

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

#### Nov 14, 2023 – 11:54 AM JST

PDB ID	:	5Z4W
Title	:	Crystal structure of signalling protein from buffalo (SPB-40) with an altered
		conformation of Trp78 at 1.79 A resolution
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Deposited on		
Resolution	:	1.79 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

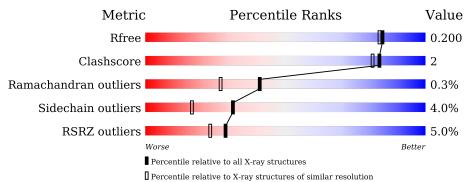
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.79 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 >=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	361	86%	12%	•



#### $5\mathrm{Z4W}$

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3284 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.

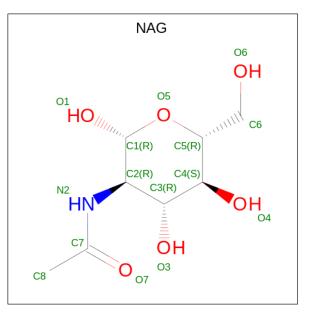
• Molecule 1 is a protein called Chitinase-3-like protein 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	361	Total 2874	C 1841	N 499	O 525	${ m S} 9$	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	?	-	ASP	deletion	UNP Q7YS85

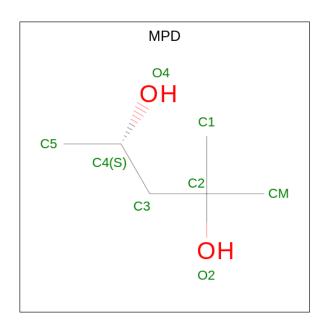
• Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	А	1	Total 14	C 8	N 1	O 5	0	0

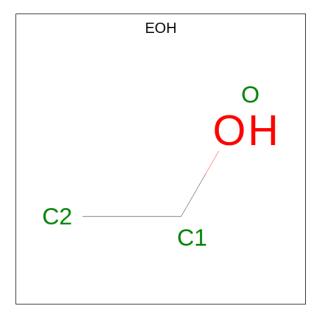
• Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	А	1	Total 8	С 6	O 2	0	0

• Molecule 4 is ETHANOL (three-letter code: EOH) (formula:  $C_2H_6O$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	А	1	Total 3	С 2	0 1	0	0

• Molecule 5 is water.

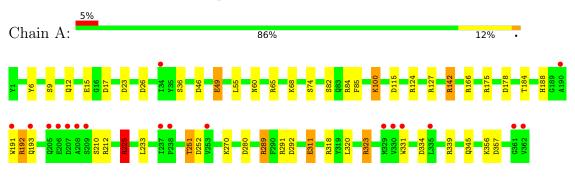


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	А	385	Total 385	O 385	0	0



# 3 Residue-property plots (i)

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: Chitinase-3-like protein 1



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	61.07Å 66.73Å 106.07Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	56.49 - 1.79	Depositor
Resolution (A)	31.24 - 1.79	EDS
% Data completeness	98.6 (56.49-1.79)	Depositor
(in resolution range)	98.6(31.24-1.79)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.06	Depositor
$< I/\sigma(I) > 1$	$2.39 (at 1.79 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
D D.	0.150 , $0.186$	Depositor
$R, R_{free}$	0.163 , $0.200$	DCC
$R_{free}$ test set	2058 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	23.6	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35, 45.1	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3284	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 5.57% 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: MPD, EOH, NAG

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).

Mal	Chain	Bo	nd lengths	Bo	ond angles
Mol Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	1.50	22/2952~(0.7%)	1.54	39/4005~(1.0%)

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	А	0	1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	311	GLU	CD-OE1	11.55	1.38	1.25
1	А	311	GLU	CG-CD	8.95	1.65	1.51
1	А	166	ARG	CZ-NH1	8.03	1.43	1.33
1	А	289	ARG	CD-NE	-7.57	1.33	1.46
1	А	82	SER	CB-OG	7.33	1.51	1.42

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	289	ARG	NE-CZ-NH2	-21.97	109.32	120.30
1	А	323	ARG	NE-CZ-NH2	-19.90	110.35	120.30
1	А	318	ARG	NE-CZ-NH2	-17.56	111.52	120.30
1	А	166	ARG	NE-CZ-NH1	16.62	128.61	120.30
1	А	318	ARG	NE-CZ-NH1	15.07	127.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	289	ARG	Sidechain

### 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	2874	0	2805	13	0
2	А	14	0	13	1	0
3	А	8	0	14	0	0
4	А	3	0	6	0	0
5	А	385	0	0	7	0
All	All	3284	0	2838	14	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 2.

The worst 5 of 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)	
1:A:192:ARG:O	1:A:193:GLN:HB2	1.68	0.91	
2:A:401:NAG:O3	5:A:501:HOH:O	2.00	0.80	
1:A:311:GLU:HG2	5:A:787:HOH:O	1.92	0.68	
1:A:251:THR:HG23	5:A:703:HOH:O	2.09	0.52	
1:A:49:GLU:OE2	5:A:502:HOH:O	2.20	0.48	

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	359/361~(99%)	350~(98%)	8 (2%)	1 (0%)	41 27		

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	212	ARG

#### 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	302/302~(100%)	290~(96%)	12~(4%)	31 16

5 of 12 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	225	ARG
1	А	251	THR
1	А	345	GLN
1	А	270	LYS
1	А	100	LYS

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

#### 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

3 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	pe Chain	Chain	Chain	nain Res	Link	Bo	Bond lengths			Bond angles		
IVIOI	туре	De Chain Res Link		LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2			
4	EOH	А	403	-	2,2,2	0.54	0	$1,\!1,\!1$	0.22	0			
2	NAG	А	401	1	14,14,15	1.19	2 (14%)	17,19,21	1.09	2 (11%)			
3	MPD	А	402	-	7,7,7	0.59	0	9,10,10	0.87	0			

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
2	NAG	А	401	1	-	0/6/23/26	0/1/1/1
3	MPD	А	402	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	401	NAG	O5-C1	-2.42	1.39	1.43
2	А	401	NAG	C2-N2	-2.09	1.42	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	401	NAG	O3-C3-C2	-2.14	105.04	109.47
2	А	401	NAG	C3-C4-C5	-2.07	106.54	110.24

There are no chirality outliers.



All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	402	MPD	C2-C3-C4-O4
3	А	402	MPD	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	401	NAG	1	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,  $95^{th}$  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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	361/361~(100%)	0.09	18 (4%) 28 23	16, 26, 47, 126	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	209	SER	8.2
1	А	206	GLU	8.1
1	А	208	ALA	7.9
1	А	362	VAL	7.2
1	А	207	ASP	6.9

### 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)

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	B-factors(Å <sup>2</sup> )	Q < 0.9
3	MPD	А	402	8/8	0.90	0.13	20,28,29,37	0
2	NAG	А	401	14/15	0.92	0.13	32,36,43,44	0
4	EOH	А	403	3/3	0.95	0.25	38,38,40,40	0



## 6.5 Other polymers (i)

There are no such residues in this entry.

