



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 2, 2026 – 12:47 AM UTC

PDB ID : 6H2F / pdb_00006h2f
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

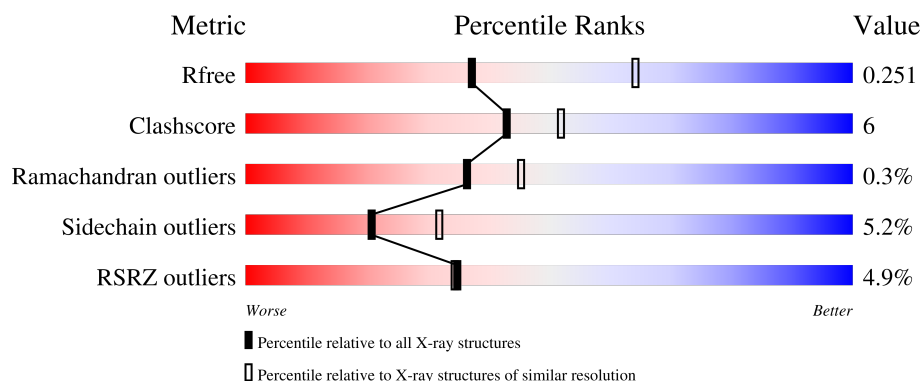
1 Overall quality at a glance

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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 $\leq 5\%$. 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	 3% 75% 13% • 10%
1	B	367	 6% 78% 14% • 6%
1	C	367	 3% 75% 14% • 8%
1	D	367	 6% 71% 19% • 8%
1	E	367	 2% 70% 17% • 10%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

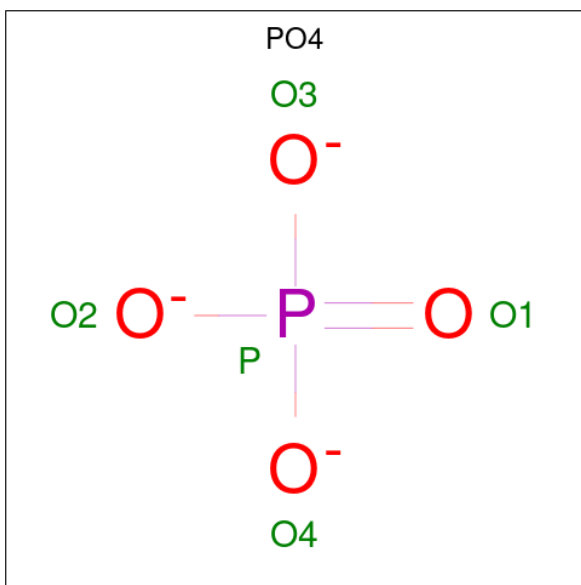
Chain	Residue	Modelled	Actual	Comment	Reference
B	361	GLU	-	expression tag	UNP A0A081US78
B	362	HIS	-	expression tag	UNP A0A081US78
B	363	HIS	-	expression tag	UNP A0A081US78
B	364	HIS	-	expression tag	UNP A0A081US78
B	365	HIS	-	expression tag	UNP A0A081US78
B	366	HIS	-	expression tag	UNP A0A081US78
B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

Continued on next page...

Continued from previous page...

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 (CCD ID: PO4) (formula: O₄P).

