



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 08:00 pm BST

PDB ID : 2XVN  
Title : A. fumigatus chitinase A1 phenyl-methylguanylurea complex  
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Deposited on : 2010-10-26  
Resolution : 2.35 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

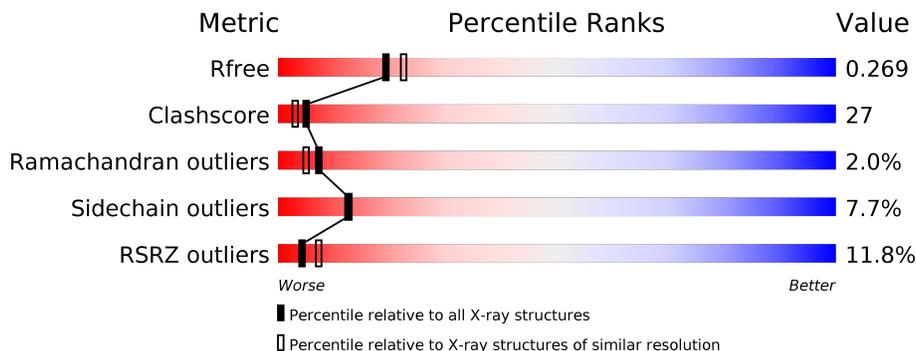
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	309	 3% 75% 22% ..
1	B	309	 2% 72% 25% .
1	C	309	 27% 28% 30% 8% . 32%

## 2 Entry composition i

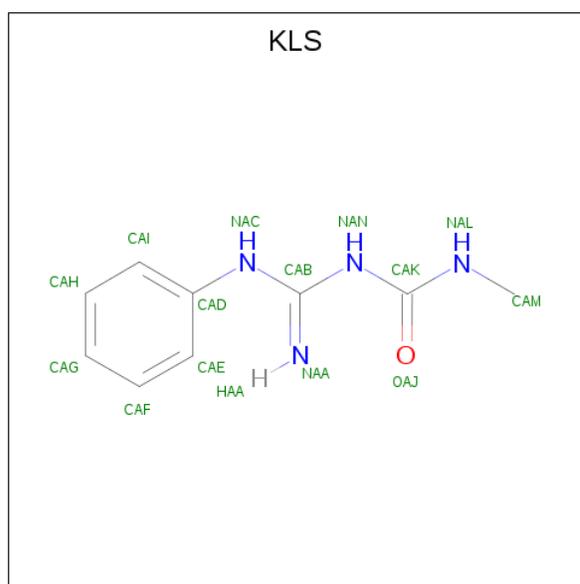
There are 4 unique types of molecules in this entry. The entry contains 6669 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ASPERGILLUS FUMIGATUS CHITINASE A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	Total 2396	C 1541	N 382	O 461	S 12	0	0	0
1	B	309	Total 2396	C 1541	N 382	O 461	S 12	0	0	0
1	C	210	Total 1631	C 1062	N 253	O 307	S 9	0	0	0

- Molecule 2 is 1-METHYL-3-(N-PHENYLCARBAMIMIDOYL)UREA (three-letter code: KLS) (formula: C<sub>9</sub>H<sub>12</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 14	C 9	N 4	O 1	0	0
2	B	1	Total 14	C 9	N 4	O 1	0	0

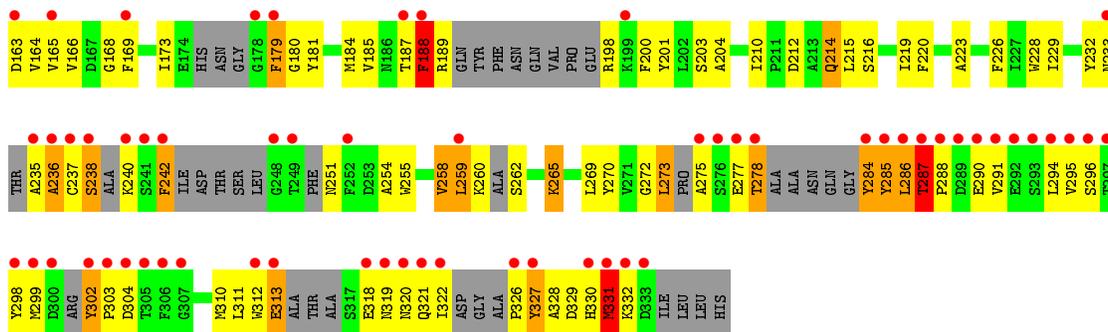
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Cl 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	89	Total O 89 89	0	0
4	B	95	Total O 95 95	0	0
4	C	32	Total O 32 32	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.98Å 99.98Å 111.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 2.35 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (12.00-2.35) 96.9 (10.00-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.259 , 0.299 0.252 , 0.269	Depositor DCC
$R_{free}$ test set	465 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.49 , 27.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.449 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
Reported twinning fraction	0.460 for H, K, L 0.540 for K, H, -L	Depositor
Outliers	0 of 46543 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	6669	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, KLS

