



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 04:50 pm BST

PDB ID : 3VA6  
Title : Crystal Structure of the extracellular domain of the putative hybrid two component system BT4673 from *B. thetaiotaomicron*  
Authors : Zhang, Z.; Liu, Q.; Hendrickson, W.A.  
Deposited on : 2011-12-28  
Resolution : 2.80 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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

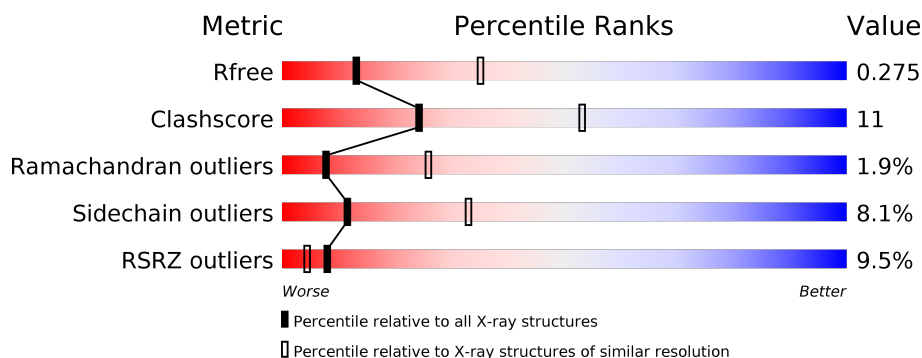
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	758	<div> <div>13%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>..</div> </div> </div>
1	B	758	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>...</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12203 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 Two-component system sensor histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			6077	3855	1043	1162	17			
1	B	743	Total	C	N	O	S	0	0	0
			6032	3828	1028	1158	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	LEU	-	EXPRESSION TAG	UNP Q89YQ8
A	29	GLU	-	EXPRESSION TAG	UNP Q89YQ8
A	778	LEU	-	EXPRESSION TAG	UNP Q89YQ8
A	779	GLU	-	EXPRESSION TAG	UNP Q89YQ8
A	780	HIS	-	EXPRESSION TAG	UNP Q89YQ8
A	781	HIS	-	EXPRESSION TAG	UNP Q89YQ8
A	782	HIS	-	EXPRESSION TAG	UNP Q89YQ8
A	783	HIS	-	EXPRESSION TAG	UNP Q89YQ8
A	784	HIS	-	EXPRESSION TAG	UNP Q89YQ8
A	785	HIS	-	EXPRESSION TAG	UNP Q89YQ8
B	28	LEU	-	EXPRESSION TAG	UNP Q89YQ8
B	29	GLU	-	EXPRESSION TAG	UNP Q89YQ8
B	778	LEU	-	EXPRESSION TAG	UNP Q89YQ8
B	779	GLU	-	EXPRESSION TAG	UNP Q89YQ8
B	780	HIS	-	EXPRESSION TAG	UNP Q89YQ8
B	781	HIS	-	EXPRESSION TAG	UNP Q89YQ8
B	782	HIS	-	EXPRESSION TAG	UNP Q89YQ8
B	783	HIS	-	EXPRESSION TAG	UNP Q89YQ8
B	784	HIS	-	EXPRESSION TAG	UNP Q89YQ8
B	785	HIS	-	EXPRESSION TAG	UNP Q89YQ8

