



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID : 2BHV  
Title : STRUCTURE OF COMB10 OF THE COM TYPE IV SECRETION SYSTEM OF HELICOBACTER PYLORI  
Authors : Terradot, L.; Oomen, C.; Bayliss, R.; Leonard, G.; Waksman, G.  
Deposited on : 2005-01-18  
Resolution : 3.00 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.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

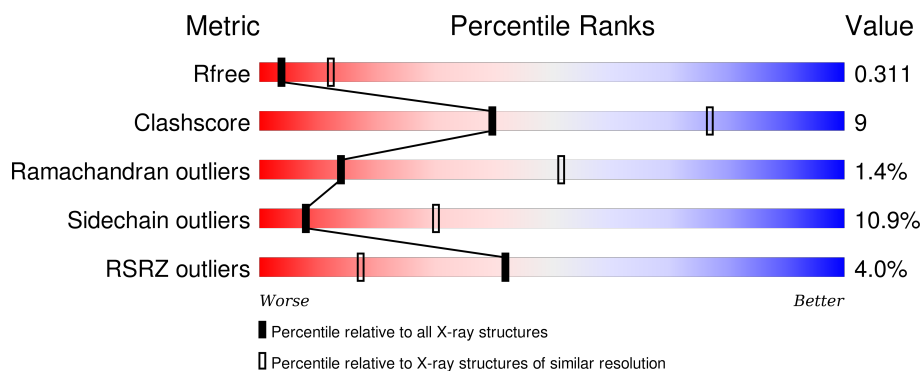
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



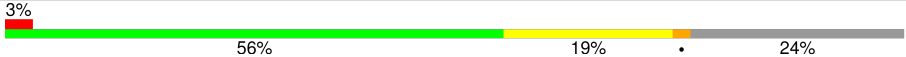
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	246	 56% 17% • 22%
1	B	246	 59% 15% • • 22%
1	C	246	 60% 14% • 24%
1	D	246	 54% 19% • 23%
1	E	246	 55% 19% • 23%

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Mol	Chain	Length	Quality of chain
1	F	246	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '3%', followed by a long green segment labeled '56%', a yellow segment labeled '19%', and a final grey segment labeled '24%'. A small black dot is located on the boundary between the yellow and grey segments.

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8759 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.

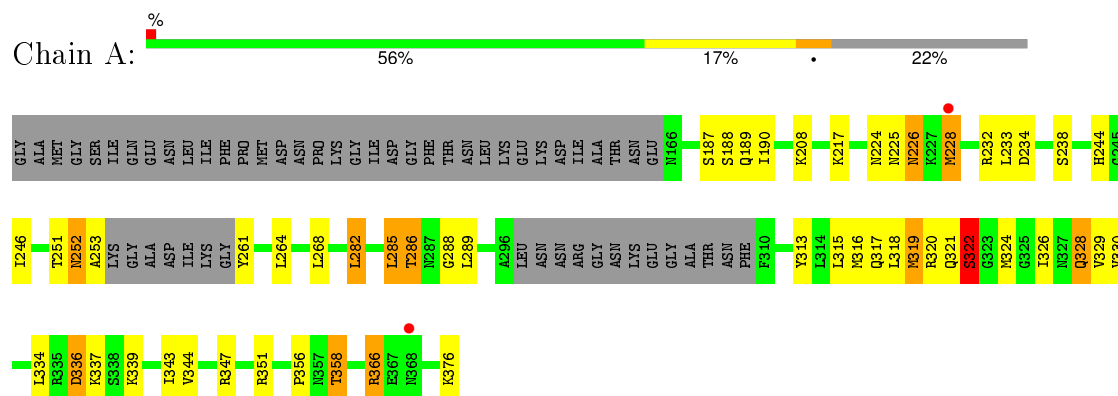
- Molecule 1 is a protein called COMB10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1468	945	253	263	7			
1	B	192	Total	C	N	O	S	0	0	0
			1466	944	254	261	7			
1	C	188	Total	C	N	O	S	0	0	0
			1457	941	250	259	7			
1	D	189	Total	C	N	O	S	0	0	0
			1464	944	251	262	7			
1	E	190	Total	C	N	O	S	0	0	0
			1447	931	251	258	7			
1	F	188	Total	C	N	O	S	0	0	0
			1457	939	250	261	7			

