



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2016 – 01:47 PM EDT

PDB ID : 5CYL  
Title : Crystal structure of the CupB6 tip adhesin from *Pseudomonas aeruginosa*  
Authors : Rasheed, M.; Garnett, J.A.; Perez-Dorado, I.; Matthews, S.J.  
Deposited on : 2015-07-30  
Resolution : 2.77 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

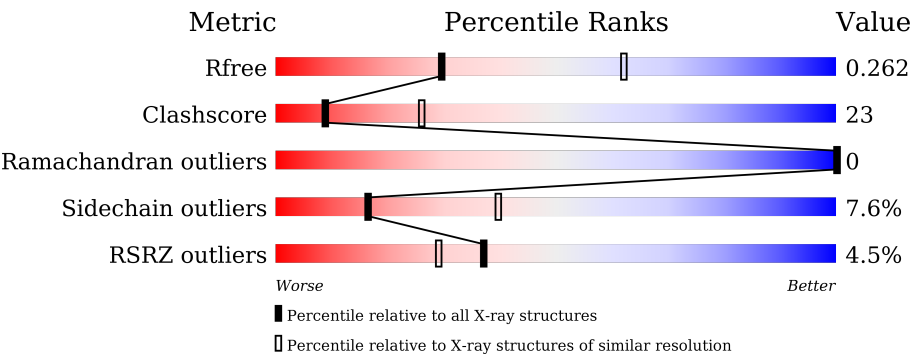
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

