



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 07:10 am BST

PDB ID : 8A1H  
Title : Bacterial 6-4 photolyase from *Vibrio cholerae*  
Authors : Essen, L.-O.; Emmerich, H.J.  
Deposited on : 2022-06-01  
Resolution : 1.65 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 : 2.35.1  
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) : 2.35.1

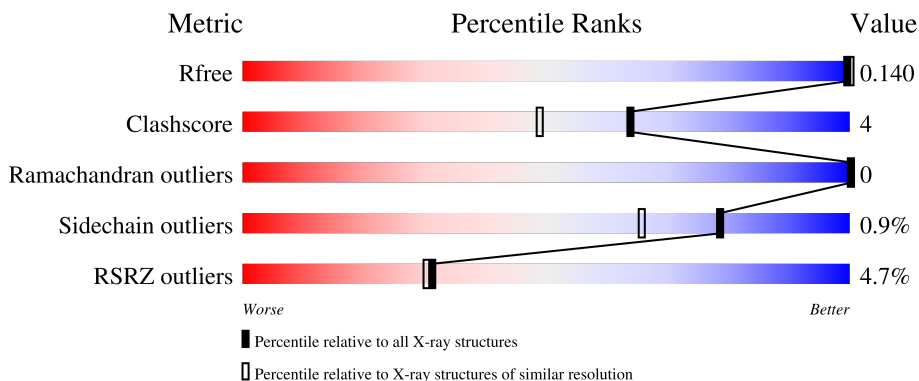
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

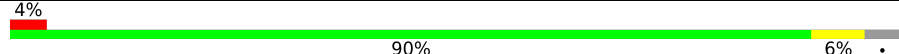
The reported resolution of this entry is 1.65 Å.

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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	536	

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
6	GOL	A	612	-	X	-	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9432 atoms, of which 4302 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 6-4 photolyase (FeS-BCP, CryPro).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	516	8468	2744	4173	757	766	28	0	22	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9KLD7
A	2	GLY	-	expression tag	UNP Q9KLD7
A	3	SER	-	expression tag	UNP Q9KLD7
A	4	SER	-	expression tag	UNP Q9KLD7
A	5	HIS	-	expression tag	UNP Q9KLD7
A	6	HIS	-	expression tag	UNP Q9KLD7
A	7	HIS	-	expression tag	UNP Q9KLD7
A	8	HIS	-	expression tag	UNP Q9KLD7
A	9	HIS	-	expression tag	UNP Q9KLD7
A	10	HIS	-	expression tag	UNP Q9KLD7
A	11	SER	-	expression tag	UNP Q9KLD7
A	12	SER	-	expression tag	UNP Q9KLD7
A	13	GLY	-	expression tag	UNP Q9KLD7
A	14	LEU	-	expression tag	UNP Q9KLD7
A	15	VAL	-	expression tag	UNP Q9KLD7
A	16	PRO	-	expression tag	UNP Q9KLD7
A	17	ARG	-	expression tag	UNP Q9KLD7
A	18	GLY	-	expression tag	UNP Q9KLD7
A	19	SER	-	expression tag	UNP Q9KLD7
A	20	HIS	-	expression tag	UNP Q9KLD7

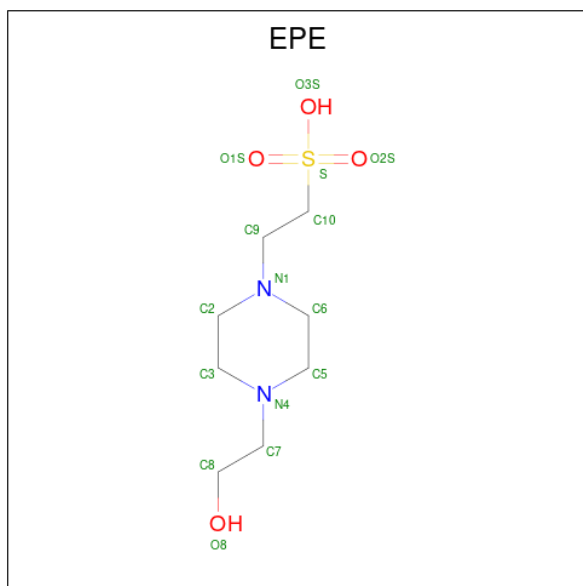
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
6	A	1	Total	C	H	O	0	0
			9	3	3	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			13	3	7	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	Na	0	0
			6	6		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		

- Molecule 10 is water.