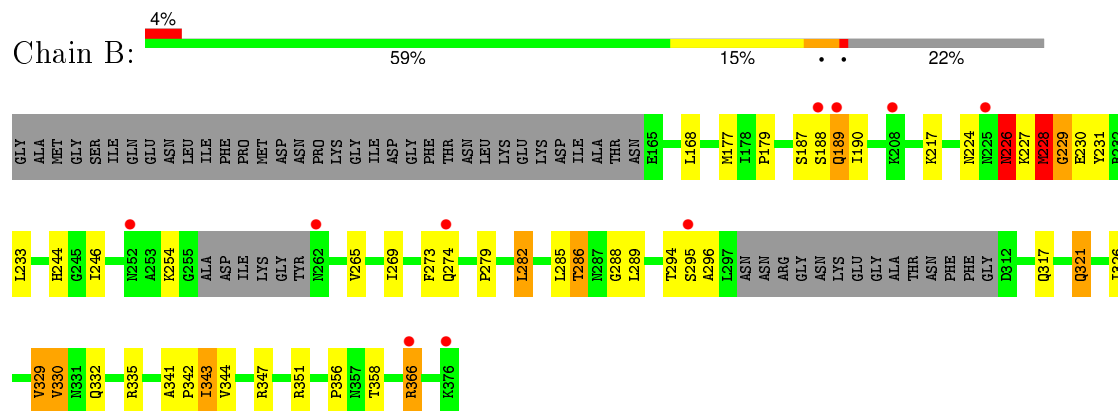
### 3 Residue-property plots [i](#)

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.

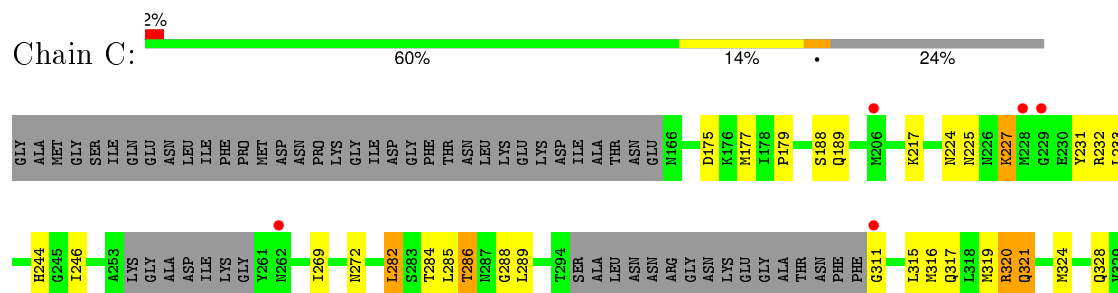
#### • Molecule 1: COMB10

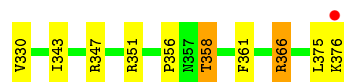


#### • Molecule 1: COMB10

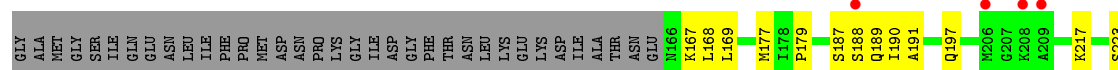


#### • Molecule 1: COMB10

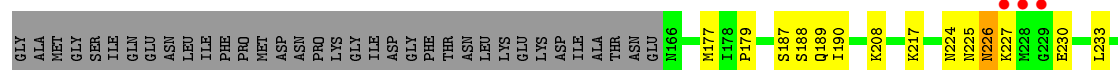




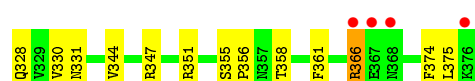
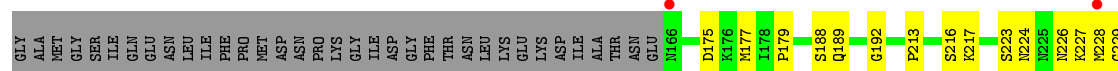
• Molecule 1: COMB10



• Molecule 1: COMB10



• Molecule 1: COMB10



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.73Å 139.41Å 168.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.64 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-3.00) 98.3 (29.64-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.257 , 0.293 0.286 , 0.311	Depositor DCC
$R_{free}$ test set	1672 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.0	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 25.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 33062 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.67	2/1490 (0.1%)	0.64	1/2016 (0.0%)
1	B	0.56	0/1487	0.65	1/2012 (0.0%)
1	C	0.62	1/1480 (0.1%)	0.63	1/2002 (0.0%)
1	D	0.51	0/1487	0.63	1/2011 (0.0%)
1	E	1.14	14/1468 (1.0%)	0.77	3/1986 (0.2%)
1	F	0.49	0/1480	0.61	0/2002
All	All	0.70	17/8892 (0.2%)	0.66	7/12029 (0.1%)

