

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

#### May 23, 2023 – 10:30 pm BST

PDB ID	:	8B61
Title	:	Crystal structure of BfrC protein from Bacteroides fragilis NCTC 9343
Authors	:	Antonyuk, S.V.; Barnett, K.; Strange, R.W.; Olczak, T.
Deposited on		
Resolution	:	1.81 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:

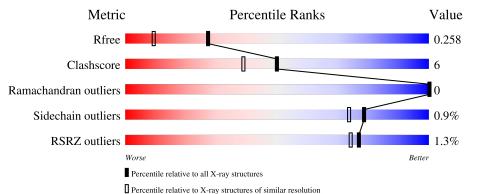
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

# 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 1.81 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	238	% 71%	12%	17%		
1	В	238	% <b>7</b> 5%	8%	16%		

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
2	GOL	А	301	-	-	Х	-



# 2 Entry composition (i)

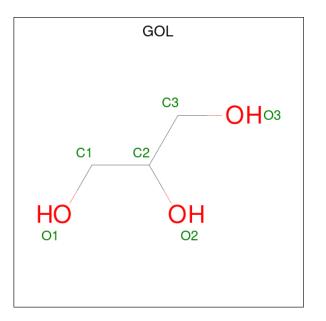
There are 4 unique types of molecules in this entry. The entry contains 6761 atoms, of which 3017 are hydrogens and 0 are deuteriums.

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 Conserved hypothetical lipoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	Δ	197	Total	С	Η	Ν	0	S	48	9	0
1	I A		3053	1001	1475	268	303	6	40	2	0
1	В	200	Total	С	Η	Ν	0	S	50	2	0
	D	200	3117	1025	1502	271	313	6	50	0	0

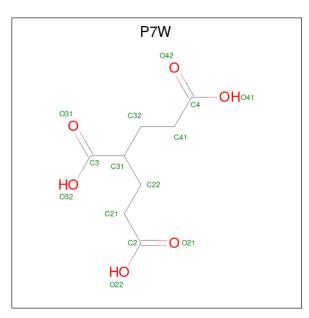
• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total         C         H         O           14         3         8         3	2	0
2	А	1	Total         C         H         O           14         3         8         3	2	0
2	В	1	Total         C         H         O           14         3         8         3	2	0

• Molecule 3 is pentane-1,3,5-tricarboxylic acid (three-letter code: P7W) (formula:  $C_8H_{12}O_6$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total         C         H           22         8         8	0	0
3	В	1	Total         C         H           22         8         8	0	0

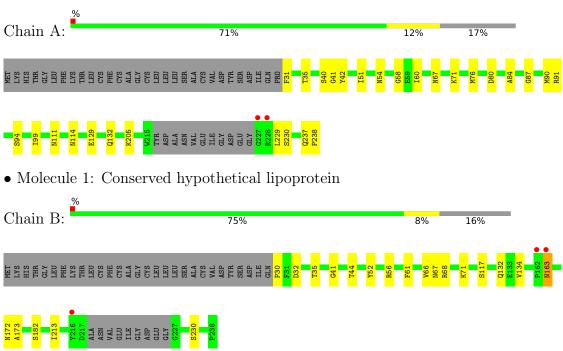
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	246	Total O 247 247	0	5
4	В	258	Total         O           258         258	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: Conserved hypothetical lipoprotein



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	52.08Å 89.84Å 99.06Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	66.55 - 1.81	Depositor
Resolution (A)	66.55 - 1.81	EDS
% Data completeness	99.2 (66.55-1.81)	Depositor
(in resolution range)	$99.1 \ (66.55 - 1.81)$	EDS
R <sub>merge</sub>	0.15	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.48 (at 1.81 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.201 , $0.251$	Depositor
$R, R_{free}$	0.207 , $0.258$	DCC
$R_{free}$ test set	2215 reflections $(5.15\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	21.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39 , $47.7$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6761	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 23.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3464e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: GOL,  $\rm P7W$ 

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	Bo	nd lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.82	1/1628~(0.1%)	0.92	1/2219~(0.0%)	
1	В	0.83	0/1673	0.94	0/2282	
All	All	0.82	1/3301~(0.0%)	0.93	1/4501~(0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	40	SER	CA-CB	-5.09	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	91	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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	1578	1475	1467	19	0
1	В	1615	1502	1500	17	0
2	А	12	16	16	6	0
2	В	6	8	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes					
3	А	14	8	0	1	0					
3	В	14	8	0	0	0					
4	А	247	0	0	6	0					
4	В	258	0	0	6	0					
All	All	3744	3017	2991	36	0					

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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 6.

