



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 08:58 am BST

PDB ID : 4Z2U  
Title : Crystal Structure of 2-hydroxybiphenyl 3-monooxygenase R242Q from *Pseudomonas azelaica*  
Authors : Kanteev, M.; Bregman-Cohen, A.; Fishman, A.  
Deposited on : 2015-03-30  
Resolution : 2.50 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  
buster-report : 1.1.7 (2018)  
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

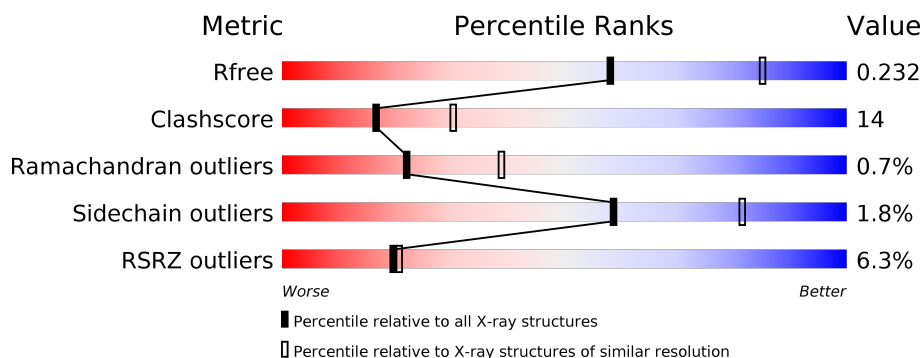
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	592	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• 5%</div> </div> </div>
1	B	592	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	601	X	-	-	-
2	FAD	B	601	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9413 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.

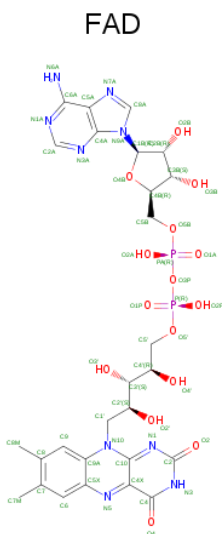
- Molecule 1 is a protein called 2-hydroxybiphenyl-3-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4330	2737	759	814	20			
1	B	563	Total	C	N	O	S	0	0	0
			4330	2737	759	814	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP O06647
A	-4	HIS	-	expression tag	UNP O06647
A	-3	HIS	-	expression tag	UNP O06647
A	-2	HIS	-	expression tag	UNP O06647
A	-1	HIS	-	expression tag	UNP O06647
A	0	HIS	-	expression tag	UNP O06647
A	1	HIS	-	expression tag	UNP O06647
A	242	GLN	ARG	engineered mutation	UNP O06647
B	-5	MET	-	initiating methionine	UNP O06647
B	-4	HIS	-	expression tag	UNP O06647
B	-3	HIS	-	expression tag	UNP O06647
B	-2	HIS	-	expression tag	UNP O06647
B	-1	HIS	-	expression tag	UNP O06647
B	0	HIS	-	expression tag	UNP O06647
B	1	HIS	-	expression tag	UNP O06647
B	242	GLN	ARG	engineered mutation	UNP O06647

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	313	Total O 313 313	0	0
3	B	334	Total O 334 334	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.14Å 131.54Å 79.00Å 90.00° 98.28° 90.00°	Depositor
Resolution (Å)	32.37 – 2.50 38.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.2 (32.37-2.50) 92.2 (38.33-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.67 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, $R_{free}$	0.204 , 0.237 0.201 , 0.232	Depositor DCC
$R_{free}$ test set	2528 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9413	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% 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: 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	0.55	4/4425 (0.1%)	0.74	11/5998 (0.2%)
1	B	0.50	3/4425 (0.1%)	0.60	2/5998 (0.0%)
All	All	0.52	7/8850 (0.1%)	0.67	13/11996 (0.1%)