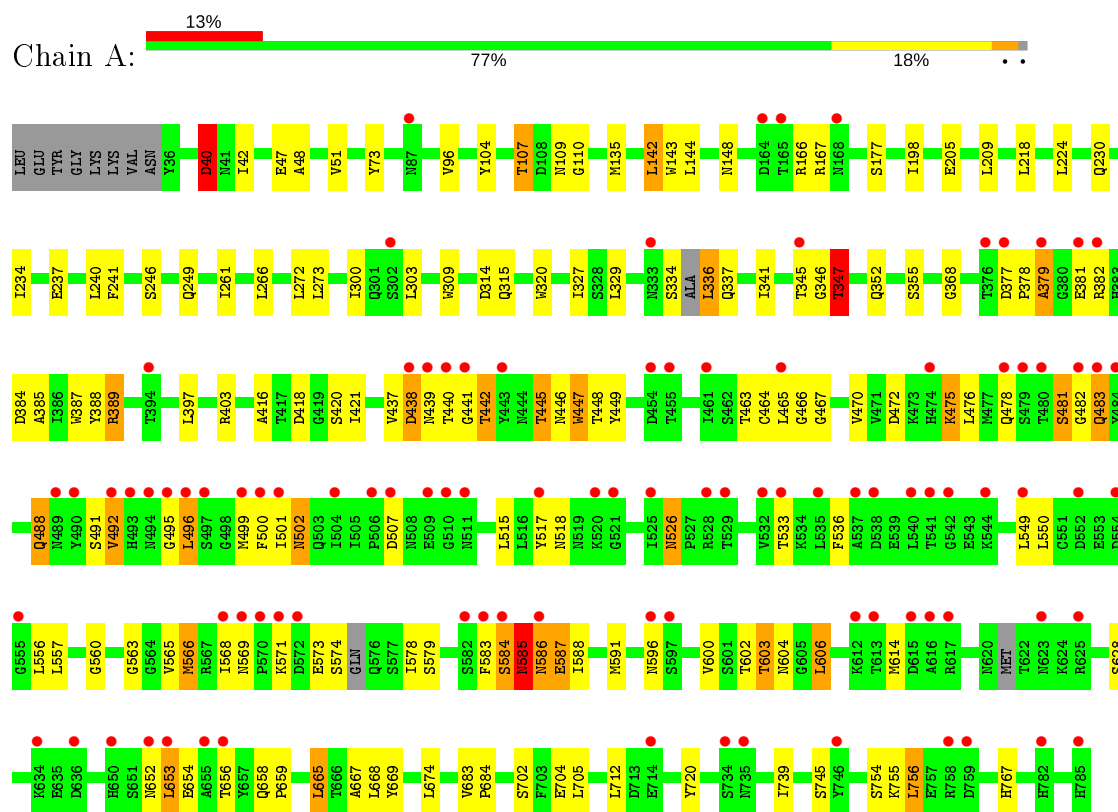
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total 48	O 48	0	0
2	B	46	Total 46	O 46	0	0

