



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 06:11 PM EDT

PDB ID : 6H2F  
Title : Structure of the pre-pore AhlB of the tripartite alpha-pore forming toxin, AHL, from *Aeromonas hydrophila*.  
Authors : Churchill-Angus, A.M.; Wilson, J.S.; Baker, P.J.  
Deposited on : 2018-07-13  
Resolution : 2.55 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

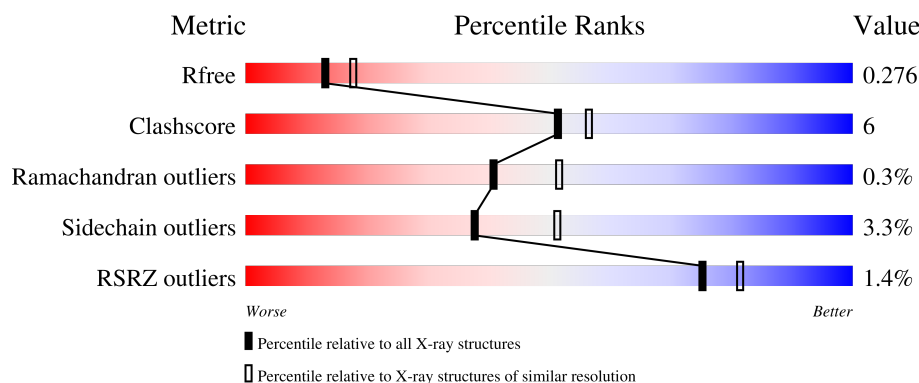
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 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	367	<div> <div>79%</div> <div>10% • 10%</div> </div>
1	B	367	<div> <div>2%</div> <div>81%</div> <div>12% • 6%</div> </div>
1	C	367	<div> <div>%</div> <div>77%</div> <div>13% • 8%</div> </div>
1	D	367	<div> <div>2%</div> <div>75%</div> <div>17% • 8%</div> </div>
1	E	367	<div> <div></div> <div>76%</div> <div>13% • 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	367	
1	G	367	
1	H	367	
1	I	367	
1	J	367	

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	PO4	C	401	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24766 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 AhlB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2436	1515	424	489	8			
1	B	344	Total	C	N	O	S	0	0	0
			2533	1584	439	504	6			
1	C	338	Total	C	N	O	S	0	0	0
			2485	1546	431	500	8			
1	D	338	Total	C	N	O	S	0	0	0
			2493	1558	433	496	6			
1	E	329	Total	C	N	O	S	0	0	0
			2424	1507	422	487	8			
1	F	326	Total	C	N	O	S	0	0	0
			2398	1498	415	479	6			
1	G	328	Total	C	N	O	S	0	0	0
			2417	1503	421	485	8			
1	H	345	Total	C	N	O	S	0	0	0
			2550	1594	444	506	6			
1	I	338	Total	C	N	O	S	0	0	0
			2485	1546	431	500	8			
1	J	343	Total	C	N	O	S	0	0	0
			2525	1578	438	503	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	LEU	-	expression tag	UNP A0A081US78
A	361	GLU	-	expression tag	UNP A0A081US78
A	362	HIS	-	expression tag	UNP A0A081US78
A	363	HIS	-	expression tag	UNP A0A081US78
A	364	HIS	-	expression tag	UNP A0A081US78
A	365	HIS	-	expression tag	UNP A0A081US78
A	366	HIS	-	expression tag	UNP A0A081US78
A	367	HIS	-	expression tag	UNP A0A081US78
B	360	LEU	-	expression tag	UNP A0A081US78