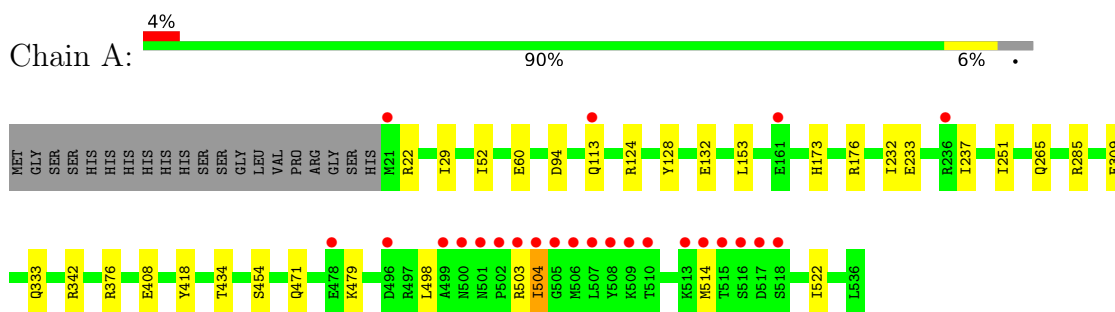
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	622	Total 628	O 628	0	6



### 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: 6-4 photolyase (FeS-BCP, CryPro)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.69Å 199.69Å 77.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.59 – 1.65 34.59 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.59-1.65) 100.0 (34.59-1.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 1.65Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.119 , 0.136 0.123 , 0.140	Depositor DCC
$R_{free}$ test set	2158 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtrriage
Anisotropy	0.069	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 64.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: SF4, EPE, FAD, NA, DLZ, GOL, SO4, CL

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	0.79	1/4481 (0.0%)	0.82	1/6076 (0.0%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	GLU	CD-OE2	9.73	1.36	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ASP	CB-CG-OD1	5.31	123.08	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ARG	Sidechain
1	A	342	ARG	Sidechain

## 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	4295	4173	4198	30	0
2	A	53	30	31	3	0
3	A	23	0	18	1	0
4	A	8	0	0	0	0
5	A	15	17	17	4	0
6	A	66	82	84	7	1
7	A	35	0	0	1	0
8	A	6	0	0	0	0
9	A	1	0	0	1	0
10	A	628	0	0	15	5
All	All	5130	4302	4348	37	5

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 4.

All (37) 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)
6:A:611:GOL:O3	10:A:701:HOH:O	1.74	1.04
1:A:479:LYS:NZ	10:A:707:HOH:O	2.13	0.79
5:A:604:EPE:O2S	10:A:702:HOH:O	2.01	0.77
1:A:408:GLU:OE1	10:A:703:HOH:O	2.02	0.77
5:A:604:EPE:O3S	10:A:704:HOH:O	2.05	0.75
6:A:611:GOL:O2	10:A:705:HOH:O	2.06	0.71
1:A:233:GLU:OE1	10:A:706:HOH:O	2.12	0.68
6:A:609:GOL:O1	9:A:629:CL:CL	2.50	0.66
7:A:619:SO4:O4	10:A:709:HOH:O	2.14	0.61
1:A:265[B]:GLN:NE2	10:A:718:HOH:O	2.36	0.58
1:A:514:MET:HE1	1:A:522:ILE:HD12	1.87	0.57
1:A:471[A]:GLN:NE2	10:A:720:HOH:O	2.38	0.55
1:A:285:ARG:HH12	5:A:604:EPE:H82	1.72	0.54
1:A:29:ILE:HB	1:A:52[B]:ILE:HG12	1.90	0.54
1:A:514:MET:HE3	1:A:522:ILE:CD1	2.37	0.53
1:A:418:TYR:CE2	2:A:601:FAD:HM73	2.43	0.52
1:A:376[B]:ARG:NH2	6:A:608:GOL:H32	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:OE1	10:A:710:HOH:O	2.19	0.51
1:A:498:LEU:HB3	1:A:504:ILE:HD13	1.92	0.51
1:A:514:MET:CE	1:A:522:ILE:HD12	2.40	0.50
1:A:232:ILE:HG23	1:A:237:ILE:HB	1.96	0.48
1:A:454:SER:OG	6:A:615:GOL:H12	2.13	0.48
1:A:434:THR:HA	2:A:601:FAD:HM72	1.96	0.47
3:A:602:DLZ:H7	3:A:602:DLZ:H1'	1.79	0.46
1:A:333:GLN:HB3	2:A:601:FAD:C8A	2.46	0.45
1:A:251:ILE:C	1:A:251:ILE:HD12	2.37	0.45
1:A:376[B]:ARG:CZ	6:A:608:GOL:H32	2.47	0.45
1:A:514:MET:CE	1:A:522:ILE:CD1	2.95	0.44
1:A:176:ARG:NH2	10:A:728:HOH:O	2.45	0.44
1:A:498:LEU:HB3	1:A:504:ILE:CD1	2.47	0.43
1:A:285:ARG:HH12	5:A:604:EPE:C8	2.31	0.43
1:A:265[B]:GLN:HG3	10:A:718:HOH:O	2.19	0.43
1:A:60:GLU:OE2	10:A:711:HOH:O	2.22	0.41
1:A:514:MET:HE3	1:A:522:ILE:HD11	2.02	0.41
1:A:128:TYR:CE2	1:A:132:GLU:HG3	2.55	0.41
1:A:153:LEU:HD23	6:A:610:GOL:H11	2.02	0.40
1:A:173:HIS:HB2	10:A:709:HOH:O	2.20	0.40