# 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 2.77 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))
$R_{free}$	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	370	<div><div>2%</div><div><div></div><div>66%</div><div>29%</div><div>• •</div></div></div>
1	B	370	<div><div>4%</div><div><div></div><div>65%</div><div>28%</div><div>• •</div></div></div>
1	C	370	<div><div>4%</div><div><div></div><div>64%</div><div>28%</div><div>• 5%</div></div></div>
1	D	370	<div><div>6%</div><div><div></div><div>61%</div><div>34%</div><div>• •</div></div></div>
1	E	370	<div><div>4%</div><div><div></div><div>63%</div><div>28%</div><div>5% •</div></div></div>
1	F	370	<div><div>4%</div><div><div></div><div>54%</div><div>35%</div><div>• 8%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	370	<div><div></div><div>9%</div><div>58%</div><div>34%</div><div>• 5%</div></div>
1	H	370	<div><div></div><div>2%</div><div>75%</div><div>20%</div><div>• •</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20981 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 Fimbrial subunit CupB6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2637	1664	455	513	5			
1	B	355	Total	C	N	O	S	0	0	0
			2608	1650	444	509	5			
1	C	353	Total	C	N	O	S	0	0	0
			2574	1630	439	500	5			
1	D	359	Total	C	N	O	S	0	0	0
			2616	1654	446	511	5			
1	E	355	Total	C	N	O	S	0	0	0
			2602	1643	448	506	5			
1	F	342	Total	C	N	O	S	0	0	0
			2452	1549	419	479	5			
1	G	353	Total	C	N	O	S	0	0	0
			2550	1617	434	494	5			
1	H	359	Total	C	N	O	S	0	0	0
			2644	1673	455	511	5			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q9HWU7
A	345	SER	-	expression tag	UNP Q9HWU7
A	346	ASP	-	expression tag	UNP Q9HWU7
A	347	ASN	-	expression tag	UNP Q9HWU7
A	348	LYS	-	expression tag	UNP Q9HWU7
A	349	VAL	-	expression tag	UNP Q9HWU7
A	350	ASP	-	expression tag	UNP Q9HWU7
A	351	GLY	-	expression tag	UNP Q9HWU7
A	352	ILE	-	expression tag	UNP Q9HWU7
A	353	VAL	-	expression tag	UNP Q9HWU7
A	354	ASN	-	expression tag	UNP Q9HWU7
A	355	PHE	-	expression tag	UNP Q9HWU7
A	356	SER	-	expression tag	UNP Q9HWU7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	GLY	-	expression tag	UNP Q9HWU7
A	358	ASN	-	expression tag	UNP Q9HWU7
A	359	ILE	-	expression tag	UNP Q9HWU7
A	360	THR	-	expression tag	UNP Q9HWU7
A	361	GLU	-	expression tag	UNP Q9HWU7
A	362	LEU	-	expression tag	UNP Q9HWU7
A	363	GLU	-	expression tag	UNP Q9HWU7
A	364	HIS	-	expression tag	UNP Q9HWU7
A	365	HIS	-	expression tag	UNP Q9HWU7
A	366	HIS	-	expression tag	UNP Q9HWU7
A	367	HIS	-	expression tag	UNP Q9HWU7
A	368	HIS	-	expression tag	UNP Q9HWU7
A	369	HIS	-	expression tag	UNP Q9HWU7
B	0	MET	-	initiating methionine	UNP Q9HWU7
B	345	SER	-	expression tag	UNP Q9HWU7
B	346	ASP	-	expression tag	UNP Q9HWU7
B	347	ASN	-	expression tag	UNP Q9HWU7
B	348	LYS	-	expression tag	UNP Q9HWU7
B	349	VAL	-	expression tag	UNP Q9HWU7
B	350	ASP	-	expression tag	UNP Q9HWU7
B	351	GLY	-	expression tag	UNP Q9HWU7
B	352	ILE	-	expression tag	UNP Q9HWU7
B	353	VAL	-	expression tag	UNP Q9HWU7
B	354	ASN	-	expression tag	UNP Q9HWU7
B	355	PHE	-	expression tag	UNP Q9HWU7
B	356	SER	-	expression tag	UNP Q9HWU7
B	357	GLY	-	expression tag	UNP Q9HWU7
B	358	ASN	-	expression tag	UNP Q9HWU7
B	359	ILE	-	expression tag	UNP Q9HWU7
B	360	THR	-	expression tag	UNP Q9HWU7
B	361	GLU	-	expression tag	UNP Q9HWU7
B	362	LEU	-	expression tag	UNP Q9HWU7
B	363	GLU	-	expression tag	UNP Q9HWU7
B	364	HIS	-	expression tag	UNP Q9HWU7
B	365	HIS	-	expression tag	UNP Q9HWU7
B	366	HIS	-	expression tag	UNP Q9HWU7
B	367	HIS	-	expression tag	UNP Q9HWU7
B	368	HIS	-	expression tag	UNP Q9HWU7
B	369	HIS	-	expression tag	UNP Q9HWU7
C	0	MET	-	initiating methionine	UNP Q9HWU7
C	345	SER	-	expression tag	UNP Q9HWU7
C	346	ASP	-	expression tag	UNP Q9HWU7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	347	ASN	-	expression tag	UNP Q9HWU7
C	348	LYS	-	expression tag	UNP Q9HWU7
C	349	VAL	-	expression tag	UNP Q9HWU7
C	350	ASP	-	expression tag	UNP Q9HWU7
C	351	GLY	-	expression tag	UNP Q9HWU7
C	352	ILE	-	expression tag	UNP Q9HWU7
C	353	VAL	-	expression tag	UNP Q9HWU7
C	354	ASN	-	expression tag	UNP Q9HWU7
C	355	PHE	-	expression tag	UNP Q9HWU7
C	356	SER	-	expression tag	UNP Q9HWU7
C	357	GLY	-	expression tag	UNP Q9HWU7
C	358	ASN	-	expression tag	UNP Q9HWU7
C	359	ILE	-	expression tag	UNP Q9HWU7
C	360	THR	-	expression tag	UNP Q9HWU7
C	361	GLU	-	expression tag	UNP Q9HWU7
