



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2022 – 03:11 pm GMT

PDB ID : 8B7S  
Title : Crystal structure of the Chloramphenicol-inactivating oxidoreductase from *Novosphingobium* sp  
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Deposited on : 2022-10-03  
Resolution : 2.10 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  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

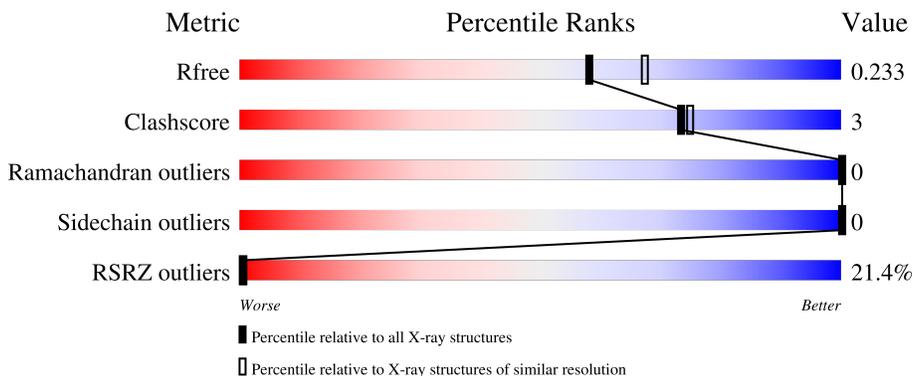
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	542	

## 2 Entry composition [i](#)

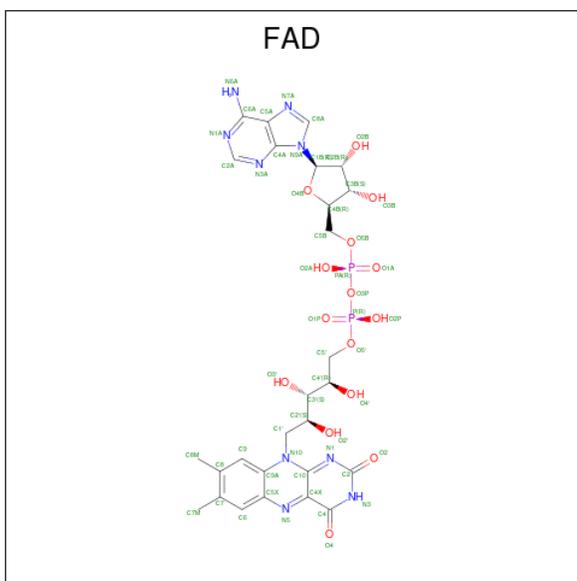
There are 3 unique types of molecules in this entry. The entry contains 7152 atoms, of which 3502 are hydrogens and 0 are deuteriums.

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 Chloramphenicol-inactivating oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	458	6953	2191	3471	621	655	15	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	84	27	31	9	15	2	0	0