All (5) 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)
10:A:1142:HOH:O	10:A:1215:HOH:O[8_555]	1.84	0.36
10:A:717:HOH:O	10:A:1045:HOH:O[10_555]	1.99	0.21
10:A:1045:HOH:O	10:A:1265:HOH:O[10_555]	1.99	0.21
10:A:1117:HOH:O	10:A:1320:HOH:O[10_555]	2.05	0.15
6:A:611:GOL:O1	10:A:705:HOH:O[10_555]	2.17	0.03

## 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 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	536/536 (100%)	521 (97%)	15 (3%)	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	461/458 (101%)	457 (99%)	4 (1%)	78 66

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	113	GLN
1	A	503	ARG
1	A	504	ILE

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

Of 29 ligands modelled in this entry, 7 are monoatomic - leaving 22 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
7	SO4	A	621	-	4,4,4	0.17	0	6,6,6	0.21	0
6	GOL	A	609	8	5,5,5	1.89	1 (20%)	5,5,5	0.68	0
7	SO4	A	617	-	4,4,4	0.38	0	6,6,6	0.69	0
6	GOL	A	610	-	5,5,5	0.77	0	5,5,5	1.04	0
6	GOL	A	612	-	5,5,5	1.58	1 (20%)	5,5,5	1.12	1 (20%)
6	GOL	A	615	-	5,5,5	0.97	0	5,5,5	0.85	0
7	SO4	A	620	-	4,4,4	0.47	0	6,6,6	0.49	0
7	SO4	A	622	-	4,4,4	0.21	0	6,6,6	0.25	0
5	EPE	A	604	-	15,15,15	0.84	0	18,20,20	1.57	3 (16%)
6	GOL	A	611	-	5,5,5	1.17	1 (20%)	5,5,5	0.86	0
7	SO4	A	616	-	4,4,4	0.43	0	6,6,6	0.26	0
3	DLZ	A	602	-	23,24,24	2.01	9 (39%)	29,35,35	2.06	11 (37%)
6	GOL	A	613	-	5,5,5	2.44	3 (60%)	5,5,5	0.62	0
4	SF4	A	603	1	0,12,12	-	-	-	-	-
7	SO4	A	618	-	4,4,4	0.18	0	6,6,6	0.42	0
6	GOL	A	606	-	5,5,5	1.85	2 (40%)	5,5,5	0.95	0
6	GOL	A	614	-	5,5,5	0.41	0	5,5,5	1.22	1 (20%)
6	GOL	A	608	-	5,5,5	1.75	2 (40%)	5,5,5	0.67	0
6	GOL	A	605	-	5,5,5	0.82	0	5,5,5	1.11	1 (20%)
2	FAD	A	601	-	53,58,58	0.84	3 (5%)	68,89,89	0.72	0
6	GOL	A	607	-	5,5,5	1.29	1 (20%)	5,5,5	0.82	0
7	SO4	A	619	-	4,4,4	0.30	0	6,6,6	0.49	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	614	-	-	0/4/4/4	-
3	DLZ	A	602	-	-	1/14/14/14	0/2/2/2
6	GOL	A	610	-	-	0/4/4/4	-
6	GOL	A	612	-	-	4/4/4/4	-
6	GOL	A	613	-	-	0/4/4/4	-
6	GOL	A	615	-	-	3/4/4/4	-
4	SF4	A	603	1	-	-	0/6/5/5
6	GOL	A	609	8	-	2/4/4/4	-
6	GOL	A	608	-	-	0/4/4/4	-
6	GOL	A	605	-	-	0/4/4/4	-
5	EPE	A	604	-	-	2/9/19/19	0/1/1/1
6	GOL	A	611	-	-	4/4/4/4	-
2	FAD	A	601	-	-	2/30/50/50	0/6/6/6
6	GOL	A	607	-	-	0/4/4/4	-
6	GOL	A	606	-	-	3/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	DLZ	C1'-C2'	4.42	1.58	1.52
3	A	602	DLZ	C7-C7A	4.03	1.55	1.49
6	A	613	GOL	O2-C2	-4.01	1.31	1.43
6	A	609	GOL	O2-C2	-3.70	1.32	1.43
6	A	608	GOL	C1-C2	3.28	1.65	1.51
6	A	612	GOL	C3-C2	3.27	1.65	1.51
3	A	602	DLZ	C8-N8	3.12	1.44	1.39
3	A	602	DLZ	C4-N3	-2.94	1.33	1.38
6	A	613	GOL	O1-C1	2.71	1.53	1.42
6	A	607	GOL	O2-C2	-2.63	1.35	1.43
3	A	602	DLZ	C7A-N8	-2.59	1.35	1.39
3	A	602	DLZ	O2-C2	-2.52	1.19	1.24
2	A	601	FAD	C4X-N5	2.49	1.35	1.30
6	A	613	GOL	C1-C2	2.42	1.61	1.51
6	A	606	GOL	C1-C2	2.41	1.61	1.51
3	A	602	DLZ	C4A-C4	2.35	1.53	1.44
3	A	602	DLZ	C2'-C3'	2.21	1.57	1.53
6	A	606	GOL	O2-C2	-2.17	1.36	1.43
3	A	602	DLZ	C2-N1	2.14	1.41	1.36
6	A	611	GOL	C1-C2	2.10	1.60	1.51
2	A	601	FAD	C2A-N3A	2.07	1.35	1.32
6	A	608	GOL	O2-C2	-2.06	1.37	1.43
2	A	601	FAD	C8A-N7A	-2.01	1.31	1.34