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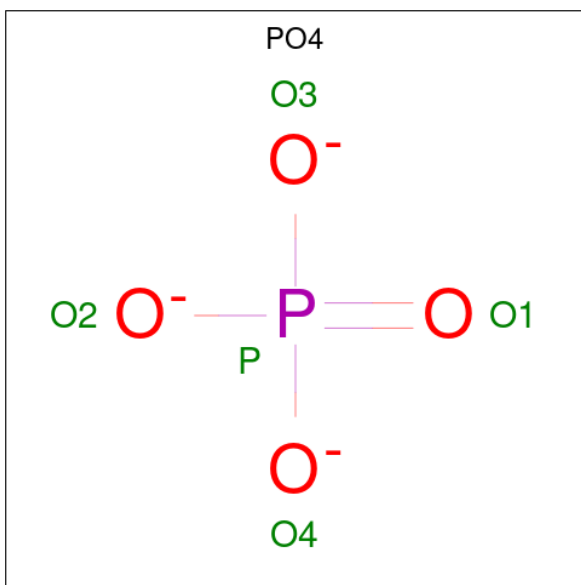
Chain	Residue	Modelled	Actual	Comment	Reference
B	361	GLU	-	expression tag	UNP A0A081US78
B	362	HIS	-	expression tag	UNP A0A081US78
B	363	HIS	-	expression tag	UNP A0A081US78
B	364	HIS	-	expression tag	UNP A0A081US78
B	365	HIS	-	expression tag	UNP A0A081US78
B	366	HIS	-	expression tag	UNP A0A081US78
B	367	HIS	-	expression tag	UNP A0A081US78
C	360	LEU	-	expression tag	UNP A0A081US78
C	361	GLU	-	expression tag	UNP A0A081US78
C	362	HIS	-	expression tag	UNP A0A081US78
C	363	HIS	-	expression tag	UNP A0A081US78
C	364	HIS	-	expression tag	UNP A0A081US78
C	365	HIS	-	expression tag	UNP A0A081US78
C	366	HIS	-	expression tag	UNP A0A081US78
C	367	HIS	-	expression tag	UNP A0A081US78
D	360	LEU	-	expression tag	UNP A0A081US78
D	361	GLU	-	expression tag	UNP A0A081US78
D	362	HIS	-	expression tag	UNP A0A081US78
D	363	HIS	-	expression tag	UNP A0A081US78
D	364	HIS	-	expression tag	UNP A0A081US78
D	365	HIS	-	expression tag	UNP A0A081US78
D	366	HIS	-	expression tag	UNP A0A081US78
D	367	HIS	-	expression tag	UNP A0A081US78
E	360	LEU	-	expression tag	UNP A0A081US78
E	361	GLU	-	expression tag	UNP A0A081US78
E	362	HIS	-	expression tag	UNP A0A081US78
E	363	HIS	-	expression tag	UNP A0A081US78
E	364	HIS	-	expression tag	UNP A0A081US78
E	365	HIS	-	expression tag	UNP A0A081US78
E	366	HIS	-	expression tag	UNP A0A081US78
E	367	HIS	-	expression tag	UNP A0A081US78
F	360	LEU	-	expression tag	UNP A0A081US78
F	361	GLU	-	expression tag	UNP A0A081US78
F	362	HIS	-	expression tag	UNP A0A081US78
F	363	HIS	-	expression tag	UNP A0A081US78
F	364	HIS	-	expression tag	UNP A0A081US78
F	365	HIS	-	expression tag	UNP A0A081US78
F	366	HIS	-	expression tag	UNP A0A081US78
F	367	HIS	-	expression tag	UNP A0A081US78
G	360	LEU	-	expression tag	UNP A0A081US78
G	361	GLU	-	expression tag	UNP A0A081US78
G	362	HIS	-	expression tag	UNP A0A081US78

