



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2024 – 02:18 PM JST

PDB ID : 8WAE  
Title : Crystal structure of a novel porphyrin-binding carbohydrate binding module  
Authors : Mei, X.W.; Chang, Y.G.  
Deposited on : 2023-09-07  
Resolution : 1.75 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

<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>.

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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 : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

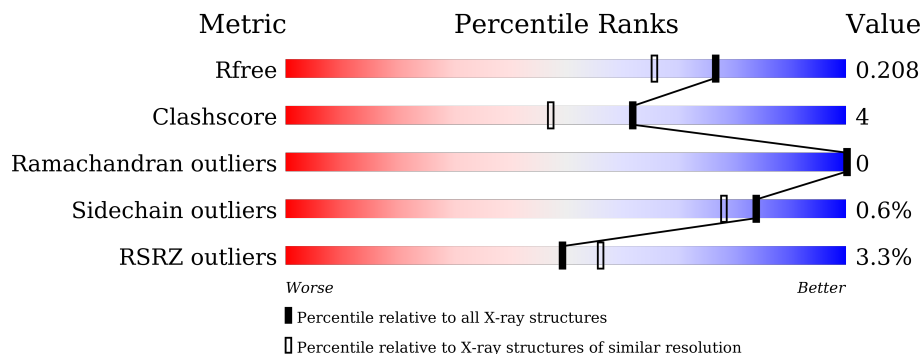
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

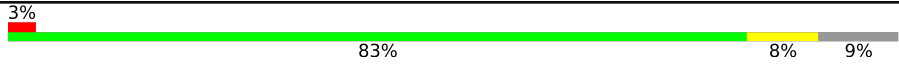

The reported resolution of this entry is 1.75 Å.

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))
$R_{free}$	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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 of 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	118	 3% 83% 8% 9%
1	B	118	 3% 83% 8% 9%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 2094 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 Beta-agarase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	107	828	509	144	175	8	6	0
1	B	107	847	521	147	179	7	9	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0D5CS34
A	2	GLY	-	expression tag	UNP A0A0D5CS34
A	111	LEU	-	expression tag	UNP A0A0D5CS34
A	112	GLU	-	expression tag	UNP A0A0D5CS34
A	113	HIS	-	expression tag	UNP A0A0D5CS34
A	114	HIS	-	expression tag	UNP A0A0D5CS34
A	115	HIS	-	expression tag	UNP A0A0D5CS34
A	116	HIS	-	expression tag	UNP A0A0D5CS34
A	117	HIS	-	expression tag	UNP A0A0D5CS34
A	118	HIS	-	expression tag	UNP A0A0D5CS34
B	1	MET	-	initiating methionine	UNP A0A0D5CS34
B	2	GLY	-	expression tag	UNP A0A0D5CS34
B	111	LEU	-	expression tag	UNP A0A0D5CS34
B	112	GLU	-	expression tag	UNP A0A0D5CS34
B	113	HIS	-	expression tag	UNP A0A0D5CS34
B	114	HIS	-	expression tag	UNP A0A0D5CS34
B	115	HIS	-	expression tag	UNP A0A0D5CS34
B	116	HIS	-	expression tag	UNP A0A0D5CS34
B	117	HIS	-	expression tag	UNP A0A0D5CS34
B	118	HIS	-	expression tag	UNP A0A0D5CS34

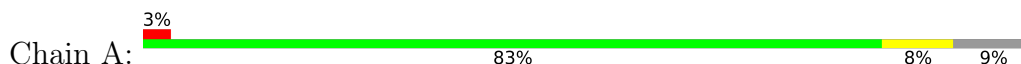
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	179	Total 179	O 179	0	0
2	B	240	Total 240	O 240	0	0