All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	EPE	C5-N4-C3	4.15	118.16	108.83
3	A	602	DLZ	O4-C4-N3	3.94	127.68	120.12
3	A	602	DLZ	C4A-C8-N8	-3.82	110.99	116.52
3	A	602	DLZ	C6-C5A-N5	3.60	118.21	112.53
3	A	602	DLZ	C1'-N8-C7A	3.04	126.63	121.74
3	A	602	DLZ	O4-C4-C4A	-2.97	118.71	126.60
3	A	602	DLZ	C7-C7A-C5A	-2.85	119.68	125.26
3	A	602	DLZ	C1'-N8-C8	-2.59	113.05	120.60
3	A	602	DLZ	C4A-C8-N1	2.53	130.61	124.73
5	A	604	EPE	O2S-S-C10	2.50	109.92	106.92
6	A	612	GOL	O3-C3-C2	-2.43	98.53	110.20
3	A	602	DLZ	O2-C2-N3	2.37	123.25	118.65
3	A	602	DLZ	C8-C4A-N5	2.37	129.79	124.85
5	A	604	EPE	C6-N1-C2	2.19	113.75	108.83
3	A	602	DLZ	C1'-C2'-C3'	2.15	115.80	109.79
6	A	605	GOL	C3-C2-C1	-2.12	103.46	111.70
6	A	614	GOL	C3-C2-C1	-2.07	103.67	111.70

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	606	GOL	O1-C1-C2-C3
6	A	611	GOL	O1-C1-C2-C3
6	A	611	GOL	C1-C2-C3-O3
6	A	612	GOL	O1-C1-C2-C3
6	A	609	GOL	O1-C1-C2-O2
6	A	609	GOL	O1-C1-C2-C3
6	A	615	GOL	O1-C1-C2-C3
6	A	606	GOL	O1-C1-C2-O2
6	A	611	GOL	O1-C1-C2-O2
6	A	615	GOL	O1-C1-C2-O2
5	A	604	EPE	N4-C7-C8-O8
6	A	611	GOL	O2-C2-C3-O3
6	A	612	GOL	O1-C1-C2-O2
3	A	602	DLZ	N8-C1'-C2'-O2'
2	A	601	FAD	C4B-C5B-O5B-PA
6	A	615	GOL	C1-C2-C3-O3
2	A	601	FAD	C4'-C5'-O5'-P
6	A	612	GOL	C1-C2-C3-O3
6	A	612	GOL	O2-C2-C3-O3