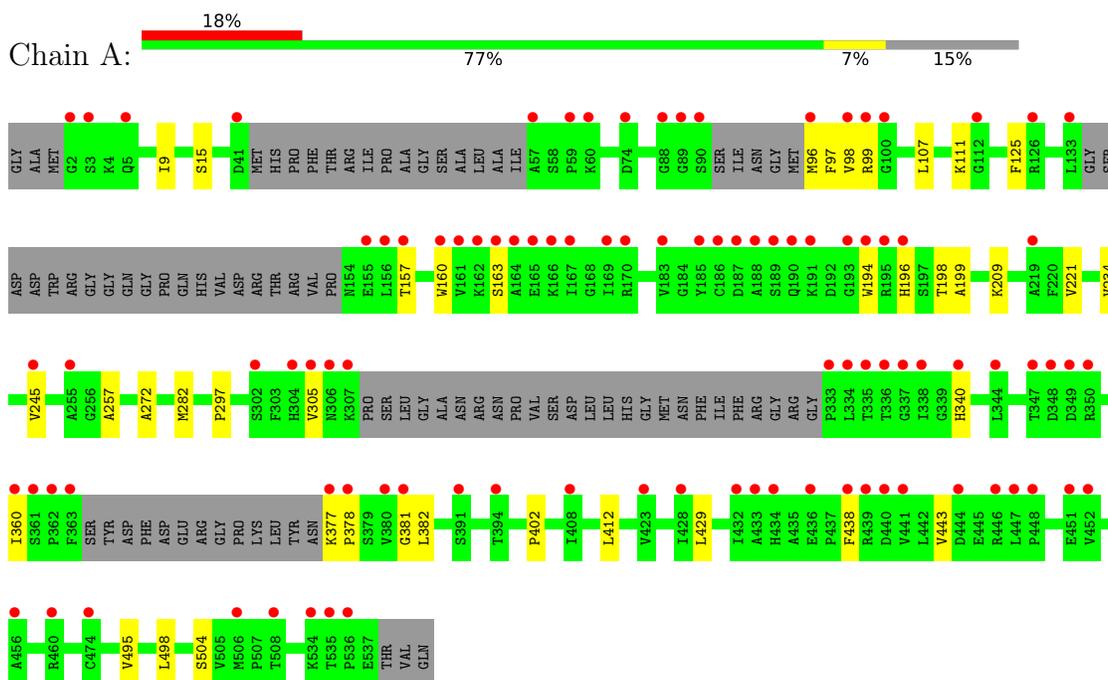
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		

### 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: Chloramphenicol-inactivating oxidoreductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.62Å 43.81Å 164.70Å 90.00° 91.06° 90.00°	Depositor
Resolution (Å)	44.61 – 2.10 44.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.61-2.10) 98.7 (44.61-2.10)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.207 , 0.232 0.208 , 0.233	Depositor DCC
$R_{free}$ test set	1636 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: FAD

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	0.32	0/3549	0.51	0/4798

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	99	ARG	Sidechain

### 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	3482	3471	3469	23	0
2	A	53	31	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	115	0	0	2	0
All	All	3650	3502	3500	23	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 3.

All (23) 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:382:LEU:HD23	1:A:429:LEU:HD22	1.66	0.78
1:A:495:VAL:HG21	1:A:498:LEU:HD23	1.72	0.69
1:A:98:VAL:HG21	1:A:125:PHE:CE1	2.31	0.65
1:A:107:LEU:HD11	1:A:111:LYS:HE2	1.87	0.55
1:A:97:PHE:CD1	1:A:194:TRP:O	2.61	0.53
1:A:272:ALA:HA	1:A:282:MET:HE3	1.91	0.53
1:A:9:ILE:HD13	1:A:245:VAL:HG13	1.92	0.52
1:A:377:LYS:HB2	1:A:378:PRO:CD	2.40	0.51
1:A:98:VAL:HG13	1:A:98:VAL:O	2.13	0.49
1:A:257:ALA:HA	1:A:504:SER:HB3	1.95	0.48
1:A:96:MET:HB2	1:A:196:HIS:CE1	2.48	0.48
1:A:377:LYS:CB	1:A:378:PRO:CD	2.92	0.47
1:A:209:LYS:NZ	3:A:705:HOH:O	2.47	0.47
1:A:160:TRP:CE3	1:A:360:ILE:HG21	2.49	0.47
1:A:157:THR:HG21	1:A:340:HIS:CB	2.45	0.47
1:A:297:PRO:HB3	1:A:412:LEU:HG	1.98	0.46
1:A:163:SER:OG	1:A:438:PHE:HB2	2.17	0.45
1:A:221:VAL:HG13	1:A:234:VAL:CG1	2.47	0.45
1:A:305:VAL:HA	1:A:443:VAL:HG23	1.99	0.44
1:A:381:GLY:C	1:A:382:LEU:HD12	2.38	0.44
1:A:198:THR:HG22	1:A:199:ALA:N	2.34	0.41
1:A:15:SER:HA	1:A:199:ALA:HB2	2.02	0.41
1:A:402:PRO:HG3	3:A:730:HOH:O	2.21	0.41

There are no symmetry-related clashes.