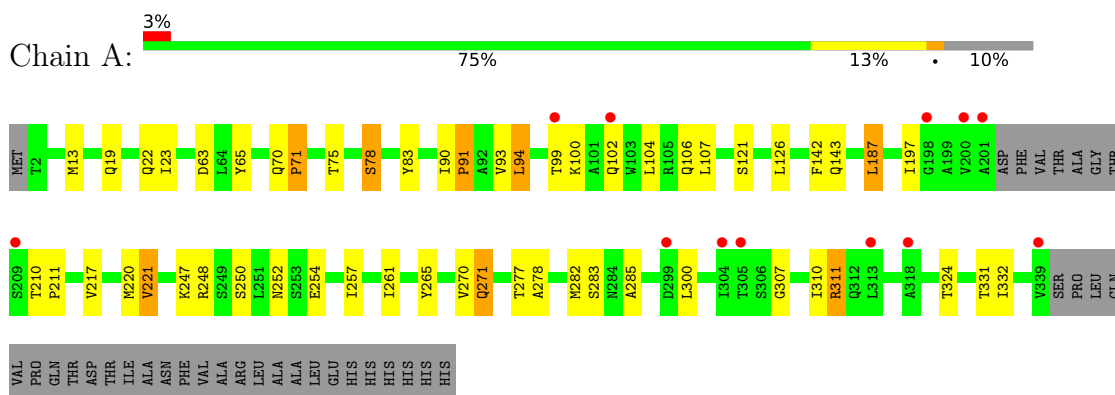


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		

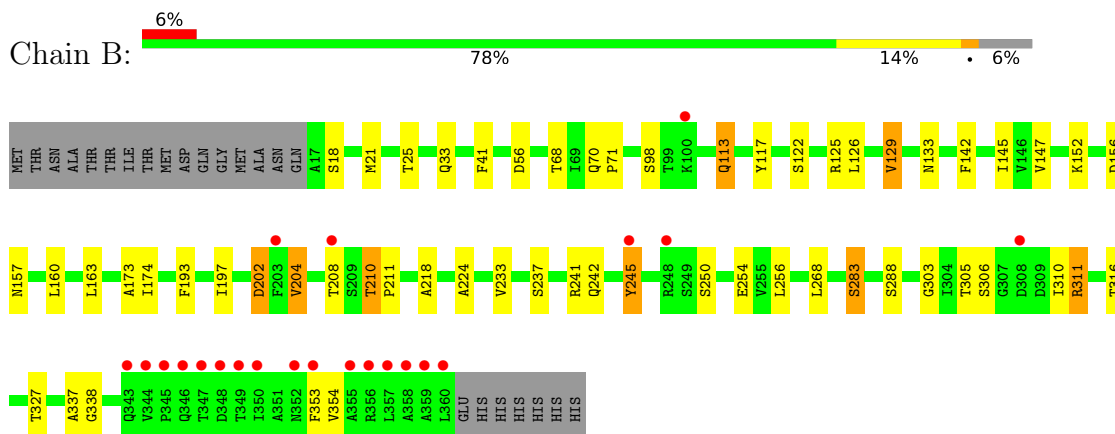
3 Residue-property plots [i](#)

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.