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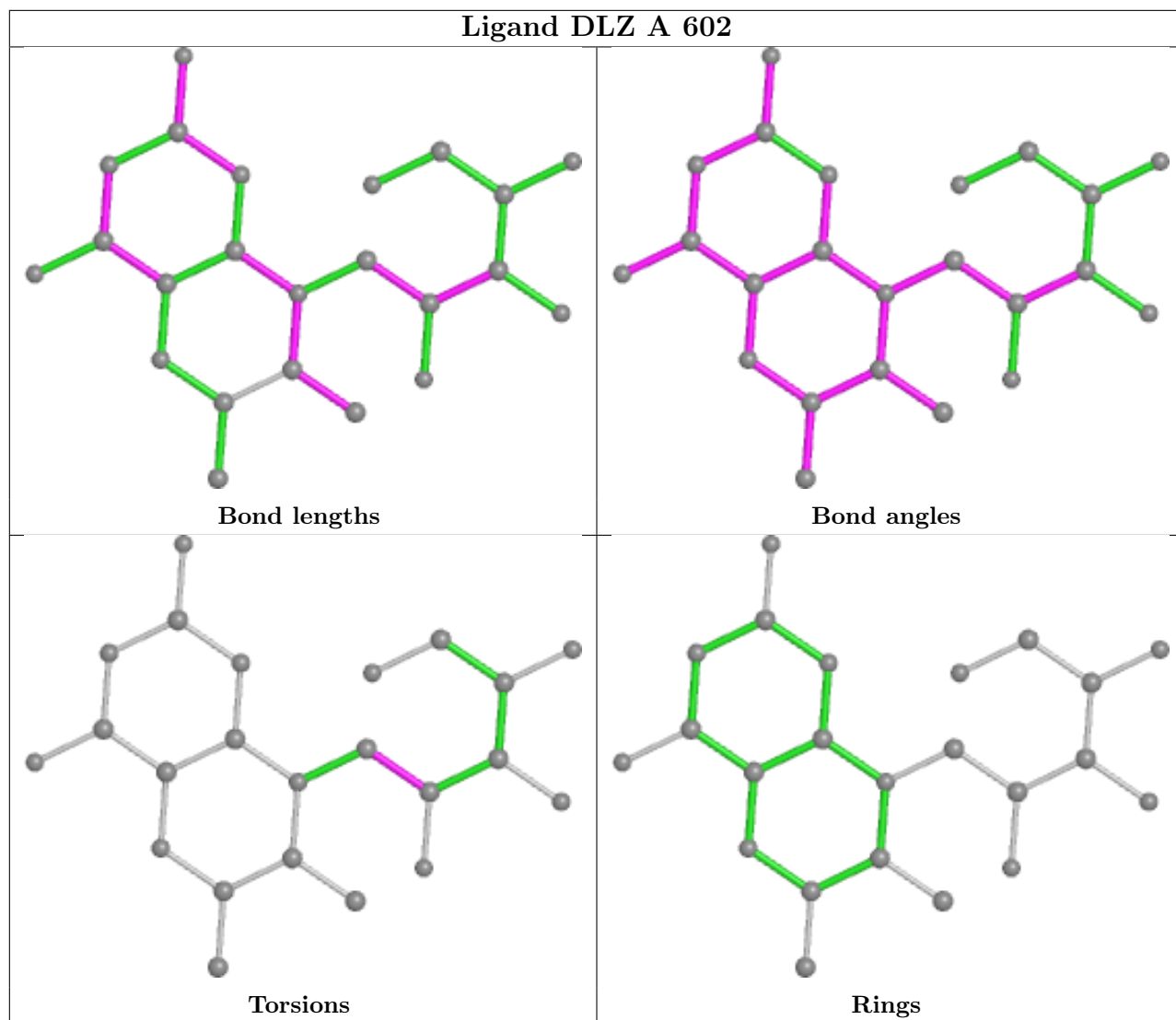
Mol	Chain	Res	Type	Atoms
5	A	604	EPE	C8-C7-N4-C3
6	A	606	GOL	O2-C2-C3-O3