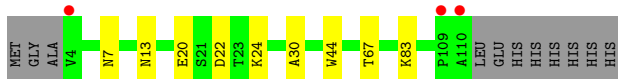
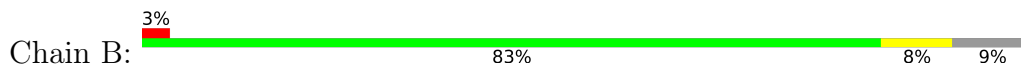
### 3 Residue-property plots [i](#)

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: Beta-agarase



- Molecule 1: Beta-agarase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	25.08Å 49.42Å 160.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.78 – 1.75 24.78 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.78-1.75) 99.1 (24.78-1.75)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.90 (at 1.75Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.157 , 0.207 0.158 , 0.208	Depositor DCC
$R_{free}$ test set	19133 reflections (9.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.6	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2094	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.24% 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	0.33	0/840	0.64	0/1155
1	B	0.34	0/860	0.63	0/1182
All	All	0.34	0/1700	0.64	0/2337

There are no bond length outliers.

There are no bond angle outliers.

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	828	0	806	7	0
1	B	847	0	820	6	0
2	A	179	0	0	4	7
2	B	240	0	0	2	5
All	All	2094	0	1626	13	7

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 4.

All (13) 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:3:ALA:N	2:A:201:HOH:O	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:ND2	2:A:203:HOH:O	2.28	0.67
1:A:20:GLU:HG2	1:A:108:ILE:HD11	1.78	0.65
1:B:22:ASP:OD1	2:B:201:HOH:O	2.15	0.64
1:A:3:ALA:N	2:A:204:HOH:O	2.31	0.63
1:A:83:LYS:NZ	2:A:206:HOH:O	2.37	0.57
1:A:10:ILE:HD11	1:A:29:LEU:HD13	1.90	0.53
1:B:20:GLU:OE2	2:B:203:HOH:O	2.19	0.50
1:B:13:ASN:HD21	1:B:30:ALA:HB2	1.78	0.49
1:B:24:LYS:NZ	1:B:67:THR:HG21	2.29	0.47
1:A:5:ILE:HD12	1:A:6:GLY:H	1.84	0.42
1:B:44:TRP:CE2	1:B:83:LYS:HE3	2.54	0.41
1:B:24:LYS:HZ2	1:B:67:THR:HG21	1.85	0.40

All (7) 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:A:351:HOH:O	2:B:396:HOH:O[4_455]	2.10	0.10
2:A:238:HOH:O	2:A:365:HOH:O[4_555]	2.12	0.08
2:A:217:HOH:O	2:A:339:HOH:O[1_655]	2.13	0.07
2:A:204:HOH:O	2:B:330:HOH:O[4_555]	2.17	0.03
2:A:297:HOH:O	2:B:363:HOH:O[2_454]	2.18	0.02
2:A:318:HOH:O	2:B:381:HOH:O[4_555]	2.19	0.01
2:A:358:HOH:O	2:B:337:HOH:O[2_454]	2.19	0.01

## 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	111/118 (94%)	106 (96%)	5 (4%)	0	100	100
1	B	114/118 (97%)	113 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	225/236 (95%)	219 (97%)	6 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	94/97 (97%)	94 (100%)	0	100	100
1	B	97/97 (100%)	95 (98%)	2 (2%)	48	29
All	All	191/194 (98%)	189 (99%)	2 (1%)	84	61

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7[A]	ASN
1	B	7[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	B	13	ASN
1	B	69	ASN

### 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 oligosaccharides 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	107/118 (90%)	-0.41	4 (3%) 45 52	4, 9, 22, 33	6 (5%)
1	B	106/118 (89%)	-0.56	3 (2%) 55 61	3, 7, 17, 54	8 (7%)
All	All	213/236 (90%)	-0.48	7 (3%) 49 56	3, 8, 22, 54	14 (6%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	VAL	5.1
1	B	110	ALA	3.8
1	B	109[A]	PRO	2.5
1	A	3	ALA	2.4
1	A	71	ASN	2.2
1	A	72	ASN	2.2
1	A	5	ILE	2.0

### 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 monosaccharides 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.