



# Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 04:13 pm BST

PDB ID : 9QW6 / pdb\_00009qw6  
Title : Urate Oxidase from Aspergillus Flavus with its Substrate Uric Acid by continuous serial electron diffraction (SerialED)  
Authors : Hofer, G.; Wang, L.; Pacoste, L.; Hager, P.; Fonjallaz, A.; Scaletti Hutchinson, E.; Stenmark, P.; Di Palma, M.; Williams, L.; Worrall, J.; Steiner, R.; Xu, H.; Zou, X.  
Deposited on : 2025-04-14  
Resolution : 1.75 Å (reported)  
Based on initial model : 4D12

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB 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/EMValidationReportHelp>

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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

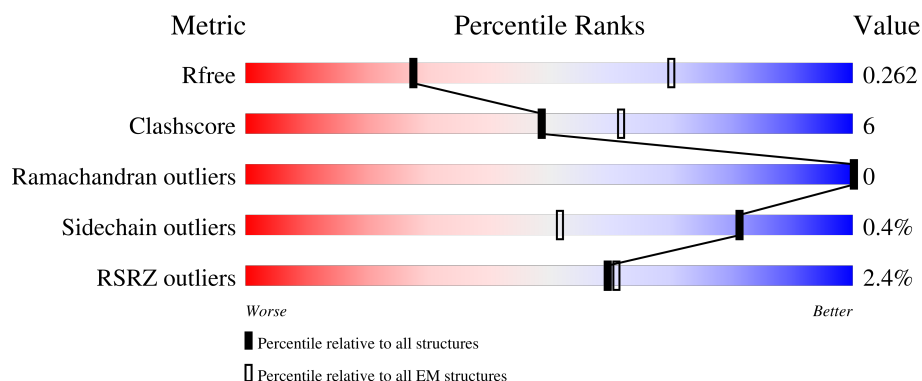
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*


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)	EM structures (#Entries)
$R_{free}$	180332	208
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RSRZ outliers	180361	209

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	302	

## 2 Entry composition [i](#)

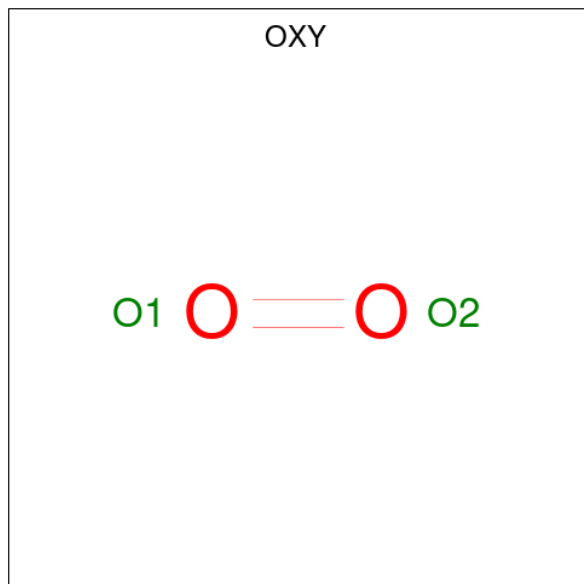
There are 4 unique types of molecules in this entry. The entry contains 5518 atoms, of which 2609 are hydrogens and 0 are deuteriums.

In the tables below, 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 Uricase.

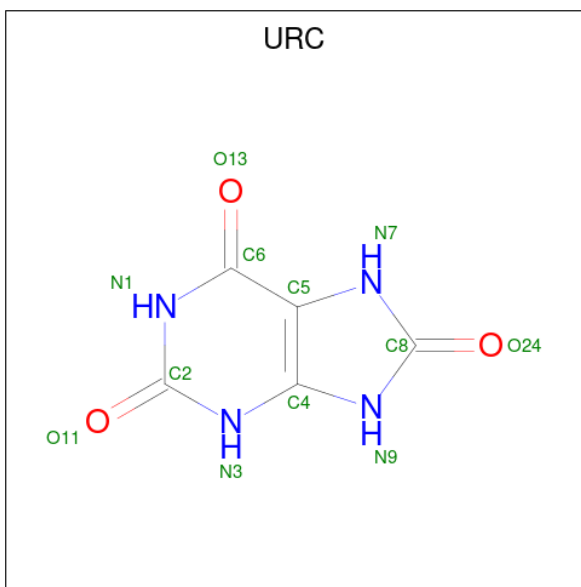
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	296	5160	1625	2605	437	483	10	37	0

- Molecule 2 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	O	0
			2	2	

- Molecule 3 is URIC ACID (CCD ID: URC) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	N	O	0
			16	5	4	4	3	