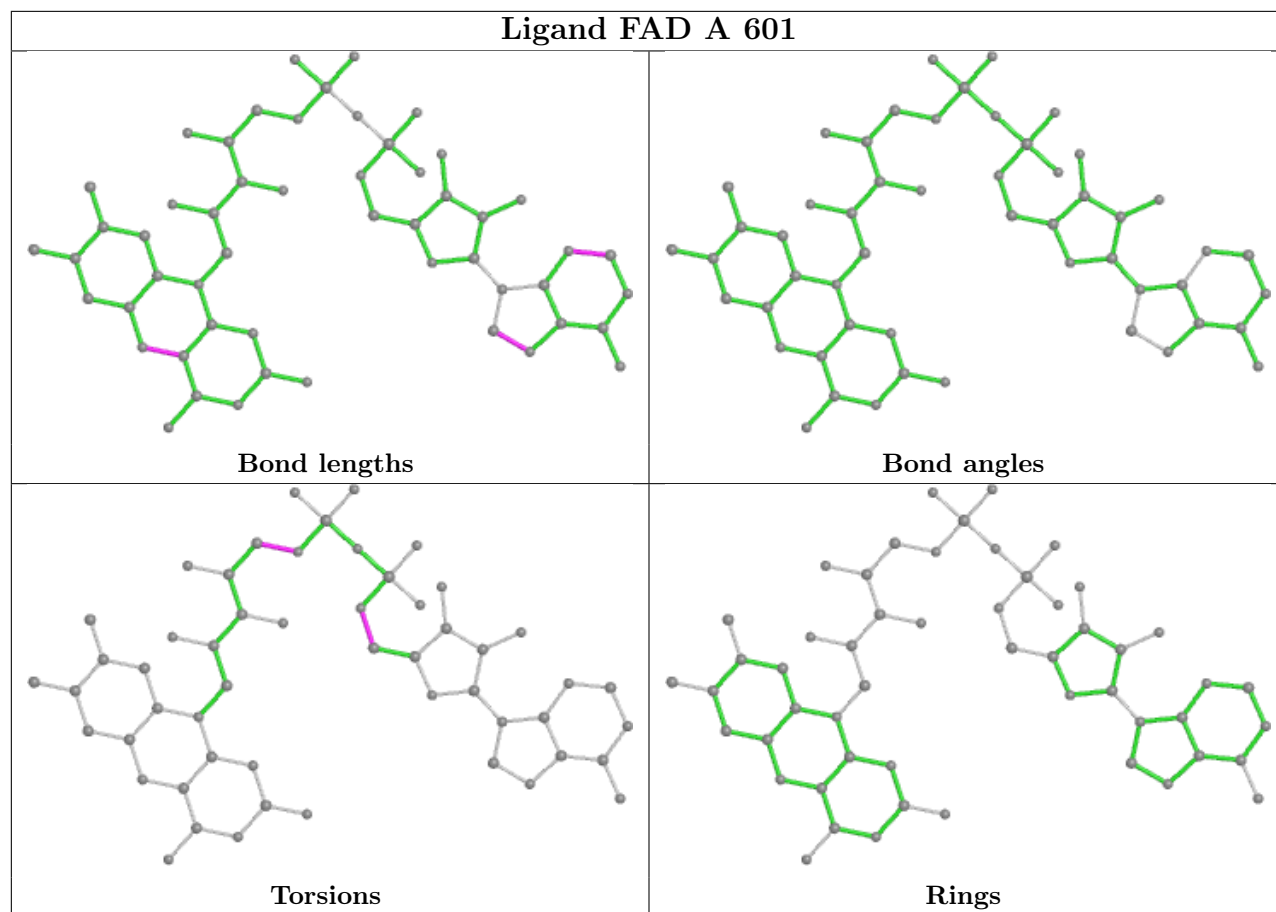
There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	609	GOL	1	0
6	A	610	GOL	1	0
6	A	615	GOL	1	0
5	A	604	EPE	4	0
6	A	611	GOL	2	1
3	A	602	DLZ	1	0
6	A	608	GOL	2	0
2	A	601	FAD	3	0
7	A	619	SO4	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.

## 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	516/536 (96%)	-0.20	24 (4%) 31 30	14, 23, 55, 123	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	PRO	9.6
1	A	21	MET	8.5
1	A	504	ILE	7.7
1	A	500	ASN	7.7
1	A	503	ARG	7.2
1	A	506	MET	6.8
1	A	505	GLY	5.7
1	A	499	ALA	5.1
1	A	513	LYS	5.0
1	A	501	ASN	4.9
1	A	516	SER	4.1
1	A	507	LEU	4.0
1	A	478	GLU	3.7
1	A	510	THR	3.7
1	A	515	THR	3.5
1	A	514	MET	3.2
1	A	496	ASP	3.1
1	A	517	ASP	3.0
1	A	518	SER	2.8
1	A	113	GLN	2.7
1	A	509	LYS	2.6
1	A	508	TYR	2.5
1	A	161	GLU	2.4
1	A	236	ARG	2.2

