



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2017 – 01:39 AM EDT

PDB ID : 5GUQ  
Title : Crystal structure of ASCH from Zymomonas mobilis  
Authors : Ha, S.C.; Park, S.Y.; Kim, J.S.  
Deposited on : unknown  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029824

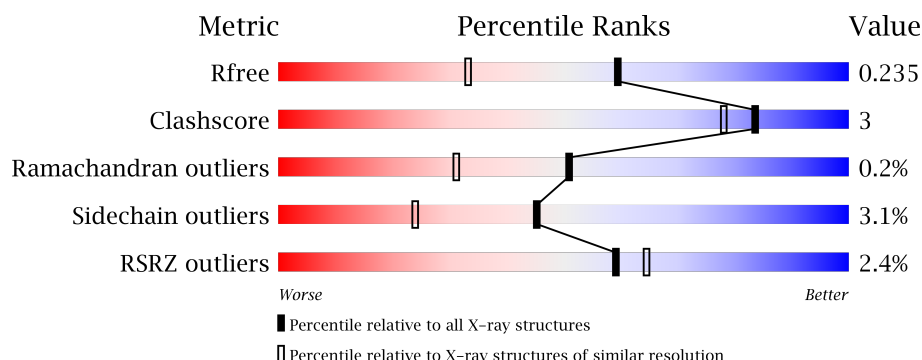
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	149	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>••</div> </div> </div>
1	B	149	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>••</div> </div> </div>
1	C	149	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>•</div> </div> </div>
1	D	149	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5566 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 Helix-turn-helix domain-containing protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	143	Total 1187	C 764	N 210	O 213	0	1	0	
1	B	143	Total 1200	C 773	N 211	O 216	0	3	0	
1	C	149	Total 1253	C 807	N 221	O 224	S 1	0	4	0
1	D	143	Total 1196	C 772	N 210	O 214		0	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A0H3G0N3
B	0	GLY	-	expression tag	UNP A0A0H3G0N3
C	0	GLY	-	expression tag	UNP A0A0H3G0N3
D	0	GLY	-	expression tag	UNP A0A0H3G0N3

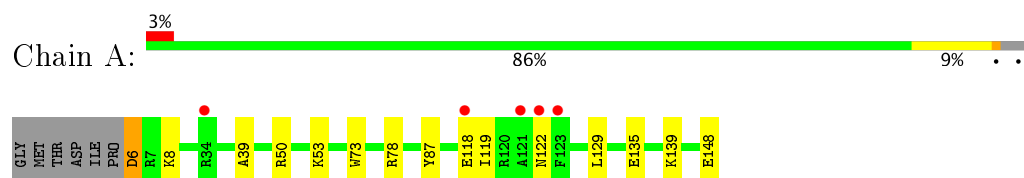
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	158	Total	O	0	0
			158	158		
2	B	163	Total	O	0	0
			163	163		
2	C	235	Total	O	0	0
			235	235		
2	D	174	Total	O	0	0
			174	174		

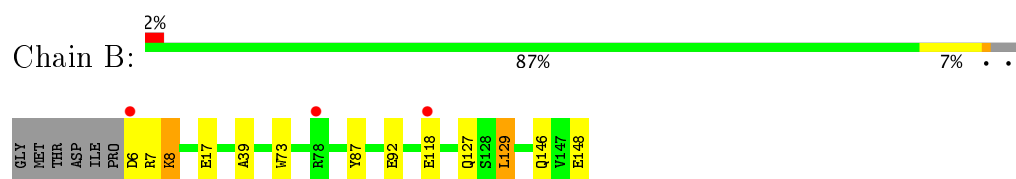
### 3 Residue-property plots [i](#)

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

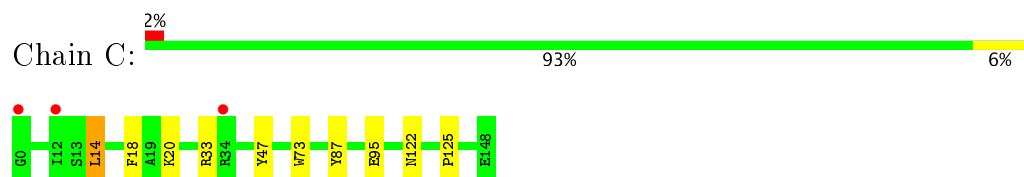
- Molecule 1: Helix-turn-helix domain-containing protein



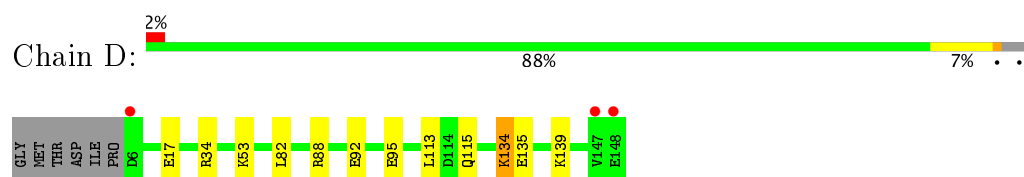
- Molecule 1: Helix-turn-helix domain-containing protein



- Molecule 1: Helix-turn-helix domain-containing protein



- Molecule 1: Helix-turn-helix domain-containing protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.91Å 52.86Å 88.67Å 90.00° 111.56° 90.00°	Depositor
Resolution (Å)	30.59 – 1.70 30.59 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.59-1.70) 98.7 (30.59-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, $R_{free}$	0.198 , 0.235 0.199 , 0.235	Depositor DCC
$R_{free}$ test set	2750 reflections (4.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.02 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.2234e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.37	0/1215	0.59	0/1646
1	B	0.35	0/1231	0.60	1/1668 (0.1%)
1	C	0.40	0/1285	0.64	0/1741
1	D	0.37	0/1230	0.59	0/1667
All	All	0.37	0/4961	0.60	1/6722 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	LEU	CA-CB-CG	6.19	129.53	115.30

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	1187	0	1203	7	0
1	B	1200	0	1217	8	0
1	C	1253	0	1280	5	0
1	D	1196	0	1221	7	0
2	A	158	0	0	2	0
2	B	163	0	0	3	0
2	C	235	0	0	1	0
2	D	174	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5566	0	4921	27	1

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 3.

