

Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 09:27 pm BST

PDB ID	:	4AYN
Title	:	Structure of the C-terminal barrel of Neisseria meningitidis FHbp Variant 2
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		Cumber, E.; Jones, R.; Newham, L.; Staunton, D.; Borrow, R.; Pickering, M.;
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Deposited on	:	2012-06-21
Resolution	:	2.06 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* 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:

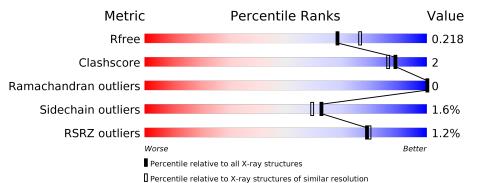
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (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 2.06 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	$egin{array}{c} \mathbf{Whole \ archive} \ (\#\mathbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R _{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	267	% • 44%	•	53%	_			
1	В	267	42%	•	55%				



4AYN

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2060 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Δ	125	Total	С	Ν	Ο	0	0	0
		120	973	605	179	189	0	0	0
1	р	119	Total	С	Ν	Ο	0	0	0
	D	119	922	574	167	181	0	0	0

• Molecule 1 is a protein called FACTOR H-BINDING PROTEIN.

Chain	Residue	Modelled	Actual	Comment	Reference
А	61	MET	-	expression tag	UNP C6KHT4
A	62	GLY	-	expression tag	UNP C6KHT4
А	63	PRO	-	expression tag	UNP C6KHT4
А	64	ASP	-	expression tag	UNP C6KHT4
А	65	SER	-	expression tag	UNP C6KHT4
А	66	ASP	-	expression tag	UNP C6KHT4
А	67	ARG	-	expression tag	UNP C6KHT4
А	68	LEU	-	expression tag	UNP C6KHT4
A	69	GLN	-	expression tag	UNP C6KHT4
А	70	GLN	-	expression tag	UNP C6KHT4
А	71	ARG	-	expression tag	UNP C6KHT4
A	72	ARG	-	expression tag	UNP C6KHT4
А	321	LEU	-	expression tag	UNP C6KHT4
А	322	GLU	-	expression tag	UNP C6KHT4
А	323	HIS	-	expression tag	UNP C6KHT4
А	324	HIS	-	expression tag	UNP C6KHT4
А	325	HIS	-	expression tag	UNP C6KHT4
А	326	HIS	-	expression tag	UNP C6KHT4
A	327	HIS	-	expression tag	UNP C6KHT4
А	328	HIS	-	expression tag	UNP C6KHT4
А	211	SER	GLY	conflict	UNP C6KHT4
В	61	MET	-	expression tag	UNP C6KHT4
В	62	GLY	-	expression tag	UNP C6KHT4
В	63	PRO	-	expression tag	UNP C6KHT4
В	64	ASP	-	expression tag	UNP C6KHT4

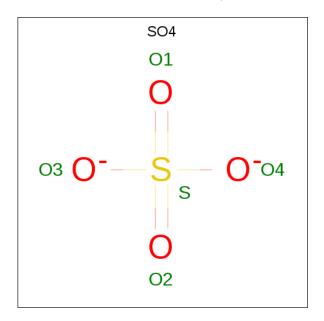
There are 42 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual Comment		Reference
В	65	SER	-	expression tag	UNP C6KHT4
В	66	ASP	-	expression tag	UNP C6KHT4
В	67	ARG	-	expression tag	UNP C6KHT4
В	68	LEU	-	expression tag	UNP C6KHT4
В	69	GLN	-	expression tag	UNP C6KHT4
В	70	GLN	-	expression tag	UNP C6KHT4
В	71	ARG	-	expression tag	UNP C6KHT4
В	72	ARG	-	expression tag	UNP C6KHT4
В	321	LEU	-	expression tag	UNP C6KHT4
В	322	GLU	-	expression tag	UNP C6KHT4
В	323	HIS	-	expression tag	UNP C6KHT4
В	324	HIS	-	expression tag	UNP C6KHT4
В	325	HIS	-	expression tag	UNP C6KHT4
В	326	HIS	-	expression tag	UNP C6KHT4
В	327	HIS	-	expression tag	UNP C6KHT4
В	328	HIS	-	expression tag	UNP C6KHT4
В	211	SER	GLY	conflict	UNP C6KHT4

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• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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



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

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	64	Total O 64 64	0	0
3	В	56	Total O 56 56	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.

