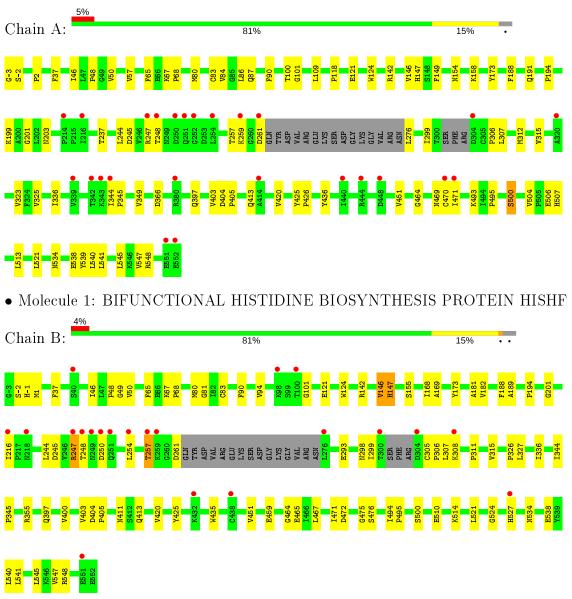
Mol	Chain	Residues	Residues Atoms		AltConf
5	А	212	Total         O           212         212	2	0
5	В	200	Total         O           200         200	0	0



## 3 Residue-property plots (i)

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: BIFUNCTIONAL HISTIDINE BIOSYNTHESIS PROTEIN HISHF





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	98.37Å 112.17Å 116.68Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	75.21 - 2.10	Depositor
Resolution (A)	80.86 - 2.11	EDS
% Data completeness	97.6 (75.21-2.10)	Depositor
(in resolution range)	$97.8 \ (80.86 - 2.11)$	EDS
R <sub>merge</sub>	0.07	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.69 (at 2.10 \text{\AA})$	Xtriage
Refinement program	CNS 1.0	Depositor
R R.	0.224 , $0.242$	Depositor
$R, R_{free}$	0.212 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	28.8	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , $42.4$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8818	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 143, POP, SO4  $\,$ 

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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.64	0/4255	0.68	0/5753	
1	В	0.62	0/4255	0.67	0/5753	
All	All	0.63	0/8510	0.68	0/11506	

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 (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	А	4185	0	4113	63	0
1	В	4185	0	4113	61	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	15	0	0	0	0
3	В	10	0	0	0	0
4	В	9	0	0	5	0
5	А	212	0	0	1	0
5	В	200	0	0	3	0
All	All	8818	0	8226	121	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 121 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:404:ASP:O	1:B:471:ILE:HD11	1.70	0.91
1:B:541:LEU:HD13	1:B:547:VAL:HG22	1.57	0.87
1:A:403:VAL:HG12	1:A:405:PRO:HD3	1.59	0.84
1:A:541:LEU:HD13	1:A:547:VAL:HG22	1.64	0.79
1:B:475:GLY:HA2	4:B:999:POP:O3	1.83	0.78

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	А	530/555~(96%)	516~(97%)	11 (2%)	3 (1%)	25 21
1	В	530/555~(96%)	516~(97%)	11 (2%)	3 (1%)	25 21
All	All	1060/1110~(96%)	1032~(97%)	22 (2%)	6 (1%)	25 21

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	259	LYS
1	А	-2	SER
1	В	-2	SER
1	А	500	SER
1	В	500	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	А	450/466~(97%)	445~(99%)	5(1%)	73 79
1	В	450/466~(97%)	436~(97%)	14(3%)	40 43
All	All	900/932~(97%)	881 (98%)	19 (2%)	53 59

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	147	HIS
1	В	216	ILE
1	В	257	THR
1	В	94	VAL
1	В	298	ASN

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

Mol	Chain	Res	Type
1	А	183	ASN
1	А	298	ASN
1	В	55	HIS
1	В	298	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)

2 non-standard protein/DNA/RNA residues 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



1

143

А

83

2 (66%)

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).										
Mol	Type	Chain	Res	Link	B	ond leng	$ agenup{sths}{\# Z >2}$	В	ond ang	gles
10101	турс	Chain	Ites		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	143	В	83	1	6,16,17	1.12	0	3.21.23	2.45	1(33%)

6, 16, 17

1.12

0

3,21,23

2.52

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).