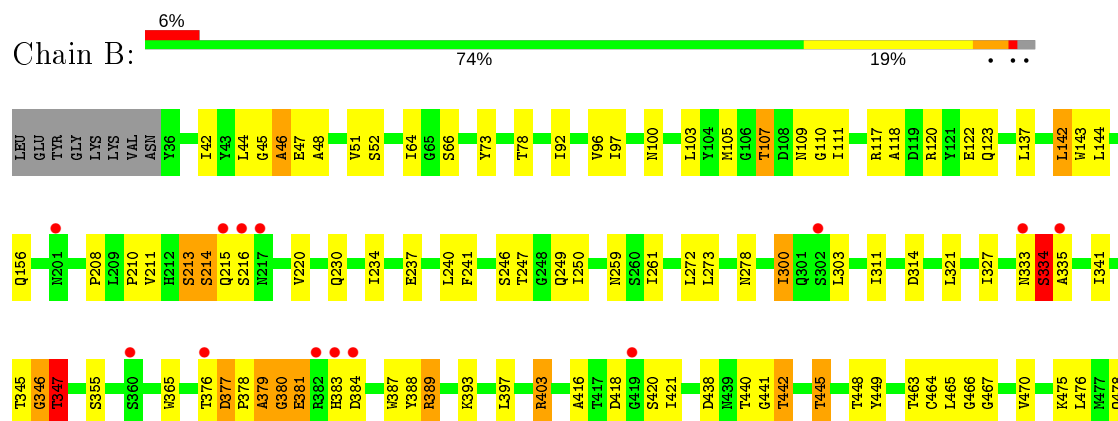
### 3 Residue-property plots

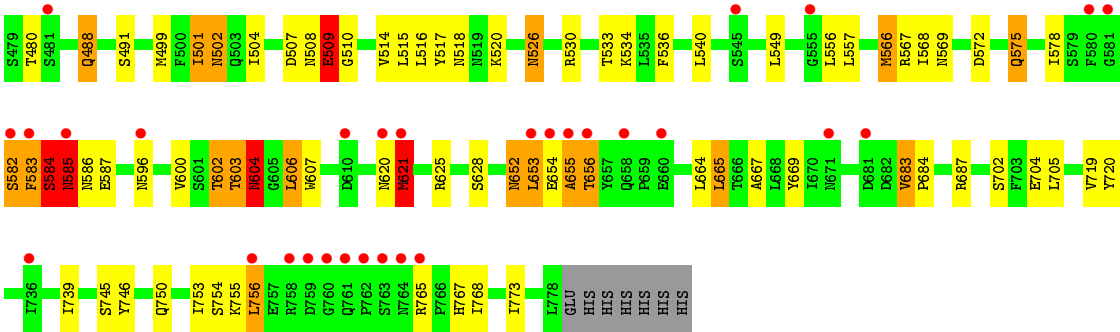
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- Molecule 1: Two-component system sensor histidine kinase



- Molecule 1: Two-component system sensor histidine kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.88Å 87.88Å 430.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.86 – 2.80 45.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (45.86-2.80) 92.3 (45.86-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.91 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.216 , 0.274 0.218 , 0.275	Depositor DCC
$R_{free}$ test set	2024 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	1.398	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12203	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

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	0.65	4/6232 (0.1%)	0.74	1/8466 (0.0%)
1	B	0.68	2/6184 (0.0%)	0.79	4/8405 (0.0%)
All	All	0.67	6/12416 (0.0%)	0.76	5/16871 (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	B	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	TRP	CD2-CE2	5.53	1.48	1.41
1	B	365	TRP	CD2-CE2	5.26	1.47	1.41
1	A	143	TRP	CD2-CE2	5.15	1.47	1.41
1	A	320	TRP	CD2-CE2	5.06	1.47	1.41
1	B	607	TRP	CD2-CE2	5.04	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	380	GLY	N-CA-C	5.32	126.39	113.10
1	B	509	GLU	N-CA-C	-5.20	96.96	111.00
1	B	530	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	40	ASP	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	213	SER	Peptide
1	B	441	GLY	Peptide
1	B	508	ASN	Peptide

## 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	6077	0	5785	119	0
1	B	6032	0	5767	146	0
2	A	48	0	0	1	0
2	B	46	0	0	4	0
All	All	12203	0	11552	260	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 11.

The worst 5 of 260 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:A:586:ASN:HB3	1:A:587:GLU:HA	1.26	1.06
1:A:166:ARG:HH11	1:A:166:ARG:HG3	1.28	0.97
1:B:46:ALA:H	1:B:47:GLU:HA	1.32	0.92
1:A:578:ILE:HG23	1:A:614:MET:CE	2.00	0.90
1:A:586:ASN:HB3	1:A:587:GLU:CA	2.02	0.89

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	739/758 (98%)	682 (92%)	46 (6%)	11 (2%)	10	33
1	B	741/758 (98%)	685 (92%)	39 (5%)	17 (2%)	6	21
All	All	1480/1516 (98%)	1367 (92%)	85 (6%)	28 (2%)	8	26

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ALA
1	A	492	VAL
1	A	585	ASN
1	A	586	ASN
1	B	46	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	666/676 (98%)	614 (92%)	52 (8%)	12	35
1	B	662/676 (98%)	607 (92%)	55 (8%)	11	32
All	All	1328/1352 (98%)	1221 (92%)	107 (8%)	11	33

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	745	SER
1	B	246	SER
1	B	628	SER
1	A	754	SER
1	B	137	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	783	HIS
1	B	215	GLN
1	B	586	ASN
1	A	784	HIS
1	B	230	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 [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	747/758 (98%)	0.87	98 (13%) <b>3</b> <b>2</b>	55, 70, 123, 152	6 (0%)
1	B	743/758 (98%)	0.58	43 (5%) <b>23</b> <b>15</b>	54, 65, 88, 112	7 (0%)
All	All	1490/1516 (98%)	0.73	141 (9%) <b>8</b> <b>4</b>	54, 67, 112, 152	13 (0%)

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ASN	5.9
1	B	384	ASP	5.8
1	B	655	ALA	5.8
1	A	583	PHE	5.5
1	A	440	THR	5.4

### 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.