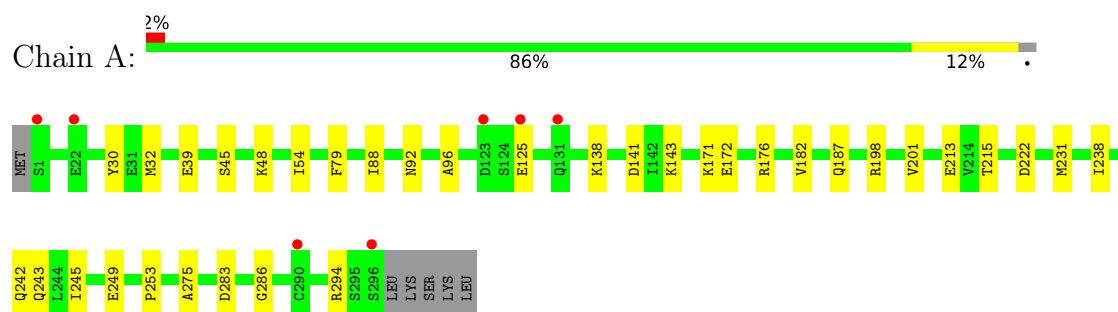
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	340	Total	O	0
			340	340	

### 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. 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. 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: Uricase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.13Å 94.44Å 103.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.48 – 1.75 17.48 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.6 (17.48-1.75) 96.5 (17.48-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 1.75Å)	Xtriage
Refinement program	unknown	Depositor
R, $R_{free}$	0.221 , 0.243 0.245 , 0.262	Depositor DCC
$R_{free}$ test set	2000 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 22.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5518	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 4.86% 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

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

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	0.31	0/2726	0.37	0/3687

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

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	2555	2605	2560	29	0
2	A	2	0	0	0	0
3	A	12	4	4	1	0
4	A	340	0	0	19	0
All	All	2909	2609	2564	30	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 6.

All (30) 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:187[B]:GLN:NE2	4:A:501:HOH:O	1.76	1.15
1:A:172:GLU:OE2	4:A:502:HOH:O	1.87	0.92
1:A:213[B]:GLU:OE1	4:A:504:HOH:O	2.01	0.79
1:A:143:LYS:NZ	1:A:249[B]:GLU:OE2	2.17	0.78
1:A:138[B]:LYS:NZ	4:A:511:HOH:O	2.21	0.72
1:A:92:ASN:OD1	4:A:506:HOH:O	2.09	0.70
1:A:141[B]:ASP:OD2	4:A:505:HOH:O	2.08	0.69
1:A:30:TYR:OH	4:A:503:HOH:O	1.97	0.64
1:A:283:ASP:OD2	4:A:508:HOH:O	2.16	0.61
1:A:39:GLU:OE1	4:A:507:HOH:O	2.16	0.59
1:A:198:ARG:HA	1:A:201:VAL:HG23	1.83	0.59
1:A:88:ILE:O	4:A:509:HOH:O	2.17	0.58
1:A:245[A]:ILE:O	1:A:294[A]:ARG:NH1	2.34	0.57
1:A:243[B]:GLN:CG	4:A:519:HOH:O	2.55	0.54
1:A:39:GLU:HB2	1:A:96:ALA:HB3	1.92	0.52
1:A:243[B]:GLN:HG3	4:A:519:HOH:O	2.10	0.51
1:A:176:ARG:HH12	3:A:402:URC:HN3	1.58	0.51
1:A:182:VAL:HG11	1:A:215:THR:HG21	1.95	0.49
1:A:45:SER:HB2	1:A:54[A]:ILE:HD11	1.97	0.47
1:A:243[B]:GLN:HG2	4:A:519:HOH:O	2.15	0.47
1:A:32[C]:MET:HE1	1:A:79:PHE:CE2	2.50	0.46
1:A:125[A]:GLU:HG2	4:A:516:HOH:O	2.15	0.45
1:A:222:ASP:OD1	4:A:510:HOH:O	2.21	0.45
1:A:238:ILE:HG22	1:A:245[B]:ILE:CD1	2.47	0.44
1:A:253:PRO:HA	1:A:286:GLY:O	2.19	0.42
1:A:275:ALA:O	4:A:513:HOH:O	2.22	0.42
1:A:48[B]:LYS:NZ	4:A:543:HOH:O	2.47	0.40
1:A:242:GLN:OE1	4:A:512:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	330/302 (109%)	322 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	298/268 (111%)	296 (99%)	2 (1%)	76	67

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

Mol	Chain	Res	Type
1	A	171[A]	LYS
1	A	171[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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
3	URC	A	402	-	11,13,13	2.24	6 (54%)	12,19,19	2.08	5 (41%)
2	OXY	A	401	-	1,1,1	0.36	0	-		