C	362	LEU	-	expression tag	UNP Q9HWU7
C	363	GLU	-	expression tag	UNP Q9HWU7
C	364	HIS	-	expression tag	UNP Q9HWU7
C	365	HIS	-	expression tag	UNP Q9HWU7
C	366	HIS	-	expression tag	UNP Q9HWU7
C	367	HIS	-	expression tag	UNP Q9HWU7
C	368	HIS	-	expression tag	UNP Q9HWU7
C	369	HIS	-	expression tag	UNP Q9HWU7
D	0	MET	-	initiating methionine	UNP Q9HWU7
D	345	SER	-	expression tag	UNP Q9HWU7
D	346	ASP	-	expression tag	UNP Q9HWU7
D	347	ASN	-	expression tag	UNP Q9HWU7
D	348	LYS	-	expression tag	UNP Q9HWU7
D	349	VAL	-	expression tag	UNP Q9HWU7
D	350	ASP	-	expression tag	UNP Q9HWU7
D	351	GLY	-	expression tag	UNP Q9HWU7
D	352	ILE	-	expression tag	UNP Q9HWU7
D	353	VAL	-	expression tag	UNP Q9HWU7
D	354	ASN	-	expression tag	UNP Q9HWU7
D	355	PHE	-	expression tag	UNP Q9HWU7
D	356	SER	-	expression tag	UNP Q9HWU7
D	357	GLY	-	expression tag	UNP Q9HWU7
D	358	ASN	-	expression tag	UNP Q9HWU7
D	359	ILE	-	expression tag	UNP Q9HWU7
D	360	THR	-	expression tag	UNP Q9HWU7
D	361	GLU	-	expression tag	UNP Q9HWU7
D	362	LEU	-	expression tag	UNP Q9HWU7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	363	GLU	-	expression tag	UNP Q9HWU7
D	364	HIS	-	expression tag	UNP Q9HWU7
D	365	HIS	-	expression tag	UNP Q9HWU7
D	366	HIS	-	expression tag	UNP Q9HWU7
D	367	HIS	-	expression tag	UNP Q9HWU7
D	368	HIS	-	expression tag	UNP Q9HWU7
D	369	HIS	-	expression tag	UNP Q9HWU7
E	0	MET	-	initiating methionine	UNP Q9HWU7
E	345	SER	-	expression tag	UNP Q9HWU7
E	346	ASP	-	expression tag	UNP Q9HWU7
E	347	ASN	-	expression tag	UNP Q9HWU7
E	348	LYS	-	expression tag	UNP Q9HWU7
E	349	VAL	-	expression tag	UNP Q9HWU7
E	350	ASP	-	expression tag	UNP Q9HWU7
E	351	GLY	-	expression tag	UNP Q9HWU7
E	352	ILE	-	expression tag	UNP Q9HWU7
E	353	VAL	-	expression tag	UNP Q9HWU7
E	354	ASN	-	expression tag	UNP Q9HWU7
E	355	PHE	-	expression tag	UNP Q9HWU7
E	356	SER	-	expression tag	UNP Q9HWU7
E	357	GLY	-	expression tag	UNP Q9HWU7
E	358	ASN	-	expression tag	UNP Q9HWU7
E	359	ILE	-	expression tag	UNP Q9HWU7
E	360	THR	-	expression tag	UNP Q9HWU7
E	361	GLU	-	expression tag	UNP Q9HWU7
E	362	LEU	-	expression tag	UNP Q9HWU7
E	363	GLU	-	expression tag	UNP Q9HWU7
E	364	HIS	-	expression tag	UNP Q9HWU7
E	365	HIS	-	expression tag	UNP Q9HWU7
E	366	HIS	-	expression tag	UNP Q9HWU7
E	367	HIS	-	expression tag	UNP Q9HWU7
E	368	HIS	-	expression tag	UNP Q9HWU7
E	369	HIS	-	expression tag	UNP Q9HWU7
F	0	MET	-	initiating methionine	UNP Q9HWU7
F	345	SER	-	expression tag	UNP Q9HWU7
F	346	ASP	-	expression tag	UNP Q9HWU7
F	347	ASN	-	expression tag	UNP Q9HWU7
F	348	LYS	-	expression tag	UNP Q9HWU7
F	349	VAL	-	expression tag	UNP Q9HWU7
F	350	ASP	-	expression tag	UNP Q9HWU7
F	351	GLY	-	expression tag	UNP Q9HWU7
F	352	ILE	-	expression tag	UNP Q9HWU7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	353	VAL	-	expression tag	UNP Q9HWU7
F	354	ASN	-	expression tag	UNP Q9HWU7
F	355	PHE	-	expression tag	UNP Q9HWU7
F	356	SER	-	expression tag	UNP Q9HWU7
F	357	GLY	-	expression tag	UNP Q9HWU7
F	358	ASN	-	expression tag	UNP Q9HWU7
F	359	ILE	-	expression tag	UNP Q9HWU7
F	360	THR	-	expression tag	UNP Q9HWU7
F	361	GLU	-	expression tag	UNP Q9HWU7
F	362	LEU	-	expression tag	UNP Q9HWU7
F	363	GLU	-	expression tag	UNP Q9HWU7
F	364	HIS	-	expression tag	UNP Q9HWU7
F	365	HIS	-	expression tag	UNP Q9HWU7
F	366	HIS	-	expression tag	UNP Q9HWU7
F	367	HIS	-	expression tag	UNP Q9HWU7
F	368	HIS	-	expression tag	UNP Q9HWU7
F	369	HIS	-	expression tag	UNP Q9HWU7
G	0	MET	-	initiating methionine	UNP Q9HWU7
G	345	SER	-	expression tag	UNP Q9HWU7
G	346	ASP	-	expression tag	UNP Q9HWU7
G	347	ASN	-	expression tag	UNP Q9HWU7
G	348	LYS	-	expression tag	UNP Q9HWU7
G	349	VAL	-	expression tag	UNP Q9HWU7
G	350	ASP	-	expression tag	UNP Q9HWU7
G	351	GLY	-	expression tag	UNP Q9HWU7
G	352	ILE	-	expression tag	UNP Q9HWU7
G	353	VAL	-	expression tag	UNP Q9HWU7
G	354	ASN	-	expression tag	UNP Q9HWU7
G	355	PHE	-	expression tag	UNP Q9HWU7
G	356	SER	-	expression tag	UNP Q9HWU7
G	357	GLY	-	expression tag	UNP Q9HWU7
G	358	ASN	-	expression tag	UNP Q9HWU7
G	359	ILE	-	expression tag	UNP Q9HWU7
G	360	THR	-	expression tag	UNP Q9HWU7
G	361	GLU	-	expression tag	UNP Q9HWU7
G	362	LEU	-	expression tag	UNP Q9HWU7
G	363	GLU	-	expression tag	UNP Q9HWU7
G	364	HIS	-	expression tag	UNP Q9HWU7
G	365	HIS	-	expression tag	UNP Q9HWU7
G	366	HIS	-	expression tag	UNP Q9HWU7
G	367	HIS	-	expression tag	UNP Q9HWU7
G	368	HIS	-	expression tag	UNP Q9HWU7