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	5
1	B	0	1
All	All	0	6

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	GLY	C-N	-13.89	1.02	1.34
1	A	46	ARG	C-N	-11.98	1.06	1.34
1	A	149	GLU	C-N	-11.72	1.07	1.34
1	B	169	VAL	C-N	-7.39	1.17	1.34
1	A	218	HIS	C-N	-7.17	1.17	1.34

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ARG	O-C-N	-16.09	96.96	122.70
1	A	150	ASP	O-C-N	-12.74	102.32	122.70
1	A	46	ARG	C-N-CA	11.94	151.55	121.70
1	A	218	HIS	O-C-N	-11.43	104.41	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	46	ARG	CA-C-N	10.58	140.49	117.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	HIS	Mainchain
1	A	46	ARG	Mainchain,Peptide
1	A	47	SER	Mainchain
1	A	495	ARG	Sidechain
1	B	255	GLY	Mainchain

## 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	4330	0	4274	141	0
1	B	4330	0	4275	104	0
2	A	53	0	30	8	0
2	B	53	0	30	8	0
3	A	313	0	0	3	4
3	B	334	0	0	1	5
All	All	9413	0	8609	246	6

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 14.

The worst 5 of 246 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
1:A:201:SER:HB3	1:A:256:TYR:O	1.39	1.22
1:A:319:THR:CG2	1:A:320:PRO:HD2	1.71	1.21
1:A:319:THR:HG23	1:A:320:PRO:HD2	1.17	1.10
1:A:511:ALA:HB1	1:A:522:LEU:HD11	1.10	1.07
1:B:75:GLU:OE1	1:B:75:GLU:N	1.95	1.00

The worst 5 of 6 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)
3:A:919:HOH:O	3:A:960:HOH:O[2_555]	1.92	0.28
3:A:935:HOH:O	3:B:849:HOH:O[4_445]	2.04	0.16
3:B:746:HOH:O	3:B:848:HOH:O[2_455]	2.06	0.14
3:A:1002:HOH:O	3:B:913:HOH:O[4_445]	2.08	0.12
3:A:975:HOH:O	3:B:911:HOH:O[4_445]	2.09	0.11

## 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	557/592 (94%)	525 (94%)	29 (5%)	3 (0%)	29	48
1	B	557/592 (94%)	520 (93%)	32 (6%)	5 (1%)	17	31
All	All	1114/1184 (94%)	1045 (94%)	61 (6%)	8 (1%)	22	39

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ILE
1	A	389	PRO
1	B	198	ILE
1	B	268	GLU
1	B	47	SER

### 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	451/473 (95%)	444 (98%)	7 (2%)	62	84
1	B	451/473 (95%)	442 (98%)	9 (2%)	55	79
All	All	902/946 (95%)	886 (98%)	16 (2%)	59	81

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	SER
1	B	47	SER
1	B	370	ARG
1	A	495	ARG
1	B	495	ARG

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	205	ASN
1	A	275	HIS
1	B	242	GLN
1	B	296	ASN
1	B	298	GLN

### 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 carbohydrates 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	$\# Z  > 2$
2	FAD	B	601	-	51,58,58	3.00	16 (31%)	60,89,89	2.64	17 (28%)
2	FAD	A	601	-	51,58,58	3.04	16 (31%)	60,89,89	2.37	11 (18%)

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	B	601	-	1/1/9/9	13/30/50/50	0/6/6/6
2	FAD	A	601	-	1/1/9/9	15/30/50/50	0/6/6/6

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C4X-C10	14.15	1.53	1.38
2	A	601	FAD	C4X-C10	13.77	1.52	1.38
2	A	601	FAD	C5X-N5	8.66	1.49	1.35
2	B	601	FAD	C5X-N5	8.36	1.49	1.35
2	A	601	FAD	C2'-C3'	5.08	1.63	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4-N3-C2	12.25	125.48	115.14
2	A	601	FAD	C4-N3-C2	10.54	124.04	115.14
2	B	601	FAD	O5'-P-O1P	-6.06	85.38	109.07
2	A	601	FAD	N3A-C2A-N1A	-5.79	119.63	128.68
2	A	601	FAD	O5'-P-O1P	-5.72	86.73	109.07