## 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.

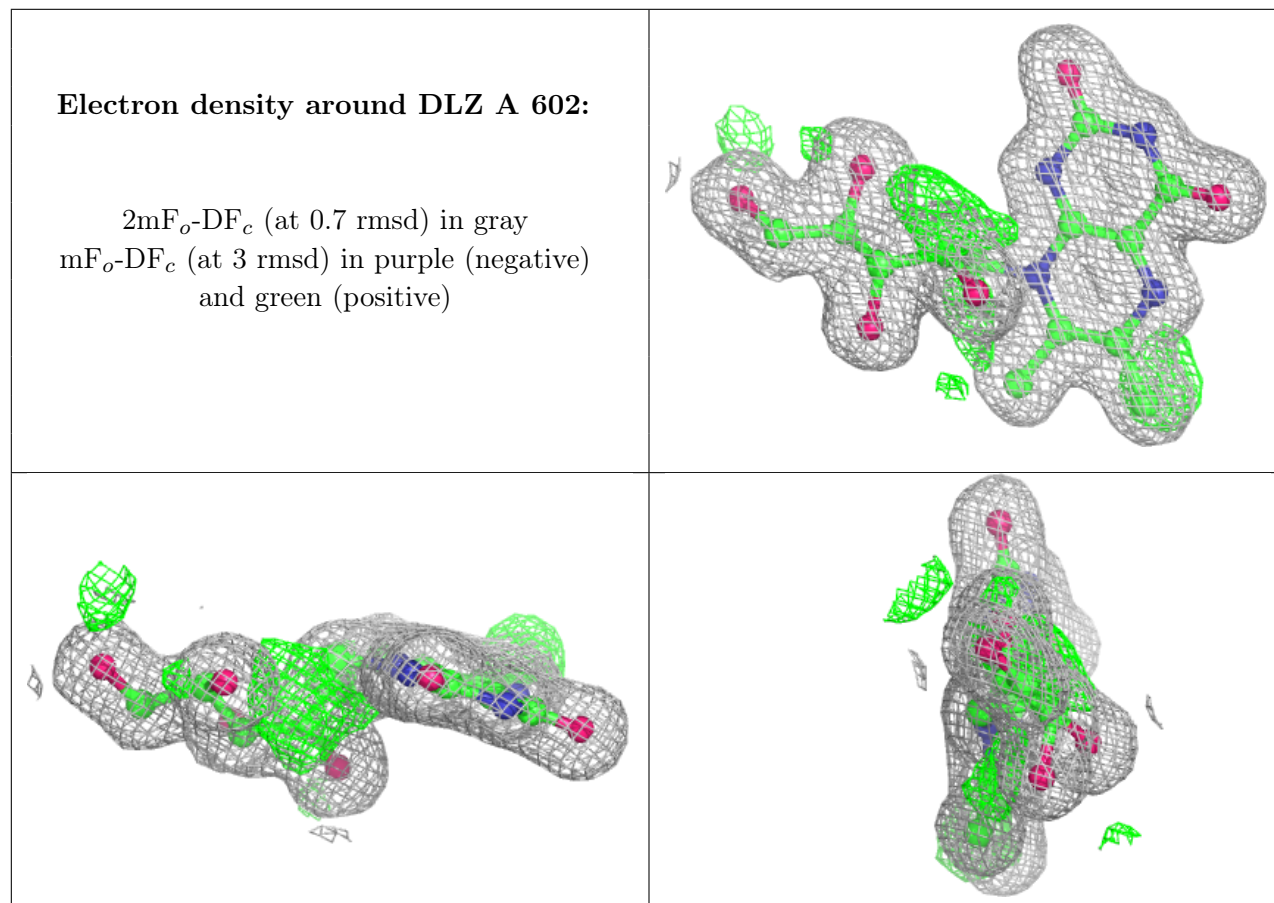
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	610	6/6	0.69	0.21	41,55,59,67	14
6	GOL	A	611	6/6	0.75	0.26	21,36,46,55	14
7	SO4	A	617	5/5	0.77	0.20	32,48,75,102	5
6	GOL	A	614	6/6	0.79	0.15	36,60,69,76	14
6	GOL	A	607	6/6	0.82	0.28	51,73,83,92	0
6	GOL	A	612	6/6	0.83	0.16	25,36,76,91	14
5	EPE	A	604	15/15	0.84	0.22	24,73,95,103	32
6	GOL	A	615	6/6	0.87	0.14	32,56,76,91	0
7	SO4	A	620	5/5	0.87	0.14	37,42,60,76	5
8	NA	A	626	1/1	0.87	0.17	64,64,64,64	1
6	GOL	A	606	6/6	0.89	0.15	24,31,41,49	14
8	NA	A	625	1/1	0.90	0.30	56,56,56,56	1
7	SO4	A	618	5/5	0.90	0.18	33,38,59,80	5
8	NA	A	627	1/1	0.91	0.63	66,66,66,66	1
8	NA	A	624	1/1	0.92	0.14	65,65,65,65	0
6	GOL	A	609	6/6	0.93	0.14	22,49,59,69	13
6	GOL	A	605	6/6	0.93	0.08	30,41,48,56	9
6	GOL	A	613	6/6	0.93	0.12	23,36,54,54	14
6	GOL	A	608	6/6	0.94	0.15	28,42,59,64	14
7	SO4	A	621	5/5	0.94	0.20	50,58,60,75	5
7	SO4	A	619	5/5	0.94	0.16	28,46,54,75	5
7	SO4	A	616	5/5	0.96	0.31	22,34,42,47	5
7	SO4	A	622	5/5	0.96	0.20	36,46,57,76	5
8	NA	A	628	1/1	0.96	0.13	67,67,67,67	1
9	CL	A	629	1/1	0.96	0.10	60,60,60,60	0
3	DLZ	A	602	23/23	0.97	0.12	15,17,19,19	0
8	NA	A	623	1/1	0.97	0.54	27,27,27,27	1