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	369	HIS	-	expression tag	UNP Q9HWU7
H	0	MET	-	initiating methionine	UNP Q9HWU7
H	345	SER	-	expression tag	UNP Q9HWU7
H	346	ASP	-	expression tag	UNP Q9HWU7
H	347	ASN	-	expression tag	UNP Q9HWU7
H	348	LYS	-	expression tag	UNP Q9HWU7
H	349	VAL	-	expression tag	UNP Q9HWU7
H	350	ASP	-	expression tag	UNP Q9HWU7
H	351	GLY	-	expression tag	UNP Q9HWU7
H	352	ILE	-	expression tag	UNP Q9HWU7
H	353	VAL	-	expression tag	UNP Q9HWU7
H	354	ASN	-	expression tag	UNP Q9HWU7
H	355	PHE	-	expression tag	UNP Q9HWU7
H	356	SER	-	expression tag	UNP Q9HWU7
H	357	GLY	-	expression tag	UNP Q9HWU7
H	358	ASN	-	expression tag	UNP Q9HWU7
H	359	ILE	-	expression tag	UNP Q9HWU7
H	360	THR	-	expression tag	UNP Q9HWU7
H	361	GLU	-	expression tag	UNP Q9HWU7
H	362	LEU	-	expression tag	UNP Q9HWU7
H	363	GLU	-	expression tag	UNP Q9HWU7
H	364	HIS	-	expression tag	UNP Q9HWU7
H	365	HIS	-	expression tag	UNP Q9HWU7
H	366	HIS	-	expression tag	UNP Q9HWU7
H	367	HIS	-	expression tag	UNP Q9HWU7
H	368	HIS	-	expression tag	UNP Q9HWU7
H	369	HIS	-	expression tag	UNP Q9HWU7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	39	Total O 39 39	0	0
2	B	62	Total O 62 62	0	0
2	C	40	Total O 40 40	0	0
2	D	68	Total O 68 68	0	0
2	E	26	Total O 26 26	0	0
2	F	13	Total O 13 13	0	0