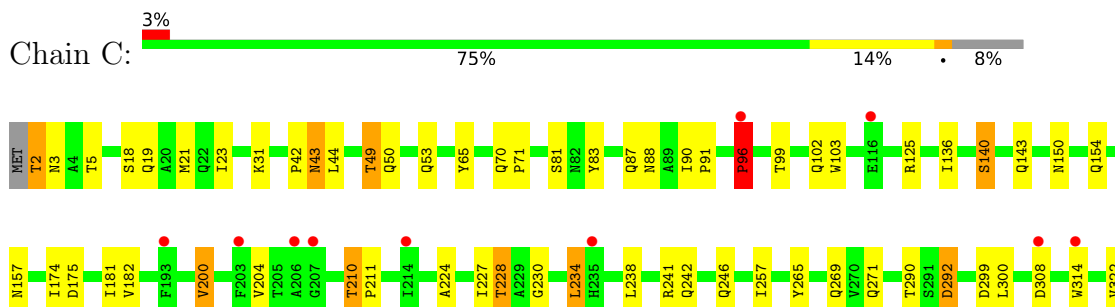
• Molecule 1: AhlB

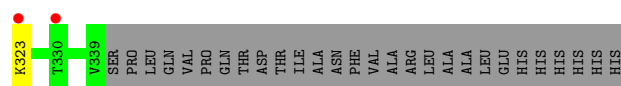


• Molecule 1: AhlB

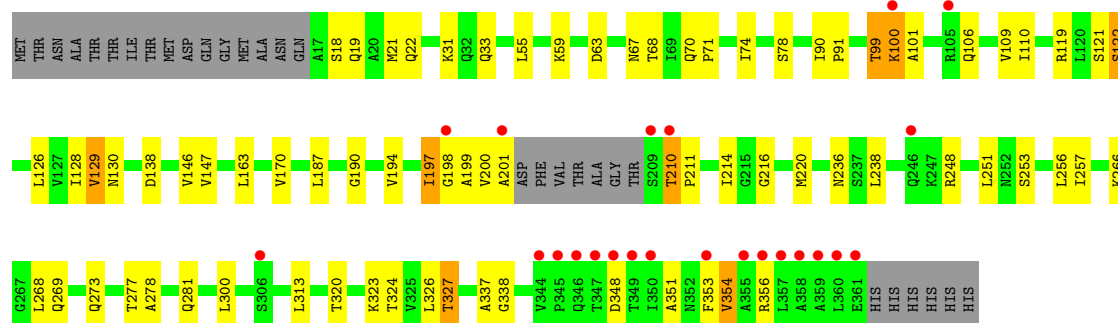


• Molecule 1: AhlB

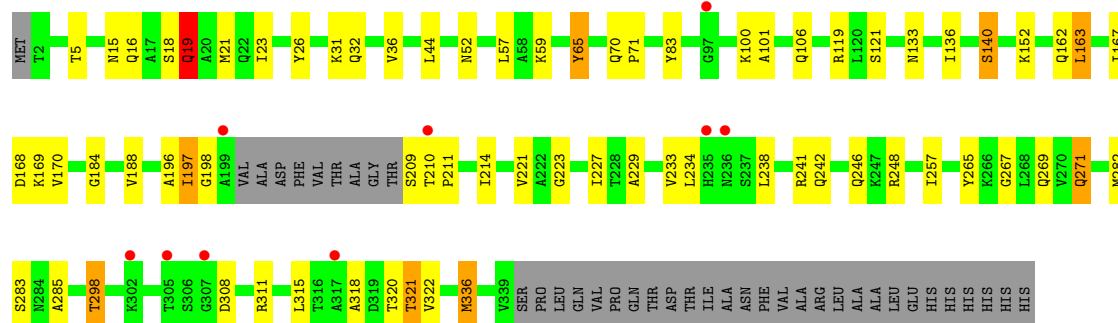




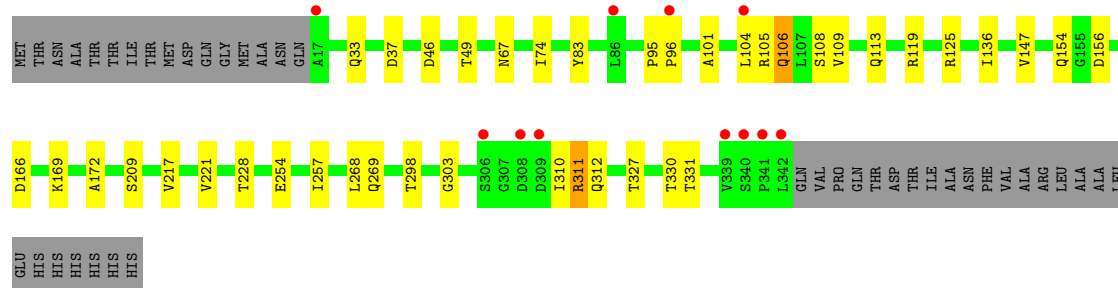
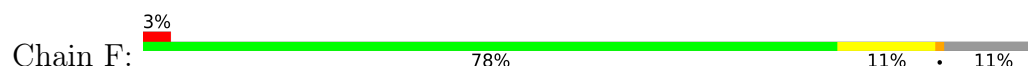
• Molecule 1: AhlB