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
3	URC	A	402	-	-	-	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	URC	C6-N1	-3.53	1.32	1.38
3	A	402	URC	C8-N7	-3.04	1.33	1.39
3	A	402	URC	C8-N9	-3.01	1.33	1.39
3	A	402	URC	O11-C2	-2.15	1.18	1.23
3	A	402	URC	C5-C6	-2.03	1.37	1.42
3	A	402	URC	O24-C8	-2.03	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	URC	C6-N1-C2	-4.31	120.12	126.34
3	A	402	URC	N3-C2-N1	3.01	120.64	115.80
3	A	402	URC	O13-C6-C5	-2.80	120.82	127.24
3	A	402	URC	C5-C6-N1	2.54	119.88	112.31
3	A	402	URC	N9-C4-N3	2.36	132.45	122.78

There are no chirality outliers.

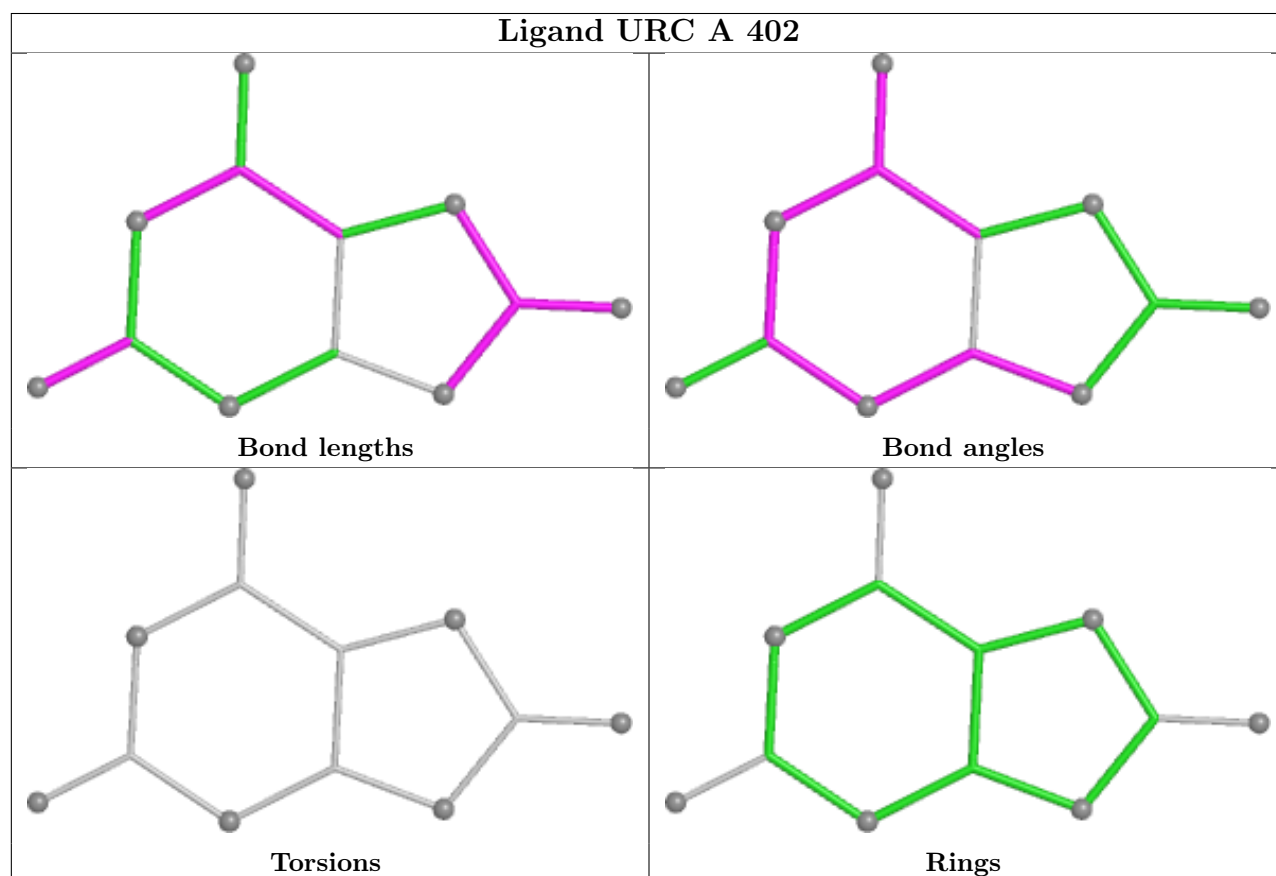
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	URC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.