*Continued on next page...*

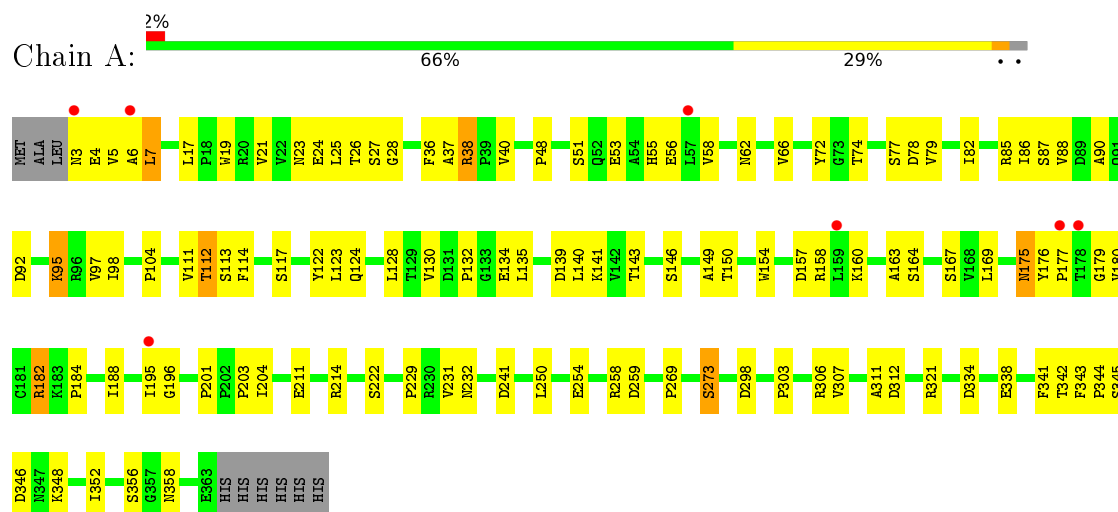
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	9	Total	O	0	0
			9	9		
2	H	41	Total	O	0	0
			41	41		