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	601	FAD	C3'
2	A	601	FAD	C3'

5 of 28 torsion outliers are listed below:

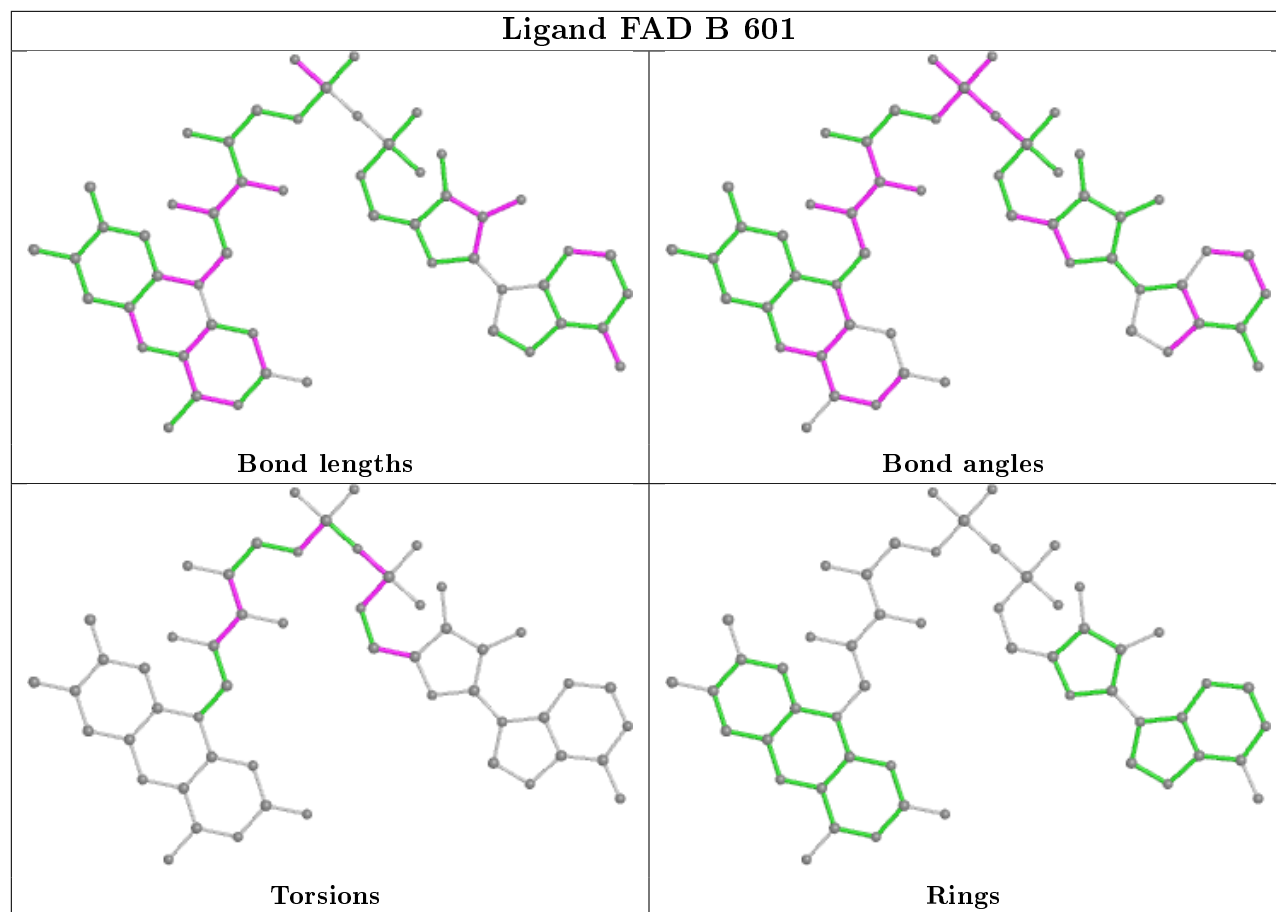
Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C1'-C2'-C3'-C4'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	B	601	FAD	C2'-C3'-C4'-O4'