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
All	All	0	2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	271	ARG	CZ-NH1	21.26	1.60	1.33
1	E	274	GLN	CD-OE1	16.42	1.60	1.24
1	C	311	GLY	N-CA	12.80	1.65	1.46
1	E	274	GLN	CD-NE2	10.80	1.59	1.32
1	E	319	MET	SD-CE	10.23	2.35	1.77

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	271	ARG	NE-CZ-NH2	-15.72	112.44	120.30
1	E	271	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	B	282	LEU	CA-CB-CG	5.31	127.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	282	LEU	CA-CB-CG	5.16	127.18	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	MET	Peptide
1	B	226	ASN	Peptide

## 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	1468	0	1517	36	3
1	B	1466	0	1519	26	0
1	C	1457	0	1513	26	2
1	D	1464	0	1515	31	0
1	E	1447	0	1493	32	0
1	F	1457	0	1506	29	1
All	All	8759	0	9063	156	3

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 9.

The worst 5 of 156 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:C:175:ASP:OD2	1:E:208:LYS:HE3	1.30	1.26
1:A:226:ASN:HB3	1:A:228:MET:HG3	1.21	1.19
1:E:319:MET:SD	1:E:319:MET:CE	2.35	1.15
1:B:326:ILE:O	1:B:330:VAL:HG12	1.78	0.84
1:D:325:GLY:O	1:D:329:VAL:HG23	1.78	0.82

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:CE	1:F:175:ASP:OD2[3_555]	1.95	0.25
1:A:232:ARG:NH1	1:C:366:ARG:CD[4_455]	2.06	0.14
1:A:234:ASP:OD1	1:C:366:ARG:NE[4_455]	2.09	0.11

### 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	185/246 (75%)	166 (90%)	15 (8%)	4 (2%)	8	38
1	B	186/246 (76%)	172 (92%)	8 (4%)	6 (3%)	5	27
1	C	182/246 (74%)	172 (94%)	10 (6%)	0	100	100
1	D	183/246 (74%)	171 (93%)	10 (6%)	2 (1%)	17	58
1	E	184/246 (75%)	166 (90%)	16 (9%)	2 (1%)	17	58
1	F	182/246 (74%)	171 (94%)	10 (6%)	1 (0%)	34	76
All	All	1102/1476 (75%)	1018 (92%)	69 (6%)	15 (1%)	14	51

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	MET
1	B	254	LYS
1	A	313	TYR
1	B	229	GLY
1	B	274	GLN

#### 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	159/209 (76%)	143 (90%)	16 (10%)	9	34
1	B	158/209 (76%)	138 (87%)	20 (13%)	5	23
1	C	159/209 (76%)	144 (91%)	15 (9%)	11	39
1	D	160/209 (77%)	139 (87%)	21 (13%)	5	22
1	E	155/209 (74%)	140 (90%)	15 (10%)	10	37
1	F	159/209 (76%)	142 (89%)	17 (11%)	8	31
All	All	950/1254 (76%)	846 (89%)	104 (11%)	8	30

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	347	ARG
1	D	261	TYR
1	F	285	LEU
1	C	351	ARG
1	D	217	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	GLN
1	C	272	ASN
1	D	274	GLN
1	A	328	GLN
1	D	197	GLN

### 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 [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 [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<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	191/246 (77%)	0.13	2 (1%) 84 60	33, 47, 56, 68	0
1	B	192/246 (78%)	0.20	10 (5%) 31 12	28, 47, 57, 68	0
1	C	188/246 (76%)	0.28	6 (3%) 51 23	32, 47, 54, 67	0
1	D	189/246 (76%)	0.17	11 (5%) 26 10	34, 47, 57, 62	0
1	E	190/246 (77%)	0.31	10 (5%) 30 12	25, 47, 56, 63	0
1	F	188/246 (76%)	0.24	7 (3%) 45 19	35, 47, 54, 67	0
All	All	1138/1476 (77%)	0.22	46 (4%) 42 17	25, 47, 56, 68	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	229	GLY	6.9
1	E	228	MET	5.5
1	C	229	GLY	5.3
1	F	376	LYS	4.8
1	A	368	ASN	4.6

### 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 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.