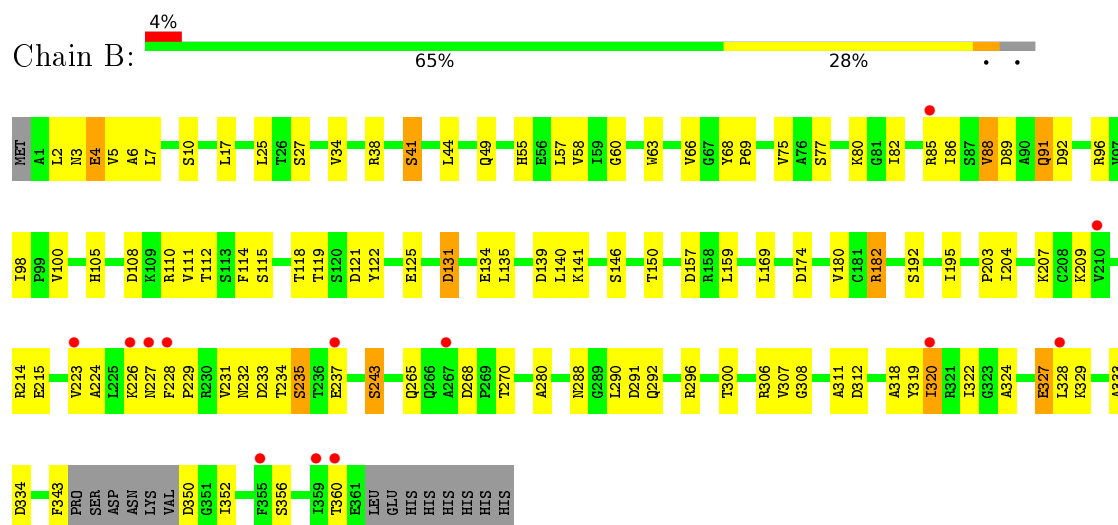
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Fimbrial subunit CupB6