• Molec	ule 1:	FAC	TOR	H-B	SINI	DIN	[G]	PRO)TI	EIN											
Chain A	A:		44	%			_	•	_	-	-	-	53%	6		-	_	-			
MET GLY PRO ASP SER	ARG LEU GLN GLN	ARG ARG VAL ALA	ALA ASP ILE GLY	ALA GLY LEU	ALA ASP AIA	LEU THR	ALA PRO 1 EII	ASP HIS	ASP	L YS SER LEU	GLN SER	LEU THR	ASP GLN	SER VAL	ARG	GLU GLU LYS	T I I I I I I I I I I I I I I I I I I I	LEU ALA ATA	GLY	ALA GLU	
THR TYR GLY GLY SN SP	SER LEU ASN THR	GLY LYS LYS	ASN ASP LYS VAL	SER ARG PHE	ASP PHE TI F	ARG GLN	ILE GLU VAT	ASP GLY	GLN GLN	THR THR LEU	GLU SER	GLU GLU	GLN GLN	TYR LYS	GLN	HIS SER ALA	VAL VAL	ALA LEU CI N	ILE GLU	LYS	1100
ASN PRO ASP LLY ILE ASP	SER IEU ILE ASN	GLN ARG SER PHE	LEU VAL SER GLY	LEU G200 G201	<mark>1208</mark>	S281	R295	2302 2302	<mark>E313</mark>	K319 0320	L321 E322	H325 1116	HIS HIS								
• Molec	ule 1:	FAC	TOR	H-B	INI	DIN	[G]	PRO)TI	EIN											
Chain E	3:		429	6			•						55%								
MET GLY PRO ASP SER ASP	ARG LEU GLN GLN	ARG ARG VAL ALA	ALA ASP ILE GLY	ALA GLY LEU	ALA ASP AIA	LEU	ALA PRO 1 EII	ASP HIS	ASP	L TEU L EU	GLN SER	THR	ASP GLN	SER VAL	ARG	GLU LYS	LEU LEU	LEU ALA ATA	GLY	ALA GLU	1
THR TYR GLY ASN GLY	SER LEU ASN THR	GLY LYS LYS	ASN ASP LYS VAL	SER ARG PHE	ASP PHE TIF	ARG GLN	ILE GLU VAT	ASP GLY	GLN	THR	GLU SER	GLU GLU	GLN GLN	TYR LYS	G LLN ASP	HIS SER ALA	VAL. VAL	ALA LEU GIN	ULE GLU	LYS	1170
ASN PRO ASP LYS ILE ASP	SER LEU ILE ASN	GLN ARG SER PHE	LEU VAL SER GLY	LEU GLY G201	E2 16	S269	H288	2302 2302	E313	K319 0320	GLU GLU	SIH SIH	SIH SIH	SIH							



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	74.79Å 75.95 Å 40.90 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 - 2.06	Depositor
Resolution (A)	53.29 - 2.06	EDS
% Data completeness	98.6 (15.00-2.06)	Depositor
(in resolution range)	$98.6\ (53.29-2.06)$	EDS
R _{merge}	0.04	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$6.10 ({\rm at}2.07{ m \AA})$	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
P. P.	0.179 , 0.213	Depositor
R, R_{free}	0.182 , 0.218	DCC
R_{free} test set	746 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	27.1	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 54.6	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2060	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.56% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: 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		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.55	0/994	0.68	0/1334	
1	В	0.52	0/940	0.68	0/1261	
All	All	0.54	0/1934	0.68	0/2595	

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	973	0	931	3	0
1	В	922	0	890	4	0
2	А	30	0	0	0	0
2	В	15	0	0	1	0
3	А	64	0	0	0	0
3	В	56	0	0	1	0
All	All	2060	0	1821	7	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.