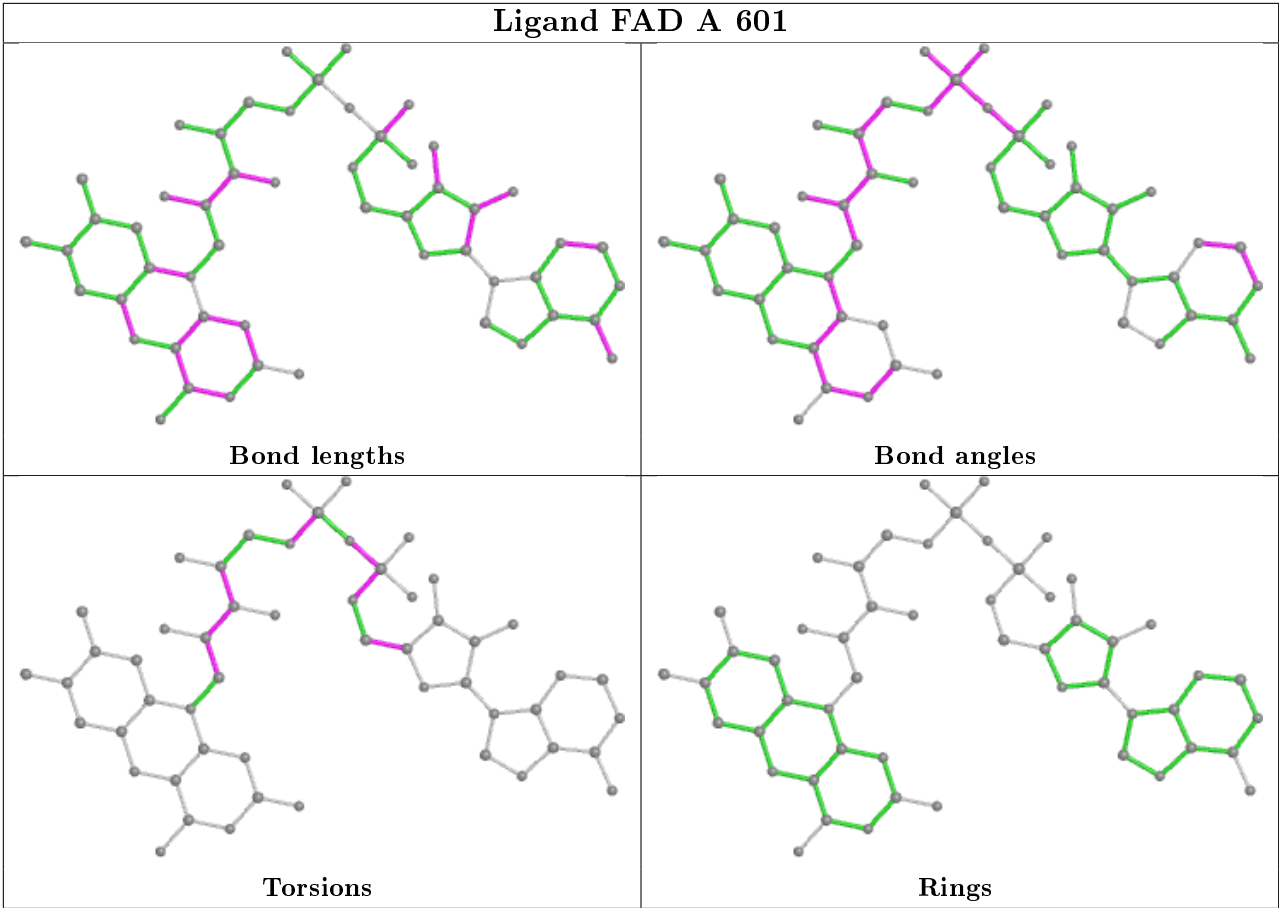
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FAD	8	0
2	A	601	FAD	8	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
1	B	3