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Chain	Residue	Modelled	Actual	Comment	Reference
G	363	HIS	-	expression tag	UNP A0A081US78
G	364	HIS	-	expression tag	UNP A0A081US78
G	365	HIS	-	expression tag	UNP A0A081US78
G	366	HIS	-	expression tag	UNP A0A081US78
G	367	HIS	-	expression tag	UNP A0A081US78
H	360	LEU	-	expression tag	UNP A0A081US78
H	361	GLU	-	expression tag	UNP A0A081US78
H	362	HIS	-	expression tag	UNP A0A081US78
H	363	HIS	-	expression tag	UNP A0A081US78
H	364	HIS	-	expression tag	UNP A0A081US78
H	365	HIS	-	expression tag	UNP A0A081US78
H	366	HIS	-	expression tag	UNP A0A081US78
H	367	HIS	-	expression tag	UNP A0A081US78
I	360	LEU	-	expression tag	UNP A0A081US78
I	361	GLU	-	expression tag	UNP A0A081US78
I	362	HIS	-	expression tag	UNP A0A081US78
I	363	HIS	-	expression tag	UNP A0A081US78
I	364	HIS	-	expression tag	UNP A0A081US78
I	365	HIS	-	expression tag	UNP A0A081US78
I	366	HIS	-	expression tag	UNP A0A081US78
I	367	HIS	-	expression tag	UNP A0A081US78
J	360	LEU	-	expression tag	UNP A0A081US78
J	361	GLU	-	expression tag	UNP A0A081US78
J	362	HIS	-	expression tag	UNP A0A081US78
J	363	HIS	-	expression tag	UNP A0A081US78
J	364	HIS	-	expression tag	UNP A0A081US78
J	365	HIS	-	expression tag	UNP A0A081US78
J	366	HIS	-	expression tag	UNP A0A081US78
J	367	HIS	-	expression tag	UNP A0A081US78

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

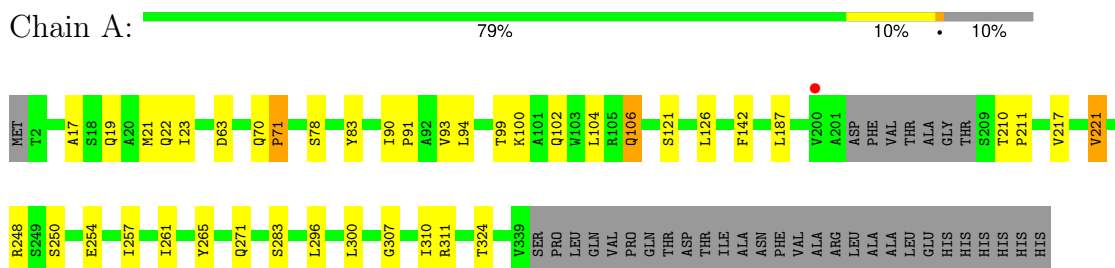


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		

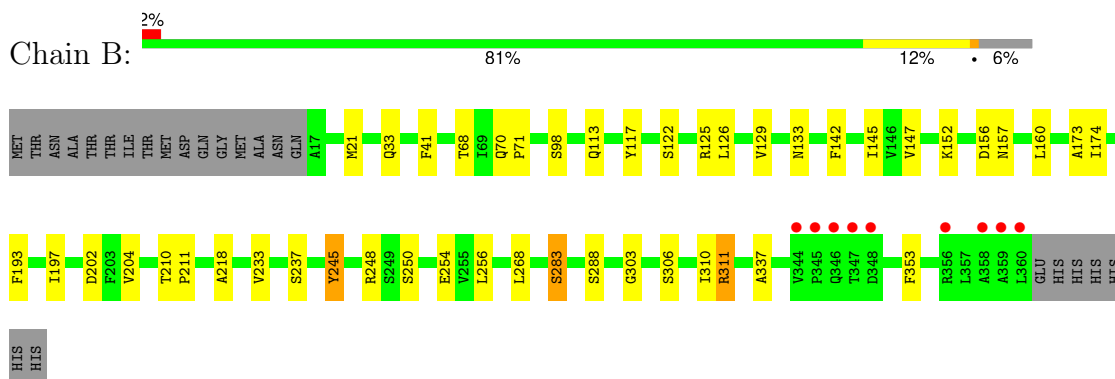
### 3 Residue-property plots

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.