## 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	446/542 (82%)	427 (96%)	19 (4%)	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	363/430 (84%)	363 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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	154	ASN
1	A	342	GLN
1	A	513	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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
2	FAD	A	601	-	53,58,58	0.53	0	68,89,89	0.57	1 (1%)

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	FAD	A	601	-	-	1/30/50/50	0/6/6/6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C5A-C6A-N6A	2.23	123.74	120.35

There are no chirality outliers.

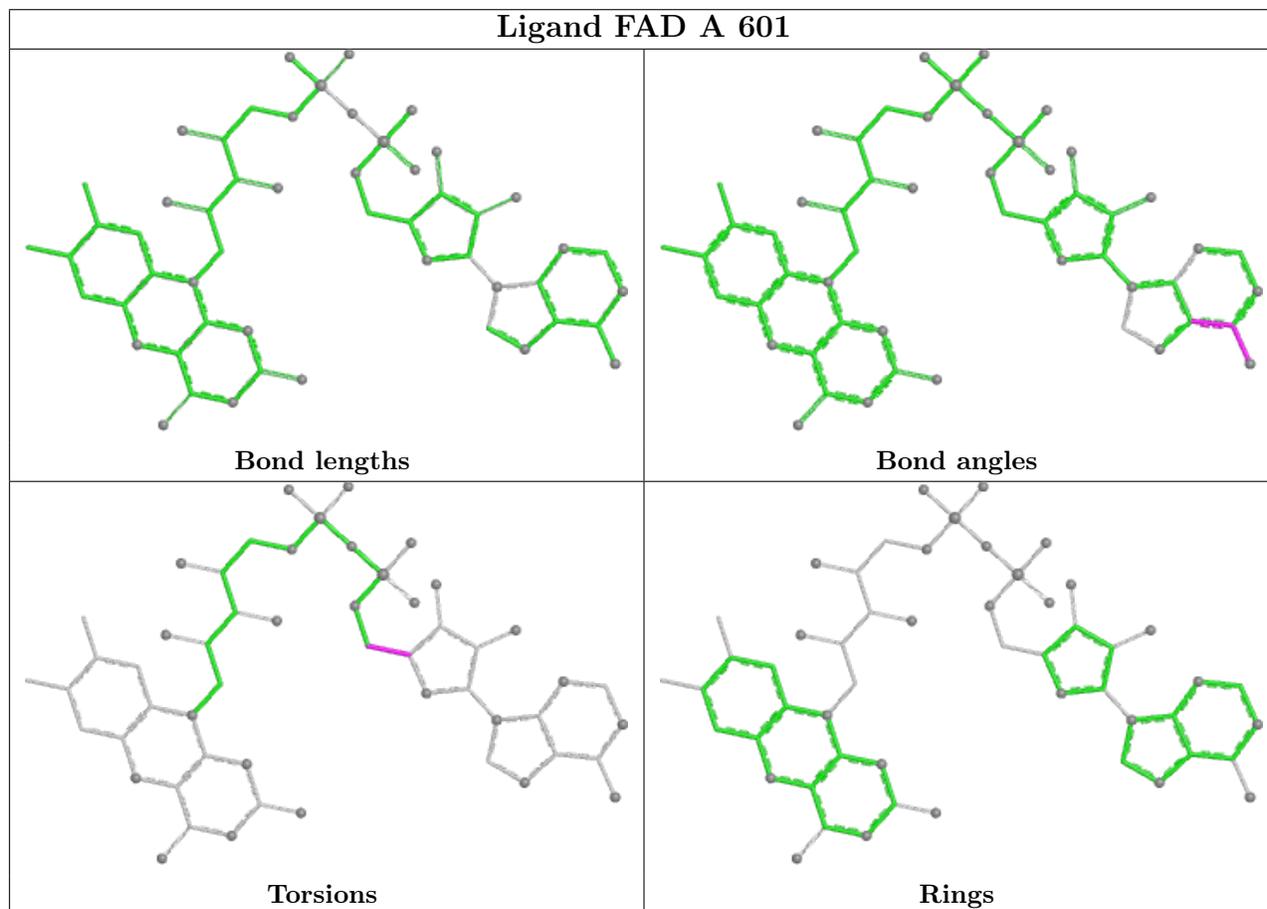
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