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	1.16	5/2468 (0.2%)	1.04	11/3368 (0.3%)
1	B	1.10	3/2468 (0.1%)	0.98	3/3368 (0.1%)
1	C	0.98	2/1655 (0.1%)	0.91	1/2218 (0.0%)
All	All	1.09	10/6591 (0.2%)	0.99	15/8954 (0.2%)

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	C	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ARG	C-N	-17.89	0.93	1.34
1	B	291	VAL	C-N	-10.51	1.09	1.34
1	B	292	GLU	C-N	7.73	1.51	1.34
1	A	327	TYR	CD2-CE2	7.31	1.50	1.39
1	B	277	GLU	C-N	-7.31	1.17	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	VAL	CB-CA-C	-12.04	88.53	111.40
1	A	198	ARG	C-N-CA	11.74	151.04	121.70
1	A	43	ARG	NE-CZ-NH1	-10.04	115.28	120.30
1	A	258	VAL	N-CA-C	-9.64	84.97	111.00
1	A	259	LEU	N-CA-C	-8.18	88.93	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	302	TYR	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	2396	0	2235	51	3
1	B	2396	0	2234	56	1
1	C	1631	0	1511	228	2
2	A	14	0	11	0	0
2	B	14	0	11	5	0
3	B	2	0	0	0	0
4	A	89	0	0	8	0
4	B	95	0	0	3	0
4	C	32	0	0	20	0
All	All	6669	0	6002	338	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 27.

The worst 5 of 338 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:286:LEU:HA	1:C:287:THR:CG2	1.40	1.50
1:C:287:THR:OG1	1:C:290:GLU:CB	1.68	1.41
1:C:133:SER:O	1:C:138:VAL:CG2	1.68	1.39
1:C:132:LEU:HA	1:C:179:PHE:CZ	1.60	1.35
1:C:286:LEU:CA	1:C:287:THR:HG23	1.58	1.33

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:323:ASP:OD2	1:B:90:ASP:O[2_554]	1.74	0.46
1:A:153:GLU:OE1	1:C:278:THR:CG2[3_555]	2.10	0.10
1:A:156:GLU:OE2	1:C:320:ASN:OD1[3_555]	2.16	0.04

### 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	307/309 (99%)	281 (92%)	24 (8%)	2 (1%)	22	23
1	B	307/309 (99%)	291 (95%)	14 (5%)	2 (1%)	22	23
1	C	169/309 (55%)	134 (79%)	23 (14%)	12 (7%)	1	0
All	All	783/927 (84%)	706 (90%)	61 (8%)	16 (2%)	7	5

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	C	61	ILE
1	C	139	ALA
1	C	147	ALA
1	C	166	VAL

#### 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	252/252 (100%)	243 (96%)	9 (4%)	35	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	252/252 (100%)	238 (94%)	14 (6%)	21	23
1	C	168/252 (67%)	139 (83%)	29 (17%)	2	1
All	All	672/756 (89%)	620 (92%)	52 (8%)	13	12

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	50	GLU
1	C	131	ILE
1	C	313	GLU
1	C	61	ILE
1	C	102	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	B	71	HIS
1	B	80	GLN
1	B	214	GLN
1	C	46	HIS

### 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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	KLS	B	1340	-	13,14,14	1.14	1 (7%)	15,17,17	0.83	0
2	KLS	A	1338	-	13,14,14	1.24	2 (15%)	15,17,17	1.30	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KLS	B	1340	-	-	1/10/10/10	0/1/1/1
2	KLS	A	1338	-	-	1/10/10/10	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1340	KLS	CAD-NAC	-2.79	1.36	1.41
2	A	1338	KLS	CAD-NAC	-2.69	1.36	1.41
2	A	1338	KLS	CAB-NAC	-2.38	1.34	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1338	KLS	CAB-NAN-CAK	4.22	132.64	125.42

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1340	KLS	NAA-CAB-NAN-CAK
2	A	1338	KLS	NAA-CAB-NAN-CAK

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1340	KLS	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	277:GLU	C	278:THR	N	1.17
1	B	291:VAL	C	292:GLU	N	1.09
1	A	198:ARG	C	199:LYS	N	0.92

## 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	309/309 (100%)	0.24	8 (2%) 56 65	2, 13, 27, 39	0
1	B	309/309 (100%)	0.08	6 (1%) 66 76	2, 10, 23, 31	0
1	C	210/309 (67%)	2.49	84 (40%) 0 0	7, 21, 63, 67	4 (1%)
All	All	828/927 (89%)	0.75	98 (11%) 4 7	2, 13, 38, 67	4 (0%)

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	291	VAL	15.0
1	C	300	ASP	11.9
1	C	288	PRO	9.8
1	C	141	ALA	9.6
1	C	275	ALA	9.5

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	KLS	B	1340	14/14	0.89	0.26	24,32,39,39	0
2	KLS	A	1338	14/14	0.93	0.18	7,11,22,22	0
3	CL	B	1339	1/1	0.93	0.10	30,30,30,30	0
3	CL	B	1338	1/1	0.98	0.08	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.