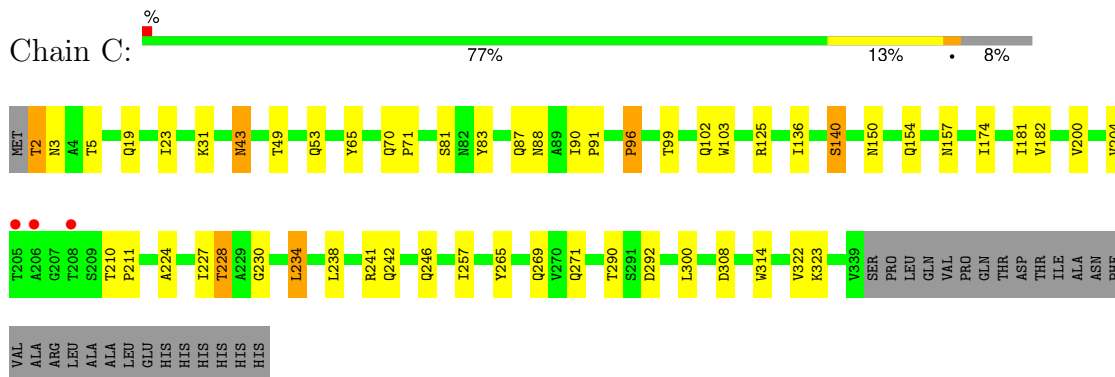
#### • Molecule 1: AhlB



#### • Molecule 1: AhlB

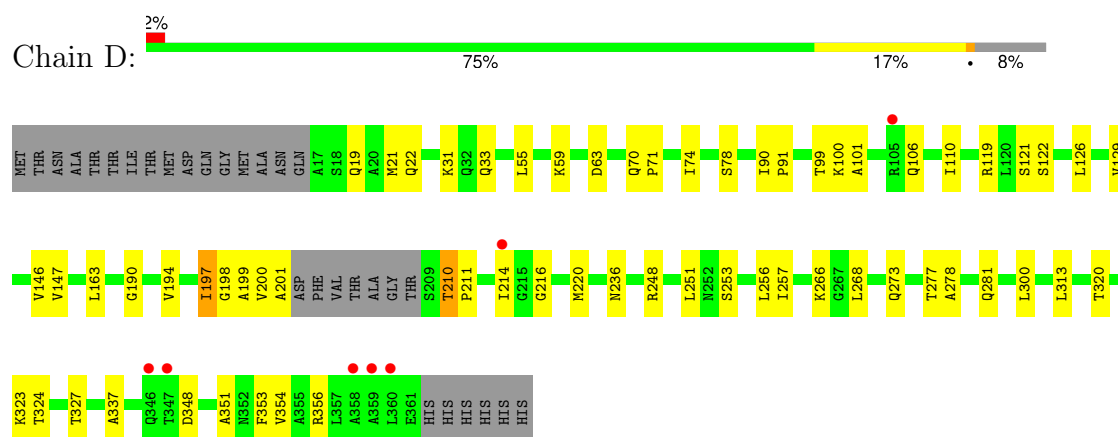


#### • Molecule 1: AhlB

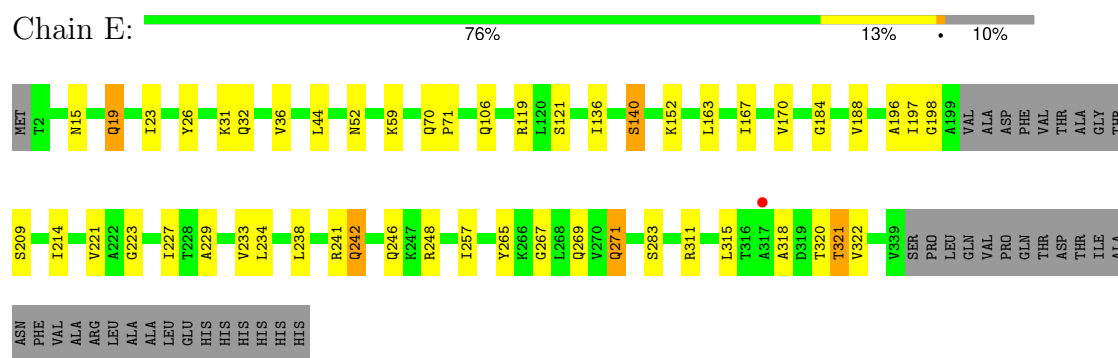


#### • Molecule 1: AhlB

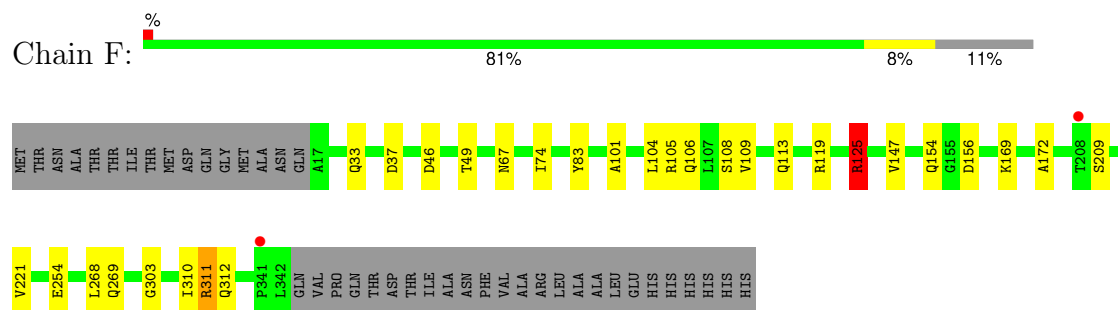




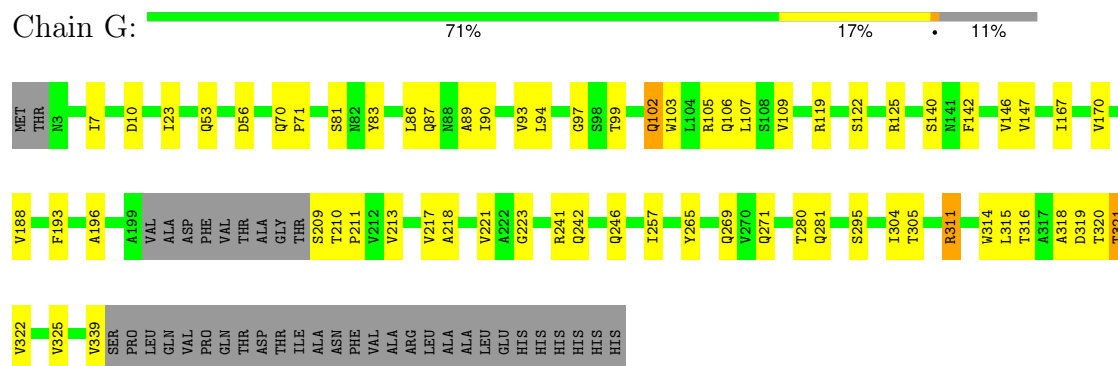
- Molecule 1: AhlB




- Molecule 1: AhlB

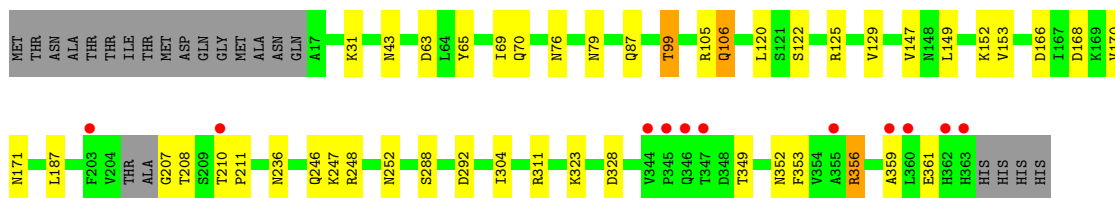


- Molecule 1: AhlB



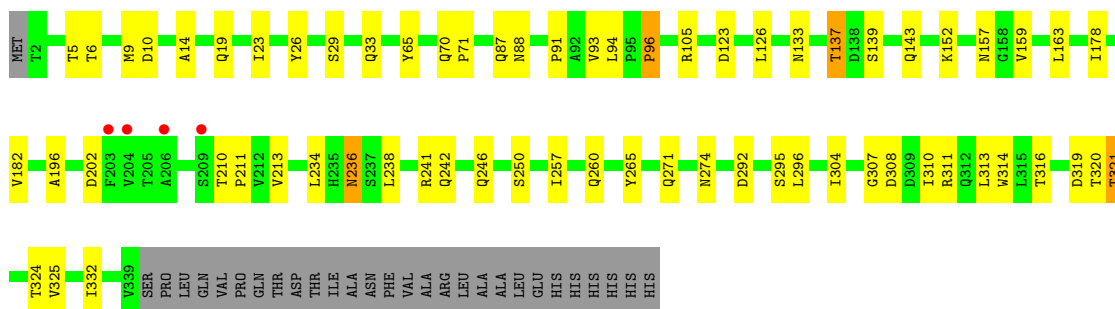
- Molecule 1: AhlB

Chain H: 




• Molecule 1: AhlB

Chain I: 



• Molecule 1: AhlB

Chain J: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.66Å 178.18Å 485.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.55 – 2.55 39.55 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.55-2.55) 99.8 (39.55-2.55)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.191 , 0.278 0.198 , 0.276	Depositor DCC
$R_{free}$ test set	8380 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.6	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	0.93	EDS