No monomer is involved in short contacts.

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.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	458/542 (84%)	1.51	98 (21%) <b>0</b> <b>0</b>	27, 52, 130, 155	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	PRO	10.7
1	A	189	SER	9.6
1	A	337	GLY	9.0
1	A	363	PHE	8.3
1	A	187	ASP	7.3
1	A	306	ASN	7.2
1	A	447	LEU	7.1
1	A	536	PRO	7.0
1	A	338	ILE	6.9
1	A	380	VAL	6.9
1	A	90	SER	6.7
1	A	334	LEU	6.4
1	A	59	PRO	6.2
1	A	3	SER	6.1
1	A	195	ARG	5.9
1	A	535	THR	5.7
1	A	89	GLY	5.1
1	A	391	SER	5.0
1	A	156	LEU	5.0
1	A	440	ASP	4.9
1	A	460	ARG	4.9
1	A	74	ASP	4.9
1	A	194	TRP	4.8
1	A	336	THR	4.7
1	A	333	PRO	4.7
1	A	428	ILE	4.4
1	A	377	LYS	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	423	VAL	4.2
1	A	456	ALA	4.0
1	A	188	ALA	4.0
1	A	98	VAL	3.9
1	A	335	THR	3.8
1	A	350	ARG	3.8
1	A	96	MET	3.7
1	A	438	PHE	3.6
1	A	360	ILE	3.6
1	A	444	ASP	3.6
1	A	436	GLU	3.5
1	A	157	THR	3.5
1	A	191	LYS	3.5
1	A	5	GLN	3.4
1	A	190	GLN	3.4
1	A	186	CYS	3.3
1	A	185	TYR	3.2
1	A	57	ALA	3.2
1	A	155	GLU	3.2
1	A	2	GLY	3.1
1	A	448	PRO	3.1
1	A	446	ARG	3.1
1	A	307	LYS	3.1
1	A	378	PRO	3.0
1	A	347	THR	3.0
1	A	304	HIS	2.9
1	A	162	LYS	2.9
1	A	349	ASP	2.8
1	A	441	VAL	2.8
1	A	41	ASP	2.8
1	A	167	ILE	2.8
1	A	305	VAL	2.7
1	A	88	GLY	2.7
1	A	381	GLY	2.7
1	A	196	HIS	2.7
1	A	99	ARG	2.7
1	A	166	LYS	2.7
1	A	169	ILE	2.6
1	A	434	HIS	2.6
1	A	451	GLU	2.6
1	A	160	TRP	2.6
1	A	161	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	163	SER	2.5
1	A	170	ARG	2.5
1	A	302	SER	2.5
1	A	433	ALA	2.4
1	A	183	VAL	2.4
1	A	394	THR	2.4
1	A	340	HIS	2.4
1	A	344	LEU	2.4
1	A	60	LYS	2.3
1	A	452	VAL	2.3
1	A	100	GLY	2.3
1	A	474	CYS	2.2
1	A	508	THR	2.2
1	A	126	ARG	2.2
1	A	439	ARG	2.2
1	A	193	GLY	2.2
1	A	361	SER	2.1
1	A	534	LYS	2.1
1	A	133	LEU	2.1
1	A	112	GLY	2.1
1	A	165	GLU	2.1
1	A	348	ASP	2.1
1	A	164	ALA	2.1
1	A	219	ALA	2.1
1	A	432	ILE	2.0
1	A	506	MET	2.0
1	A	245	VAL	2.0
1	A	255	ALA	2.0
1	A	408	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](#)