• Molecule 1: AhlB

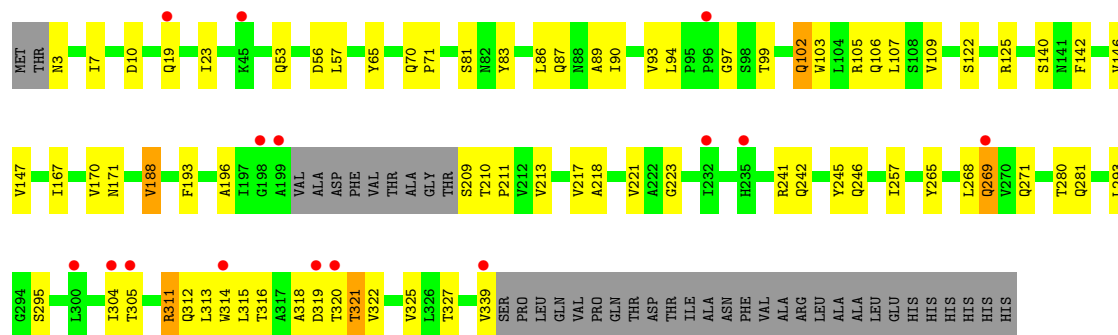


• Molecule 1: AhlB

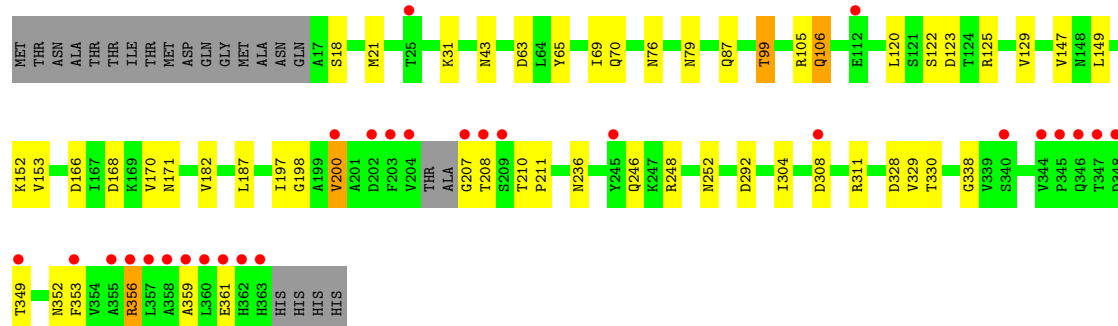
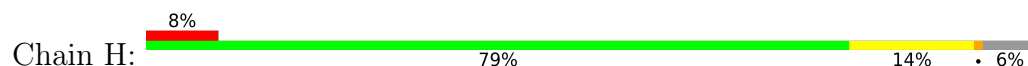


• Molecule 1: AhlB

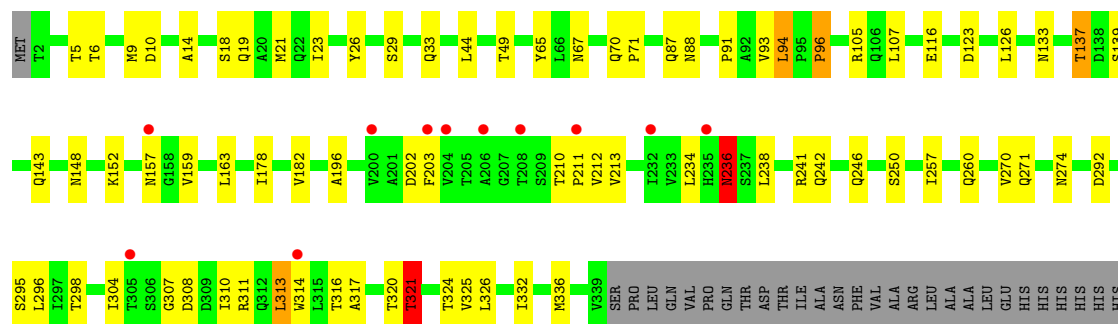




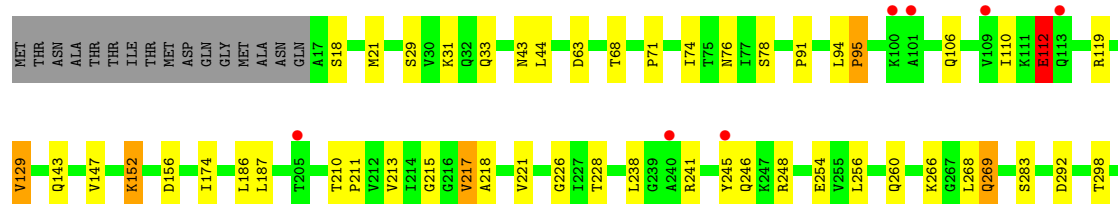
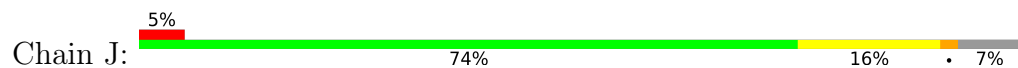
• Molecule 1: AhlB



• Molecule 1: AhlB



• Molecule 1: AhlB





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.191 , 0.278 (Not available) , 0.251	Depositor DCC
R_{free} test set	8387 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24766	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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.

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: 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	0.93	1/2460 (0.0%)	1.39	10/3350 (0.3%)
1	B	0.96	1/2562 (0.0%)	1.33	9/3495 (0.3%)
1	C	0.96	1/2511 (0.0%)	1.36	7/3422 (0.2%)
1	D	0.94	2/2520 (0.1%)	1.36	8/3435 (0.2%)
1	E	0.94	0/2448	1.37	10/3333 (0.3%)
1	F	0.93	0/2425	1.37	6/3306 (0.2%)
1	G	0.95	3/2441 (0.1%)	1.37	8/3323 (0.2%)
1	H	0.93	0/2580	1.36	8/3517 (0.2%)
1	I	0.95	1/2511 (0.0%)	1.35	7/3422 (0.2%)
1	J	0.95	1/2554 (0.0%)	1.39	15/3484 (0.4%)
All	All	0.94	10/25012 (0.0%)	1.36	88/34087 (0.3%)

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	269	GLN	N-CA	7.12	1.55	1.46
1	C	50	GLN	N-CA	6.72	1.54	1.46
1	G	97	GLY	N-CA	6.68	1.55	1.45
1	D	122	SER	N-CA	6.61	1.54	1.46
1	J	29	SER	N-CA	-5.87	1.39	1.46