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	217:GLU	C	218:HIS	N	1.18
1	A	218:HIS	C	219:ARG	N	1.17
1	B	51:ASN	C	52:GLN	N	1.17
1	B	169:VAL	C	170:ARG	N	1.17
1	A	149:GLU	C	150:ASP	N	1.07

## 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	563/592 (95%)	0.19	34 (6%) 21 22	6, 22, 62, 157	0
1	B	563/592 (95%)	0.07	37 (6%) 18 19	6, 22, 62, 157	0
All	All	1126/1184 (95%)	0.13	71 (6%) 20 21	6, 22, 62, 157	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	GLY	10.2
1	B	198	ILE	7.5
1	B	199	GLY	7.3
1	A	198	ILE	7.1
1	A	256	TYR	6.6

### 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.

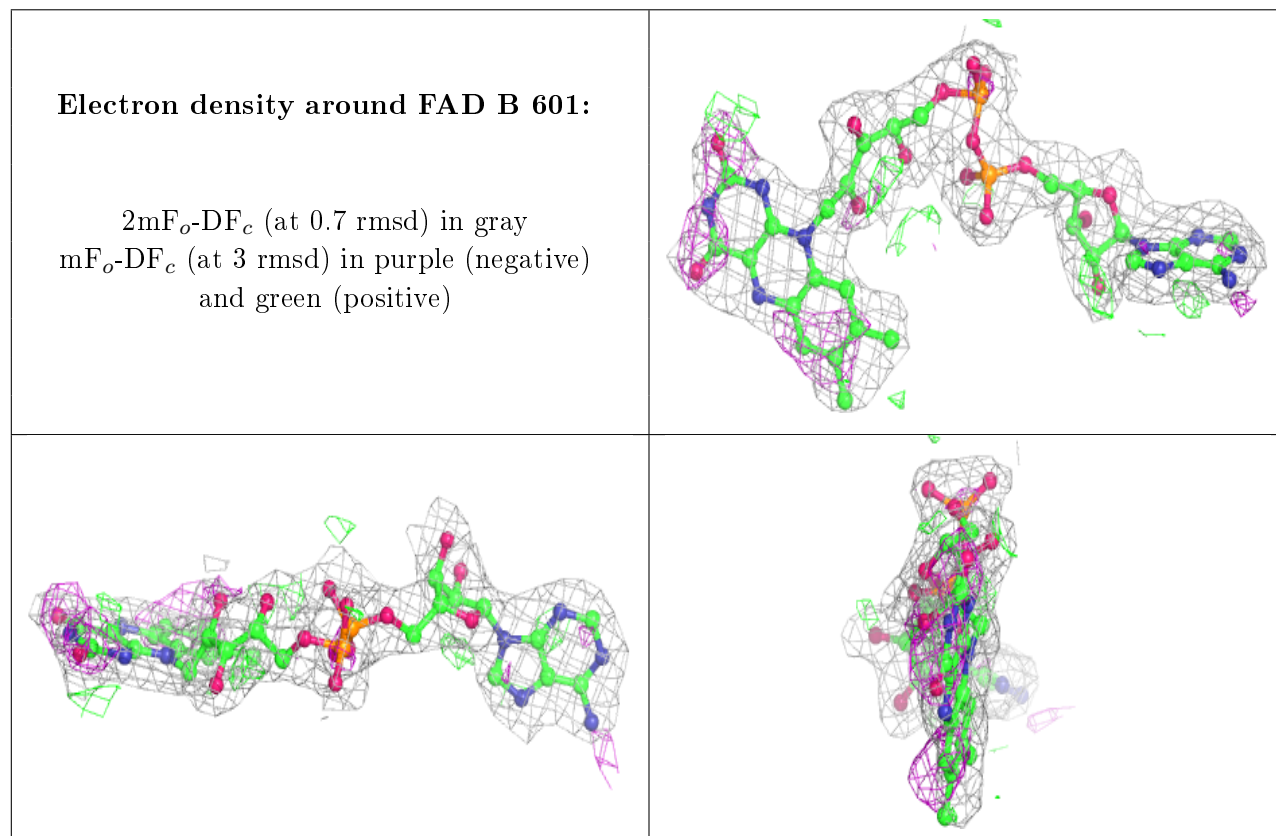
### 6.4 Ligands [i](#)