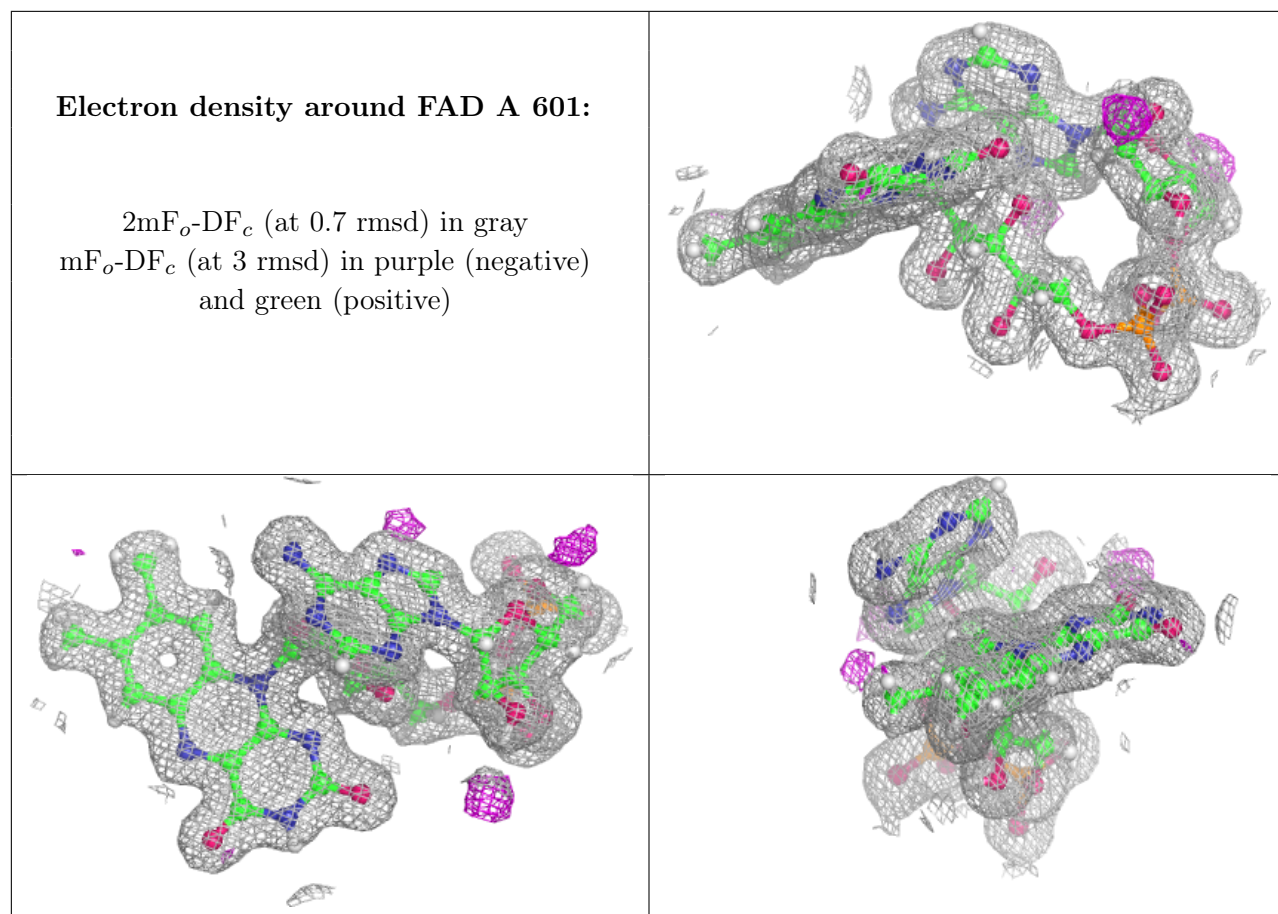
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	A	601	53/53	0.99	0.11	13,15,21,22	0
4	SF4	A	603	8/8	1.00	0.05	18,19,20,21	0

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.