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	THR	CA-CB-OG1	-7.78	97.94	109.60
1	H	308	ASP	CB-CA-C	-7.38	108.07	116.63
1	J	91	PRO	CB-CA-C	7.12	117.85	111.87
1	D	327	THR	CA-CB-OG1	-7.02	99.07	109.60
1	I	203	PHE	CA-CB-CG	6.93	120.73	113.80

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 [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	A	2436	0	2465	25	0
1	B	2533	0	2571	29	0
1	C	2485	0	2510	36	0
1	D	2493	0	2532	44	0
1	E	2424	0	2451	36	0
1	F	2398	0	2431	20	0
1	G	2417	0	2444	44	0
1	H	2550	0	2578	26	0
1	I	2485	0	2510	44	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2525	0	2560	41	0
2	A	5	0	0	0	0
2	C	5	0	0	2	0
2	G	5	0	0	0	0
2	I	5	0	0	0	0
All	All	24766	0	25052	309	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 309 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%)	36	45
1	B	342/367 (93%)	337 (98%)	4 (1%)	1 (0%)	36	45
1	C	336/367 (92%)	320 (95%)	15 (4%)	1 (0%)	36	45
1	D	334/367 (91%)	322 (96%)	8 (2%)	4 (1%)	10	13
1	E	325/367 (89%)	313 (96%)	11 (3%)	1 (0%)	36	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
1	I	336/367 (92%)	321 (96%)	14 (4%)	1 (0%)	36	45
1	J	341/367 (93%)	325 (95%)	16 (5%)	0	100	100
All	All	3330/3670 (91%)	3200 (96%)	121 (4%)	9 (0%)	36	45

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 [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	A	265/295 (90%)	250 (94%)	15 (6%)	18	28
1	B	275/295 (93%)	260 (94%)	15 (6%)	19	29
1	C	270/295 (92%)	255 (94%)	15 (6%)	19	29
1	D	271/295 (92%)	259 (96%)	12 (4%)	25	38
1	E	264/295 (90%)	245 (93%)	19 (7%)	13	18
1	F	261/295 (88%)	253 (97%)	8 (3%)	35	53
1	G	263/295 (89%)	248 (94%)	15 (6%)	18	28
1	H	277/295 (94%)	266 (96%)	11 (4%)	28	42
1	I	270/295 (92%)	252 (93%)	18 (7%)	15	21
1	J	274/295 (93%)	261 (95%)	13 (5%)	23	36
All	All	2690/2950 (91%)	2549 (95%)	141 (5%)	21	32

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	148	ASN
1	I	212	VAL
1	J	152	LYS
1	D	121	SER
1	D	109	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	40	GLN
1	H	148	ASN
1	J	269	GLN
1	J	43	ASN
1	G	82	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [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, 95th 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	A	331/367 (90%)	-0.20	12 (3%) 46 47	12, 34, 79, 230	0
1	B	344/367 (93%)	-0.20	22 (6%) 25 24	9, 31, 90, 296	0
1	C	338/367 (92%)	-0.22	12 (3%) 46 47	13, 33, 88, 153	0
1	D	338/367 (92%)	-0.05	23 (6%) 23 22	15, 36, 110, 244	0
1	E	329/367 (89%)	-0.16	9 (2%) 56 57	16, 35, 72, 155	0
1	F	326/367 (88%)	-0.15	11 (3%) 48 49	14, 35, 79, 206	0
1	G	328/367 (89%)	-0.09	15 (4%) 37 38	18, 35, 76, 159	0
1	H	345/367 (94%)	-0.04	28 (8%) 18 17	16, 33, 127, 259	0
1	I	338/367 (92%)	-0.12	11 (3%) 49 50	15, 35, 82, 177	0
1	J	343/367 (93%)	-0.07	20 (5%) 29 28	15, 35, 99, 244	0
All	All	3360/3670 (91%)	-0.13	163 (4%) 35 34	9, 34, 89, 296	0

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	THR	6.1
1	J	358	ALA	6.0
1	D	201	ALA	5.9
1	H	347	THR	5.8
1	D	359	ALA	5.6

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 oligosaccharides 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, 95th 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	0.88	0.19	18,27,28,602	0
2	PO4	C	401	5/5	0.89	0.14	45,49,95,157	0
2	PO4	G	401	5/5	0.95	0.10	39,41,102,204	0
2	PO4	I	401	5/5	0.97	0.08	16,20,24,183	0

6.5 Other polymers [i](#)

There are no such residues in this entry.