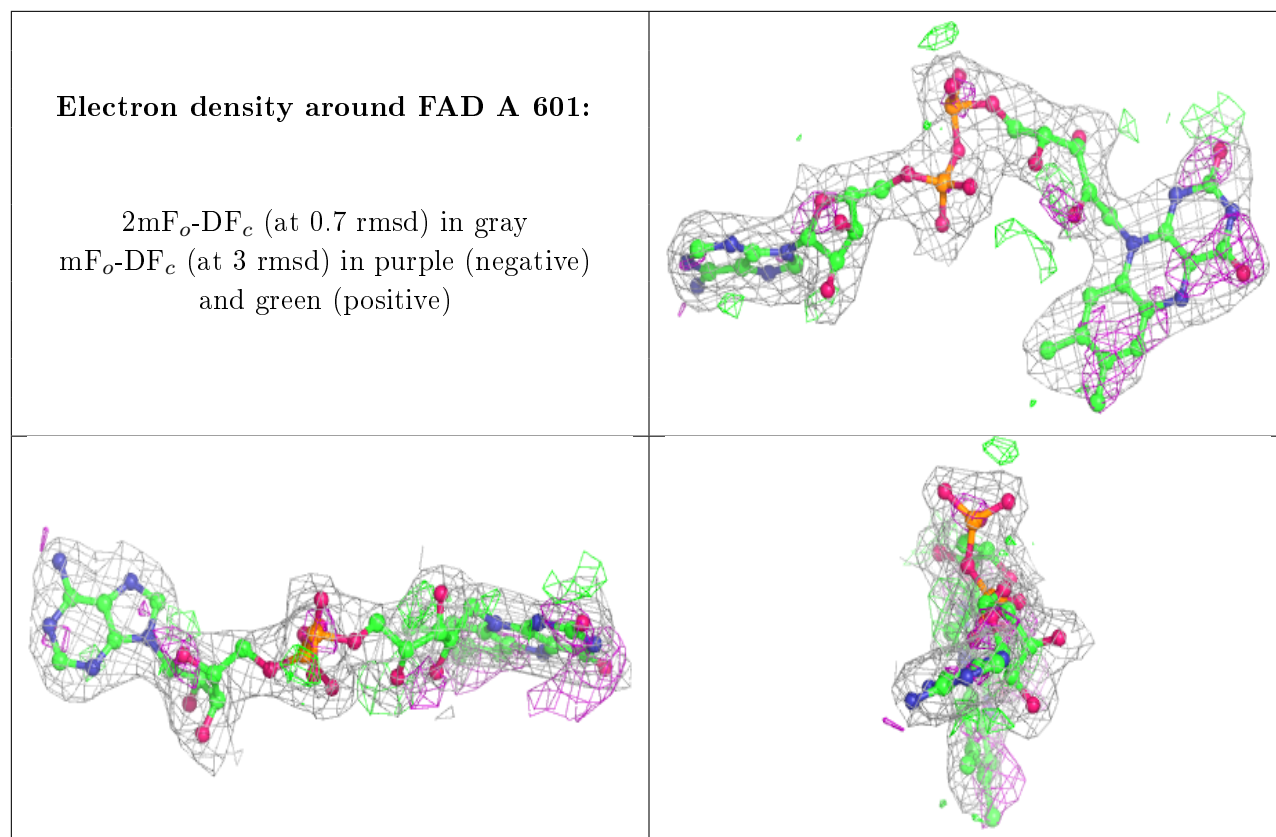
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	FAD	B	601	53/53	0.95	0.13	4,8,11,13	0
2	FAD	A	601	53/53	0.95	0.13	4,8,11,13	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.