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	143	В	83	1	-	3/5/24/26	0/1/1/1
1	143	А	83	1	-	3/5/24/26	0/1/1/1

1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	83	143	CJ-CI-CF	3.43	117.57	112.63
1	А	83	143	CJ-CI-CF	3.41	117.53	112.63
1	А	83	143	CA-CB-SG	2.12	121.16	113.58

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
1	В	83	143	CA-CB-SG-CD
1	В	83	143	OF-CF-CI-CJ
1	В	83	143	CE-CF-CI-CJ
1	А	83	143	CA-CB-SG-CD
1	А	83	143	OF-CF-CI-CJ

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	83	143	1	0
1	А	83	143	7	0



#### 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	Turne	Chain	Res	Link	B	ond leng	$\operatorname{gths}$	Bond angles		
	Type		nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	А	806	-	4, 4, 4	0.28	0	$^{6,6,6}$	0.11	0
3	SO4	А	802	-	4,4,4	0.27	0	$^{6,6,6}$	0.15	0
3	SO4	В	803	-	$4,\!4,\!4$	0.20	0	$6,\!6,\!6$	0.09	0
3	SO4	А	801	-	4,4,4	0.28	0	$6,\!6,\!6$	0.08	0
3	SO4	В	804	-	$4,\!4,\!4$	0.23	0	$^{6,6,6}$	0.11	0
4	POP	В	999	-	6,8,8	1.15	0	13, 13, 13	2.07	6 (46%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POP	В	999	-	-	0/6/6/6	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	В	999	POP	P2-O-P1	3.88	146.14	132.83
4	В	999	POP	O5-P2-O	-3.54	92.76	104.64
4	В	999	POP	O5-P2-O4	-2.83	99.61	110.68
4	В	999	POP	O-P2-O4	2.70	126.18	111.19
4	В	999	POP	O6-P2-O4	2.51	120.52	110.68

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mo	Chain	Res	Type	Clashes	Symm-Clashes
4	В	999	POP	5	0

### 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		$OWAB(Å^2)$	Q<0.9
1	А	536/555~(96%)	0.54	25 (4%) 31	37	16, 28, 50, 72	0
1	В	536/555~(96%)	0.52	21 (3%) 39	45	17, 29, 49, 72	0
All	All	1072/1110~(96%)	0.53	46 (4%) 35	41	16, 29, 49, 72	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	259	LYS	6.4
1	А	250	ASP	4.7
1	А	304	ASP	4.3
1	В	276	LEU	4.1
1	В	254	LEU	3.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$Q{<}0.9$
1	143	А	83	16/17	0.72	0.39	$20,\!25,\!49,\!51$	0
1	143	В	83	16/17	0.76	0.25	$20,\!25,\!49,\!51$	0

### 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.



### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
3	SO4	А	806	5/5	0.80	0.20	74,75,76,76	0
4	POP	В	999	9/9	0.83	0.32	$52,\!55,\!57,\!57$	0
3	SO4	А	802	5/5	0.93	0.17	$57,\!57,\!58,\!58$	0
3	SO4	А	801	5/5	0.95	0.09	$59,\!60,\!60,\!60$	0
3	SO4	В	804	5/5	0.95	0.12	$51,\!51,\!51,\!51$	0
3	SO4	В	803	5/5	0.97	0.20	49,52,52,52	0
2	NI	А	902	1/1	0.99	0.11	$26,\!26,\!26,\!26$	0
2	NI	В	901	1/1	0.99	0.08	27,27,27,27	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