All (27) 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:119:ILE:HG23	1:A:139:LYS:HE3	1.67	0.75
1:A:6:ASP:N	2:A:201:HOH:O	2.25	0.68
1:C:122:ASN:ND2	2:C:203:HOH:O	2.27	0.68
1:A:78:ARG:NH1	2:A:204:HOH:O	2.38	0.57
1:D:53:LYS:HE2	1:D:113:LEU:HD12	1.88	0.56
1:B:6:ASP:HA	1:B:7:ARG:HB2	1.91	0.53
1:D:134:LYS:H	1:D:134:LYS:HE3	1.74	0.53
1:C:47:TYR:CE2	1:C:125:PRO:HG3	2.45	0.51
1:D:115:GLN:NE2	2:D:205:HOH:O	2.39	0.50
1:B:146:GLN:NE2	2:B:212:HOH:O	2.45	0.49
1:C:14[B]:LEU:HD13	1:C:18:PHE:HB3	1.95	0.49
1:B:6:ASP:HB2	1:B:8:LYS:N	2.28	0.48
1:B:6:ASP:HB2	1:B:8:LYS:HB2	1.95	0.48
1:B:92:GLU:O	2:B:201:HOH:O	2.20	0.47
1:A:135:GLU:O	1:A:139:LYS:HE2	2.14	0.47
1:A:50:ARG:HA	1:A:53:LYS:HG3	1.96	0.47
1:D:88:ARG:O	1:D:92:GLU:HG3	2.14	0.47
1:C:73:TRP:HB2	1:C:87:TYR:CE1	2.50	0.47
1:A:8:LYS:HD3	1:A:39:ALA:HB3	1.97	0.46
1:C:95:GLU:N	1:C:95:GLU:OE2	2.34	0.46
1:D:135:GLU:O	1:D:139:LYS:HG3	2.14	0.46
1:B:127:GLN:NE2	2:B:217:HOH:O	2.48	0.46
1:B:73:TRP:HB2	1:B:87:TYR:CE1	2.52	0.44
1:A:73:TRP:HB2	1:A:87:TYR:CE2	2.54	0.42
1:D:134:LYS:CE	1:D:134:LYS:H	2.33	0.42
1:B:8:LYS:HE2	1:B:39:ALA:HB3	2.02	0.41
1:D:95:GLU:OE2	1:D:95:GLU:N	2.40	0.40

All (1) 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)
2:D:360:HOH:O	2:D:369:HOH:O[2_444]	2.17	0.03

## 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	142/149 (95%)	137 (96%)	5 (4%)	0	100	100
1	B	144/149 (97%)	141 (98%)	3 (2%)	0	100	100
1	C	151/149 (101%)	147 (97%)	3 (2%)	1 (1%)	25	9
1	D	144/149 (97%)	141 (98%)	3 (2%)	0	100	100
All	All	581/596 (98%)	566 (97%)	14 (2%)	1 (0%)	51	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	33	ARG

### 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	127/131 (97%)	122 (96%)	5 (4%)	37	15
1	B	129/131 (98%)	124 (96%)	5 (4%)	37	15
1	C	135/131 (103%)	132 (98%)	3 (2%)	57	38
1	D	129/131 (98%)	125 (97%)	4 (3%)	45	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	520/524 (99%)	503 (97%)	17 (3%)	45 21

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	118	GLU
1	A	122	ASN
1	A	129	LEU
1	A	148	GLU
1	B	8	LYS
1	B	17	GLU
1	B	118	GLU
1	B	129	LEU
1	B	148	GLU
1	C	14[A]	LEU
1	C	14[B]	LEU
1	C	20	LYS
1	D	17	GLU
1	D	34	ARG
1	D	82	LEU
1	D	134	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	143/149 (95%)	0.02	5 (3%) 44 50	16, 23, 45, 66	0
1	B	143/149 (95%)	0.01	3 (2%) 64 69	16, 23, 41, 75	0
1	C	149/149 (100%)	0.01	3 (2%) 65 71	12, 16, 31, 56	0
1	D	143/149 (95%)	0.03	3 (2%) 64 69	14, 21, 40, 54	0
All	All	578/596 (96%)	0.02	14 (2%) 59 64	12, 21, 39, 75	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ASP	6.2
1	C	0	GLY	5.8
1	A	122	ASN	3.9
1	D	6	ASP	3.6
1	C	34	ARG	3.5
1	B	78	ARG	2.9
1	D	147	VAL	2.8
1	A	123	PHE	2.7
1	A	118	GLU	2.4
1	A	121	ALA	2.3
1	A	34	ARG	2.3
1	B	118	GLU	2.3
1	D	148	GLU	2.1
1	C	12	ILE	2.1

### 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.