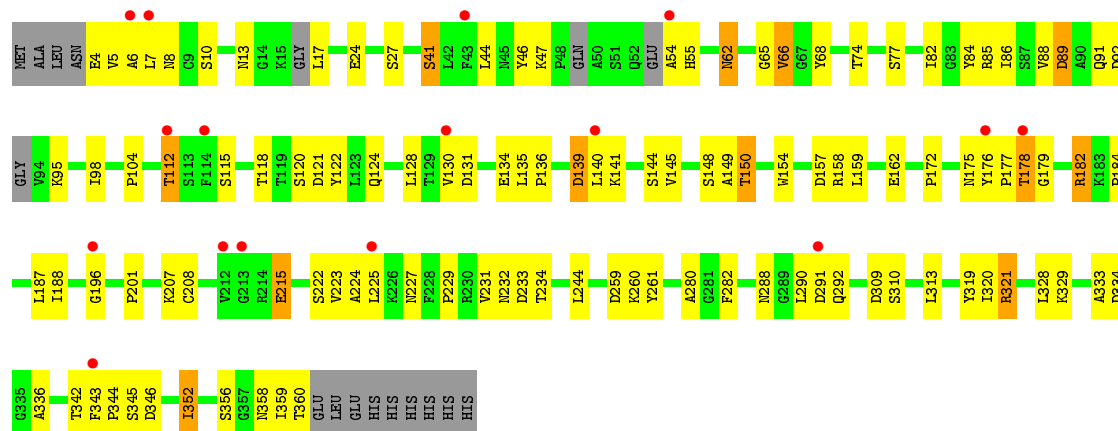


#### • Molecule 1: Fimbrial subunit CupB6

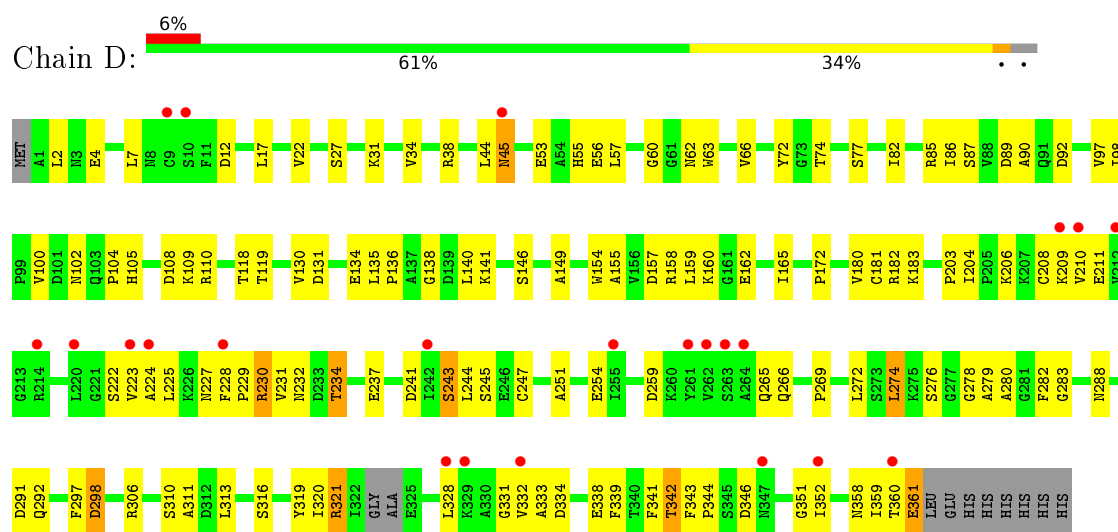


#### • Molecule 1: Fimbrial subunit CupB6

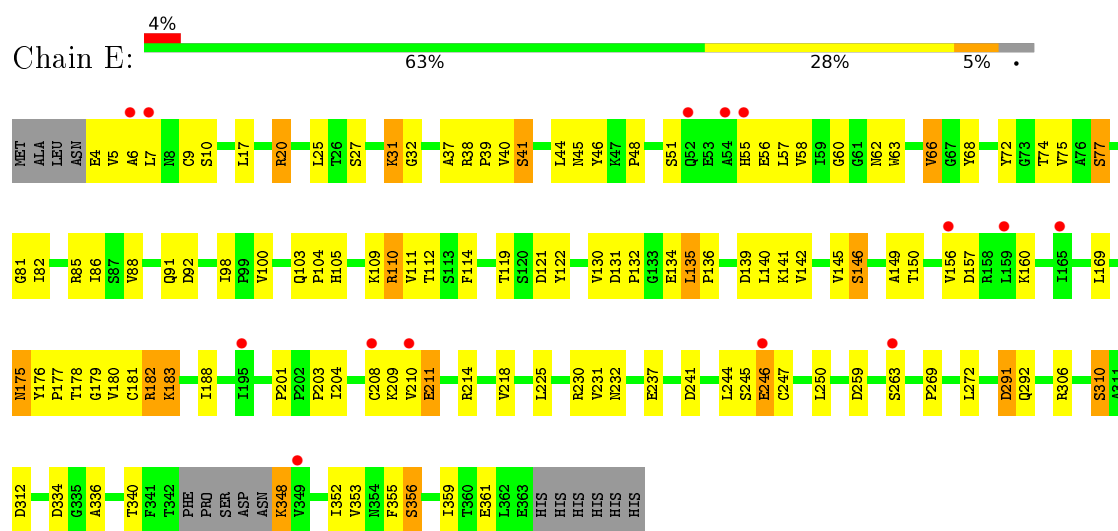




• Molecule 1: Fimbrial subunit CupB6

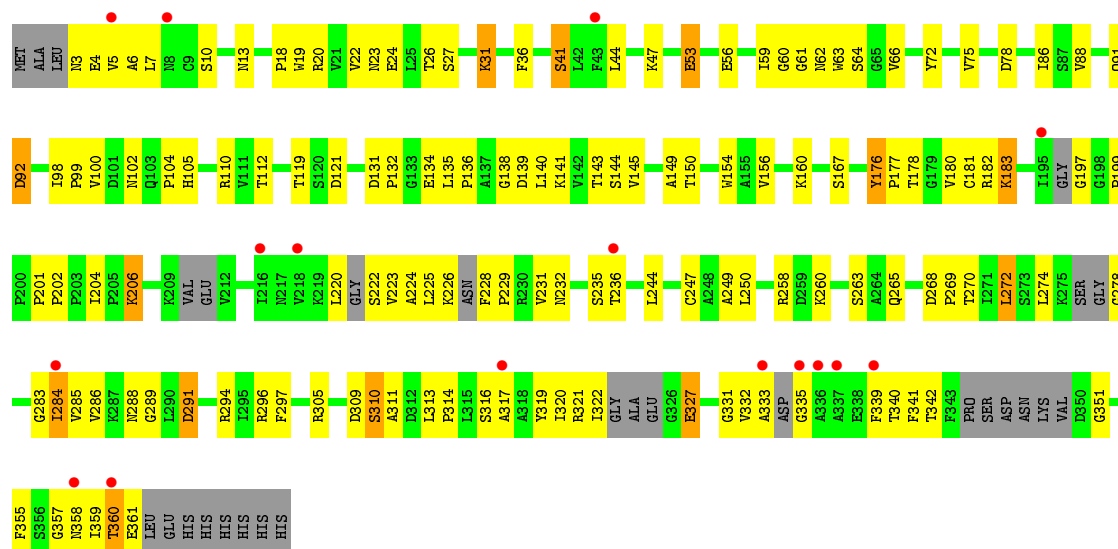


• Molecule 1: Fimbrial subunit CupB6

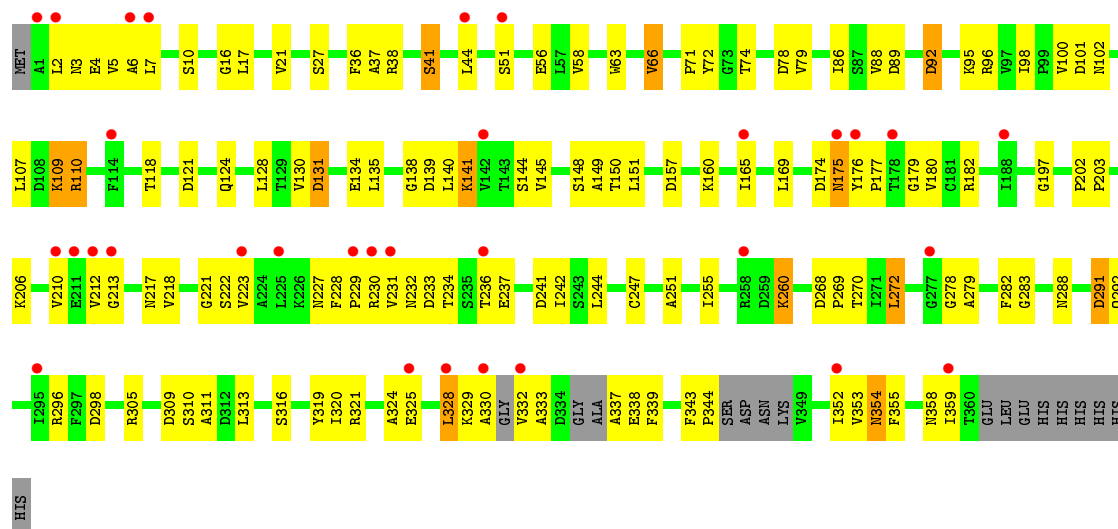


• Molecule 1: Fimbrial subunit CupB6

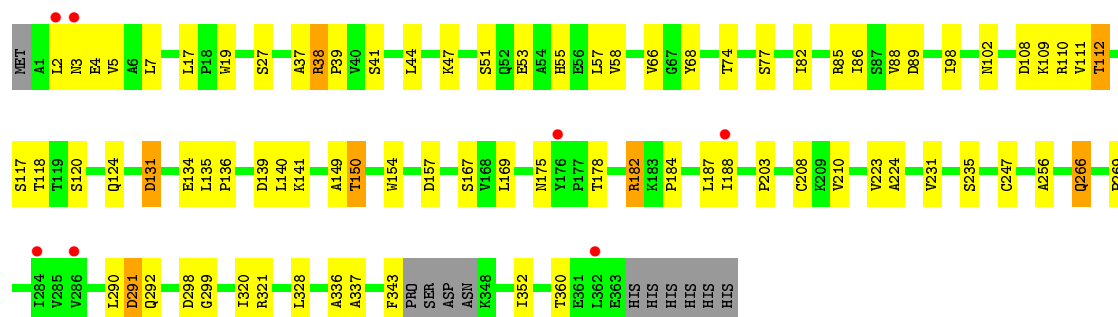
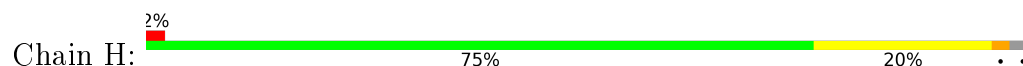




• Molecule 1: Fimbrial subunit CupB6



• Molecule 1: Fimbrial subunit CupB6



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	358.81Å 88.93Å 172.97Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	97.29 – 2.77 97.28 – 2.77	Depositor EDS
% Data completeness (in resolution range)	96.2 (97.29-2.77) 96.2 (97.28-2.77)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.238 , 0.266 0.233 , 0.262	Depositor DCC
$R_{free}$ test set	6115 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.9	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	20981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.66	0/2692	0.78	1/3671 (0.0%)
1	B	0.75	0/2661	0.85	4/3627 (0.1%)
1	C	0.74	1/2619 (0.0%)	0.84	2/3572 (0.1%)
1	D	0.73	0/2666	0.81	2/3640 (0.1%)
1	E	0.66	0/2654	0.79	2/3616 (0.1%)
1	F	0.67	0/2491	0.81	1/3396 (0.0%)
1	G	0.67	0/2603	0.82	2/3555 (0.1%)
1	H	0.66	0/2698	0.81	2/3673 (0.1%)
All	All	0.69	1/21084 (0.0%)	0.81	16/28750 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	215	GLU	CD-OE1	-5.89	1.19	1.25