Total number of atoms	24766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.58	0/2460	0.81	1/3350 (0.0%)
1	B	0.60	0/2562	0.78	1/3495 (0.0%)
1	C	0.61	0/2511	0.77	0/3422
1	D	0.59	0/2520	0.80	0/3435
1	E	0.59	0/2448	0.81	1/3333 (0.0%)
1	F	0.57	0/2425	0.78	1/3306 (0.0%)
1	G	0.60	1/2441 (0.0%)	0.79	1/3323 (0.0%)
1	H	0.57	0/2580	0.78	1/3517 (0.0%)
1	I	0.59	0/2511	0.79	0/3422
1	J	0.58	0/2554	0.80	0/3484
All	All	0.59	1/25012 (0.0%)	0.79	6/34087 (0.0%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	2
1	F	0	3
1	G	0	2
1	H	0	5
1	I	0	1
1	J	0	3
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	97	GLY	N-CA	6.00	1.55	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	119	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	248	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	F	125	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	324	THR	CA-CB-OG1	-5.27	97.94	109.00
1	E	271	GLN	CB-CA-C	5.20	120.79	110.40

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	ARG	Sidechain
1	B	311	ARG	Sidechain
1	C	125	ARG	Sidechain
1	D	119	ARG	Sidechain
1	D	248	ARG	Sidechain

## 5.2 Too-close contacts

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	2436	0	2465	22	0
1	B	2533	0	2571	25	0
1	C	2485	0	2510	33	0
1	D	2493	0	2532	40	0
1	E	2424	0	2451	29	0
1	F	2398	0	2431	19	0
1	G	2417	0	2444	42	0
1	H	2550	0	2578	23	0
1	I	2485	0	2510	41	0
1	J	2525	0	2560	39	0
2	A	5	0	0	0	0
2	C	5	0	0	2	0
2	G	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	5	0	0	0	0
All	All	24766	0	25052	278	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 6.

The worst 5 of 278 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:I:242:GLN:O	1:I:246:GLN:HG2	1.66	0.93
1:J:302:LYS:O	1:J:306:SER:OG	1.95	0.83
1:A:307:GLY:O	1:A:310:ILE:HG22	1.80	0.80
1:I:139:SER:O	1:I:143:GLN:HG2	1.84	0.77
1:G:94:LEU:O	1:G:311:ARG:NH1	2.18	0.76