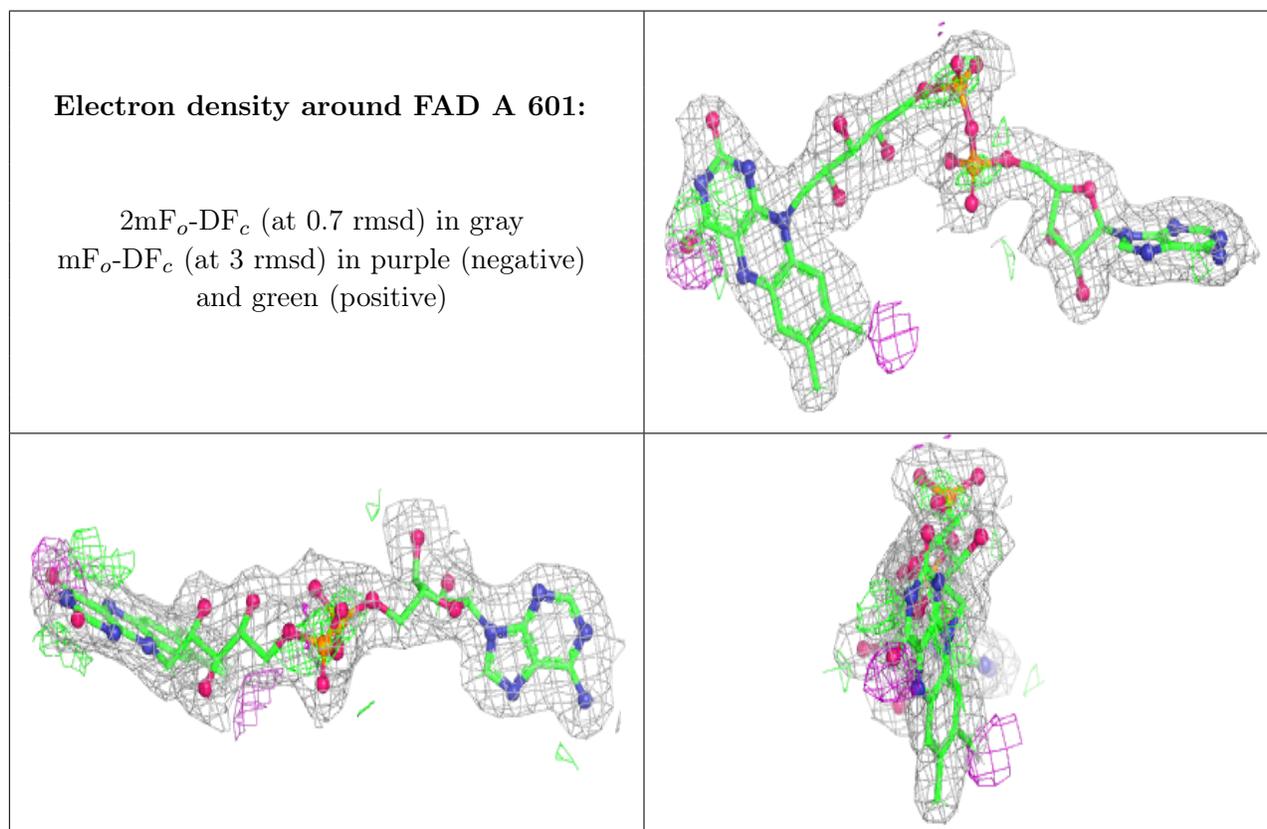
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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(Å <sup>2</sup> )	Q<0.9
2	FAD	A	601	53/53	0.94	0.17	24,36,53,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.