All (7) close contacts within the same asymmetric unit are listed below, sorted by their clash



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLU:OE2	3:B:2013:HOH:O	2.13	0.67
1:B:302:SER:HB2	1:B:313:GLU:OE2	2.03	0.58
1:A:302:SER:HB2	1:A:313:GLU:OE2	2.04	0.58
1:B:288:HIS:NE2	2:B:1322:SO4:O1	2.45	0.49
1:A:298:GLU:HG2	1:A:319:LYS:HG2	1.95	0.48
1:B:298:GLU:HG2	1:B:319:LYS:HG2	1.96	0.46
1:A:295:ARG:HD2	1:A:295:ARG:HA	1.70	0.42

magnitude.

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	123/267~(46%)	122~(99%)	1 (1%)	0	100	100
1	В	117/267~(44%)	116~(99%)	1 (1%)	0	100	100
All	All	240/534~(45%)	238~(99%)	2(1%)	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	98/220~(44%)	96~(98%)	2(2%)	55 51	



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	В	93/220~(42%)	92~(99%)	1 (1%)	73 72
All	All	191/440~(43%)	188 (98%)	3 (2%)	62 59

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

Mol	Chain	Res	Type
1	А	208	GLN
1	А	320	GLN
1	В	269	SER

Some 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 carbohydrates in this entry.

5.6 Ligand geometry (i)

9 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	Chain	Res	Link	B	ond leng	gths	В	ond ang	gles
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	А	1327	-	4,4,4	0.23	0	6,6,6	0.14	0



Mol	Turne	Chain	Res	Link	B	ond leng	gths	Bond angles		
	Type	Cham	nes	Res Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	А	1331	-	$4,\!4,\!4$	0.27	0	6,6,6	0.27	0
2	SO4	В	1323	-	$4,\!4,\!4$	0.14	0	6,6,6	0.08	0
2	SO4	В	1321	-	4,4,4	0.12	0	6,6,6	0.16	0
2	SO4	А	1326	-	4,4,4	0.20	0	6,6,6	0.20	0
2	SO4	А	1329	-	$4,\!4,\!4$	0.15	0	6,6,6	0.17	0
2	SO4	А	1328	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	В	1322	-	$4,\!4,\!4$	0.17	0	6,6,6	0.35	0
2	SO4	А	1330	-	4,4,4	0.18	0	6,6,6	0.26	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1322	SO4	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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$Q{<}0.9$
1	А	125/267~(46%)	0.02	3 (2%) 59 61	16, 26, 49, 65	0
1	В	119/267~(44%)	-0.03	0 100 100	19, 27, 50, 72	0
All	All	244/534~(45%)	-0.01	3 (1%) 79 80	16, 27, 50, 72	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	201	GLY	3.0
1	А	281	SER	2.6
1	А	322	GLU	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 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
2	SO4	В	1322	5/5	0.84	0.28	$71,\!73,\!74,\!75$	0
2	SO4	А	1329	5/5	0.90	0.19	$76,\!77,\!78,\!80$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({f A}^2)$	$\mathbf{Q}{<}0.9$
2	SO4	В	1323	5/5	0.90	0.17	109, 109, 110, 110	0
2	SO4	А	1328	5/5	0.91	0.31	73,76,77,77	0
2	SO4	В	1321	5/5	0.92	0.24	$76,\!77,\!78,\!78$	0
2	SO4	А	1330	5/5	0.94	0.22	59,60,62,63	0
2	SO4	А	1331	5/5	0.95	0.18	$57,\!59,\!59,\!60$	0
2	SO4	А	1326	5/5	0.95	0.16	49,50,51,54	0
2	SO4	А	1327	5/5	0.95	0.18	76,78,79,80	0

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6.5 Other polymers (i)

There are no such residues in this entry.