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	A	327/367 (89%)	316 (97%)	10 (3%)	1 (0%)	41	51
1	B	342/367 (93%)	337 (98%)	4 (1%)	1 (0%)	41	51
1	C	336/367 (92%)	320 (95%)	15 (4%)	1 (0%)	41	51
1	D	334/367 (91%)	322 (96%)	8 (2%)	4 (1%)	13	17
1	E	325/367 (89%)	313 (96%)	11 (3%)	1 (0%)	41	51
1	F	324/367 (88%)	305 (94%)	19 (6%)	0	100	100
1	G	324/367 (88%)	315 (97%)	9 (3%)	0	100	100
1	H	341/367 (93%)	326 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	336/367 (92%)	321 (96%)	14 (4%)	1 (0%)	41	51
1	J	341/367 (93%)	325 (95%)	16 (5%)	0	100	100
All	All	3330/3670 (91%)	3200 (96%)	121 (4%)	9 (0%)	41	51

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	ASN
1	D	199	ALA
1	E	197	ILE
1	A	100	LYS
1	D	351	ALA

### 5.3.2 Protein sidechains ⓘ

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	265/295 (90%)	255 (96%)	10 (4%)	33	45
1	B	275/295 (93%)	266 (97%)	9 (3%)	38	51
1	C	270/295 (92%)	258 (96%)	12 (4%)	28	38
1	D	271/295 (92%)	266 (98%)	5 (2%)	59	74
1	E	264/295 (90%)	255 (97%)	9 (3%)	37	50
1	F	261/295 (88%)	257 (98%)	4 (2%)	65	77
1	G	263/295 (89%)	252 (96%)	11 (4%)	30	40
1	H	277/295 (94%)	266 (96%)	11 (4%)	31	43
1	I	270/295 (92%)	259 (96%)	11 (4%)	30	41
1	J	274/295 (93%)	266 (97%)	8 (3%)	42	57
All	All	2690/2950 (91%)	2600 (97%)	90 (3%)	38	51

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	315	LEU
1	I	96	PRO
1	G	321	THR
1	H	236	ASN
1	I	202	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	269	GLN
1	J	72	GLN
1	J	269	GLN
1	J	260	GLN
1	D	269	GLN

### 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](#)

4 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PO4	C	401	-	4,4,4	1.28	0	6,6,6	0.97	0
2	PO4	I	401	-	4,4,4	0.98	0	6,6,6	1.71	2 (33%)
2	PO4	G	401	-	4,4,4	1.04	0	6,6,6	0.72	0
2	PO4	A	401	-	4,4,4	1.02	0	6,6,6	1.52	1 (16%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PO4	O3-P-O1	-2.89	100.72	110.95
2	I	401	PO4	O4-P-O2	2.37	115.29	107.91
2	I	401	PO4	O3-P-O2	-2.30	100.76	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PO4	2	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 ⓘ

### 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	331/367 (90%)	-0.56	1 (0%) 94 96	12, 34, 79, 230	0
1	B	344/367 (93%)	-0.54	9 (2%) 56 62	9, 31, 90, 296	0
1	C	338/367 (92%)	-0.57	3 (0%) 84 88	13, 33, 88, 153	0
1	D	338/367 (92%)	-0.48	7 (2%) 63 70	15, 36, 110, 244	0
1	E	329/367 (89%)	-0.49	1 (0%) 94 96	16, 35, 72, 155	0
1	F	326/367 (88%)	-0.57	2 (0%) 89 92	14, 35, 79, 206	0
1	G	328/367 (89%)	-0.56	0 100 100	18, 35, 76, 159	0
1	H	345/367 (94%)	-0.41	11 (3%) 47 55	16, 33, 127, 259	0
1	I	338/367 (92%)	-0.54	4 (1%) 79 84	15, 35, 82, 177	0
1	J	343/367 (93%)	-0.46	8 (2%) 60 67	15, 35, 99, 244	0
All	All	3360/3670 (91%)	-0.52	46 (1%) 75 81	9, 34, 89, 296	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	203	PHE	6.8
1	H	363	HIS	6.6
1	H	359	ALA	6.3
1	D	358	ALA	6.3
1	B	347	THR	6.0

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

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	PO4	A	401	5/5	0.82	0.19	18,27,28,602	0
2	PO4	C	401	5/5	0.90	0.29	45,49,95,157	0
2	PO4	G	401	5/5	0.92	0.15	39,41,102,204	0
2	PO4	I	401	5/5	0.92	0.10	16,20,24,183	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.