The worst 5 of 36 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:230:SER:HB3	4:B:454:HOH:O	1.87	0.75
2:A:301:GOL:O1	4:A:401:HOH:O	2.08	0.71
1:B:132[A]:GLN:HG2	1:B:172:ASN:ND2	2.07	0.69
1:A:42:TYR:HD1	2:A:301:GOL:H11	1.58	0.67
1:A:76:MET:O	1:A:99:ILE:HG23	1.95	0.66

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	Perce	ntiles
1	А	194/238~(82%)	193~(100%)	1 (0%)	0	100	100
1	В	199/238~(84%)	198 (100%)	1 (0%)	0	100	100
All	All	393/476~(83%)	391 (100%)	2~(0%)	0	100	100

There are no Ramachandran outliers to report.



#### 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	168/201~(84%)	168 (100%)	0	100 100		
1	В	173/201~(86%)	170 (98%)	3~(2%)	60 50		
All	All	341/402~(85%)	338~(99%)	3 (1%)	78 74		

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	117	SER
1	В	163	ASN
1	В	182	SER

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

Mol	Chain	Res	Type
1	А	114	ASN
1	А	164	ASN
1	А	172	ASN
1	В	172	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 monosaccharides in this entry.



### 5.6 Ligand geometry (i)

5 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	Turne	Chain	Res	Link	Bo	Bond lengths			Bond angles		
Moi Type	Type		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
2	GOL	А	301	-	$5,\!5,\!5$	0.20	0	$5,\!5,\!5$	0.81	0	
3	P7W	В	302	-	$13,\!13,\!13$	1.06	0	16, 16, 16	1.12	1 (6%)	
2	GOL	А	302	-	$5,\!5,\!5$	0.17	0	$5,\!5,\!5$	0.38	0	
2	GOL	В	301	-	$5,\!5,\!5$	0.21	0	$5,\!5,\!5$	0.47	0	
3	P7W	А	303	-	$13,\!13,\!13$	1.20	2 (15%)	16, 16, 16	1.12	2 (12%)	

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	GOL	А	301	-	-	2/4/4/4	-
3	P7W	В	302	-	-	7/14/14/14	-
2	GOL	А	302	-	-	2/4/4/4	-
2	GOL	В	301	-	-	2/4/4/4	-
3	P7W	А	303	-	-	5/14/14/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	А	303	P7W	O22-C2	-2.33	1.22	1.30
3	А	303	P7W	O42-C4	2.28	1.29	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	303	P7W	O31-C3-C31	-2.35	117.19	122.93
3	В	302	P7W	O21-C2-C21	-2.08	116.40	123.08

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	303	P7W	C22-C21-C2	-2.05	107.06	112.51

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	301	GOL	O1-C1-C2-C3
2	В	301	GOL	O1-C1-C2-O2
2	В	301	GOL	O1-C1-C2-C3
3	А	303	P7W	O31-C3-C31-C32
3	А	303	P7W	O32-C3-C31-C32

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	301	GOL	5	0
2	А	302	GOL	1	0
2	В	301	GOL	1	0
3	А	303	P7W	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	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	197/238~(82%)	-0.14	2 (1%) 82 80	16, 27, 48, 74	4 (2%)
1	В	200/238~(84%)	-0.25	3 (1%) 73 70	16, 25, 49, 78	2 (1%)
All	All	397/476~(83%)	-0.20	5 (1%) 77 74	16, 26, 48, 78	6 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	216	TYR	6.0
1	В	163	ASN	3.5
1	А	228	ARG	2.9
1	А	227	GLY	2.9
1	В	162	PRO	2.2

#### 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
3	P7W	В	302	14/14	0.62	0.27	$55,\!63,\!71,\!77$	0
3	P7W	А	303	14/14	0.74	0.24	54,59,66,73	0
2	GOL	А	302	6/6	0.82	0.19	20,46,49,49	2
2	GOL	А	301	6/6	0.88	0.14	20,40,44,46	2
2	GOL	В	301	6/6	0.91	0.15	20,37,39,41	2

## 6.5 Other polymers (i)

There are no such residues in this entry.