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	96	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	B	96	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	E	259	ASP	CB-CG-OD1	6.32	123.99	118.30
1	C	259	ASP	CB-CG-OD1	6.15	123.83	118.30
1	E	135	LEU	C-N-CD	5.34	139.62	128.40

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	A	2637	0	2592	103	0
1	B	2608	0	2565	104	0
1	C	2574	0	2501	142	0
1	D	2616	0	2548	164	0
1	E	2602	0	2573	109	0
1	F	2452	0	2334	141	0
1	G	2550	0	2482	157	0
1	H	2644	0	2628	61	0
2	A	39	0	0	1	0
2	B	62	0	0	2	0
2	C	40	0	0	1	0
2	D	68	0	0	0	0
2	E	26	0	0	2	0
2	F	13	0	0	1	0
2	G	9	0	0	0	0
2	H	41	0	0	0	0
All	All	20981	0	20223	957	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 23.

The worst 5 of 957 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:G:228:PHE:CE2	1:G:282:PHE:HE1	1.21	1.57
1:G:325:GLU:HA	1:G:328:LEU:CD2	1.35	1.55
1:D:224:ALA:CA	1:D:360:THR:HB	1.11	1.54
1:G:279:ALA:CA	1:G:330:ALA:HB2	1.37	1.52
1:G:228:PHE:CE2	1:G:282:PHE:CE1	2.00	1.50

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	359/370 (97%)	349 (97%)	10 (3%)	0	100	100
1	B	351/370 (95%)	343 (98%)	8 (2%)	0	100	100
1	C	343/370 (93%)	339 (99%)	4 (1%)	0	100	100
1	D	355/370 (96%)	343 (97%)	12 (3%)	0	100	100
1	E	351/370 (95%)	348 (99%)	3 (1%)	0	100	100
1	F	324/370 (88%)	318 (98%)	6 (2%)	0	100	100
1	G	345/370 (93%)	341 (99%)	4 (1%)	0	100	100
1	H	355/370 (96%)	348 (98%)	7 (2%)	0	100	100
All	All	2783/2960 (94%)	2729 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	278/297 (94%)	260 (94%)	18 (6%)	21	49
1	B	274/297 (92%)	254 (93%)	20 (7%)	17	42
1	C	267/297 (90%)	247 (92%)	20 (8%)	17	40
1	D	272/297 (92%)	252 (93%)	20 (7%)	17	41
1	E	275/297 (93%)	251 (91%)	24 (9%)	13	33
1	F	249/297 (84%)	225 (90%)	24 (10%)	10	28
1	G	265/297 (89%)	243 (92%)	22 (8%)	14	36
1	H	280/297 (94%)	264 (94%)	16 (6%)	25	56
All	All	2160/2376 (91%)	1996 (92%)	164 (8%)	16	40

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	321	ARG
1	E	211	GLU
1	H	53	GLU
1	D	346	ASP
1	E	77	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	55	HIS
1	D	175	ASN
1	G	175	ASN
1	D	91	GLN
1	E	49	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	361/370 (97%)	0.46	7 (1%) 70 63	26, 50, 83, 129	0
1	B	355/370 (95%)	0.59	13 (3%) 45 37	26, 46, 79, 105	0
1	C	353/370 (95%)	0.57	16 (4%) 37 29	23, 55, 92, 109	0
1	D	359/370 (97%)	0.75	23 (6%) 23 16	18, 42, 98, 128	0
1	E	355/370 (95%)	0.50	14 (3%) 43 35	29, 56, 82, 102	0
1	F	342/370 (92%)	0.42	16 (4%) 35 27	28, 65, 102, 124	0
1	G	353/370 (95%)	0.69	32 (9%) 11 7	26, 69, 98, 117	0
1	H	359/370 (97%)	0.32	7 (1%) 70 63	34, 56, 83, 112	0
All	All	2837/2960 (95%)	0.54	128 (4%) 37 29	18, 56, 94, 129	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	359	ILE	6.3
1	C	176	TYR	5.4
1	G	330	ALA	4.8
1	D	262	VAL	4.7
1	D	10	SER	4.3

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.