



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 12, 2021 – 06:07 PM JST

PDB ID : 5XWF  
Title : Crystal structure of chitinase (RmChi1) from *Rhizomucor miehei* (SP3221/SAD)  
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Deposited on : 2017-06-29  
Resolution : 2.58 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
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) : 2.23.1

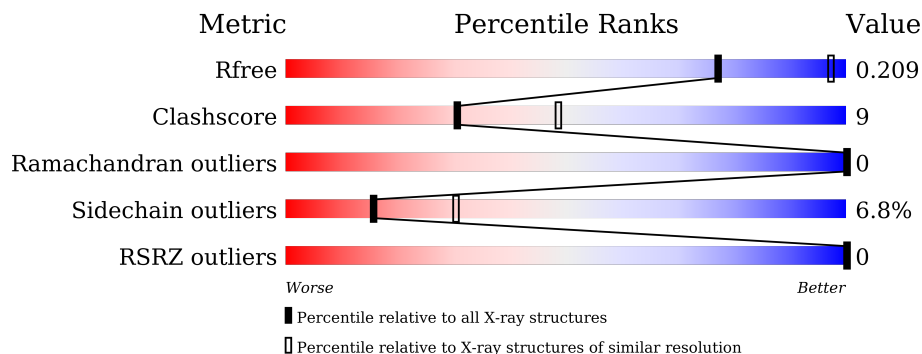
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	378	 78% 18% ..

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2957 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 Fungal chitinase from *Rhizomucor miehei* (SeMet-substituted proteins).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	369	2869	1816	465	583	2	3	0	3	0

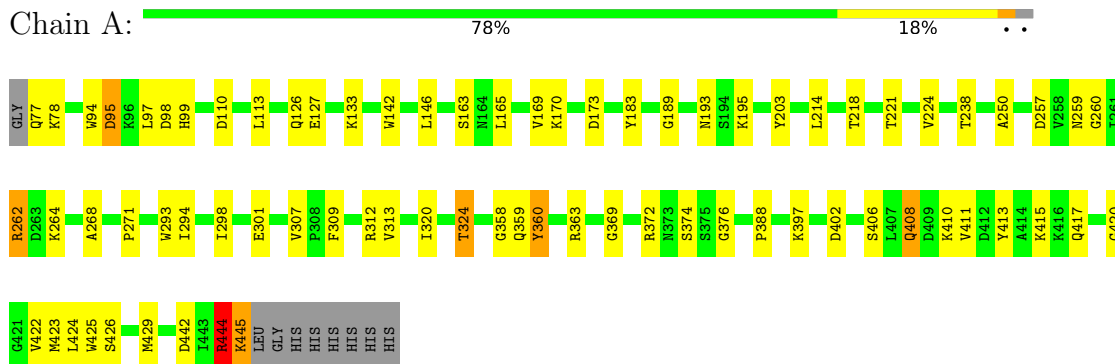
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	88	Total	O	0	0
			88	88		

### 3 Residue-property plots

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: Fungal chitinase from *Rhizomucor miehei* (SeMet-substituted proteins)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.81Å 48.81Å 247.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.27 – 2.58 42.27 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.27-2.58) 99.3 (42.27-2.58)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.57 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.172 , 0.206 0.172 , 0.209	Depositor DCC
$R_{free}$ test set	1150 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtrriage
Anisotropy	0.781	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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	0.69	2/2933 (0.1%)	0.69	2/3991 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	GLU	CD-OE1	-6.48	1.18	1.25
1	A	301	GLU	CD-OE2	-5.15	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	444	ARG	C-N-CA	6.87	138.86	121.70

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	2869	0	2756	52	0
2	A	88	0	0	6	1
All	All	2957	0	2756	52	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 9.

All (52) 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:408:GLN:O	1:A:408:GLN:NE2	1.89	1.06
1:A:442:ASP:O	1:A:445:LYS:CB	2.10	0.98
1:A:183:TYR:O	2:A:501:HOH:O	1.83	0.97
1:A:259:ASN:O	2:A:502:HOH:O	1.84	0.96
1:A:442:ASP:O	1:A:445:LYS:HB3	1.66	0.92
1:A:445:LYS:N	1:A:445:LYS:HD3	1.86	0.90
1:A:98:ASP:OD1	2:A:503:HOH:O	1.93	0.87
1:A:442:ASP:C	1:A:445:LYS:HB2	2.02	0.80
1:A:442:ASP:O	1:A:445:LYS:HB2	1.83	0.79
1:A:445:LYS:HD3	1:A:445:LYS:H	1.46	0.79
1:A:320:ILE:HA	1:A:324:THR:HG21	1.68	0.75
1:A:110:ASP:OD2	2:A:505:HOH:O	2.07	0.73
1:A:95:ASP:N	1:A:95:ASP:OD1	2.25	0.70
1:A:411:VAL:O	1:A:415:LYS:HG3	1.90	0.69
1:A:257:ASP:OD1	1:A:312:ARG:NH2	2.30	0.65
1:A:408:GLN:HE21	1:A:408:GLN:C	1.96	0.58
1:A:98:ASP:OD1	1:A:444:ARG:NH2	2.31	0.58
1:A:363:ARG:HG3	1:A:429:MSE:O	2.04	0.56
1:A:95:ASP:O	1:A:444:ARG:NH1	2.38	0.54
1:A:307:VAL:HG12	1:A:410:LYS:HD3	1.88	0.54
1:A:142:TRP:CH2	1:A:189:GLY:HA2	2.44	0.53
1:A:376:GLY:N	2:A:506:HOH:O	2.07	0.51
1:A:94:TRP:CZ2	1:A:127:GLU:HB3	2.45	0.51
1:A:142:TRP:CZ3	1:A:189:GLY:HA2	2.46	0.51
1:A:78:LYS:HD3	1:A:420:GLY:O	2.11	0.51
1:A:442:ASP:CA	1:A:445:LYS:HB2	2.41	0.50
1:A:442:ASP:C	1:A:445:LYS:CB	2.70	0.49
1:A:369:GLY:O	1:A:374:SER:HB2	2.13	0.49
1:A:442:ASP:HA	1:A:445:LYS:HB2	1.96	0.48
1:A:415:LYS:HE3	1:A:415:LYS:HB3	1.60	0.47
1:A:309:PHE:CE2	1:A:424:LEU:HD13	2.51	0.46
1:A:97:LEU:O	1:A:133:LYS:NZ	2.47	0.45
1:A:262:ARG:HE	1:A:262:ARG:HB3	1.56	0.45
1:A:442:ASP:HA	1:A:445:LYS:CB	2.46	0.45
1:A:146:LEU:HD23	1:A:193:ASN:HA	1.99	0.44
1:A:442:ASP:HA	1:A:445:LYS:HG2	1.98	0.44
1:A:359:GLN:HG2	1:A:360:TYR:N	2.32	0.44
1:A:224:VAL:HB	1:A:293:TRP:CZ2	2.52	0.44
1:A:260:GLY:HA3	1:A:262:ARG:CZ	2.48	0.43
1:A:313:VAL:HG22	1:A:358:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ILE:HA	1:A:298:ILE:O	2.18	0.43
1:A:214:LEU:HD13	1:A:218:THR:HG21	2.01	0.42
1:A:268:ALA:HB3	1:A:271:PRO:HB3	2.02	0.42
1:A:413:TYR:CZ	1:A:417:GLN:HG3	2.53	0.42
1:A:257:ASP:HA	1:A:312:ARG:HH21	1.85	0.42
1:A:221:THR:HG22	1:A:250:ALA:HB3	2.02	0.42
1:A:127:GLU:OE1	2:A:508:HOH:O	2.22	0.41
1:A:165:LEU:O	1:A:169:VAL:HG23	2.21	0.41
1:A:388:PRO:HD3	1:A:406:SER:HB3	2.03	0.41
1:A:77:GLN:CG	1:A:99:HIS:HB2	2.51	0.40
1:A:77:GLN:HG3	1:A:99:HIS:HB2	2.03	0.40
1:A:425:TRP:HA	1:A:426:SER:HA	1.86	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:A:561:HOH:O	2:A:585:HOH:O[1_445]	1.82	0.38

## 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	370/378 (98%)	358 (97%)	12 (3%)	0	<b>100</b> <b>100</b>

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	314/315 (100%)	293 (93%)	21 (7%)	16 31

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASP
1	A	113	LEU
1	A	126	GLN
1	A	163	SER
1	A	170	LYS
1	A	173	ASP
1	A	195	LYS
1	A	203	TYR
1	A	238	THR
1	A	262	ARG
1	A	264	LYS
1	A	324	THR
1	A	360	TYR
1	A	372	ARG
1	A	397	LYS
1	A	402	ASP
1	A	408	GLN
1	A	422	VAL
1	A	423	MSE
1	A	444	ARG
1	A	445	LYS

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

### 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 monosaccharides 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	366/378 (96%)	-0.29	0 <a href="#">100</a> <a href="#">100</a>	13, 24, 38, 53	0

There are no RSRZ outliers to report.

### 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.