



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2026 – 01:26 pm BST

PDB ID : 9RDR / pdb\_00009rdr  
Title : Nicotine Glucoside Synthase (BBL) in complex with FAD and Nicotine Glucoside  
Authors : Schwabe, B.T.W.; Lichman, B.R.; Grogan, G.  
Deposited on : 2025-06-03  
Resolution : 2.56 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

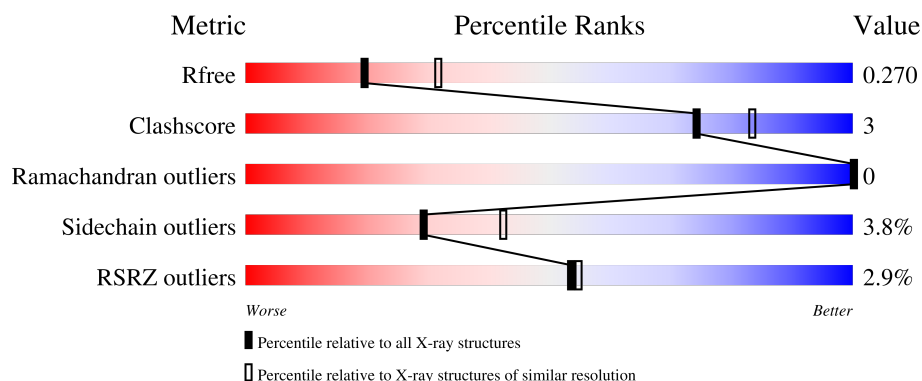
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

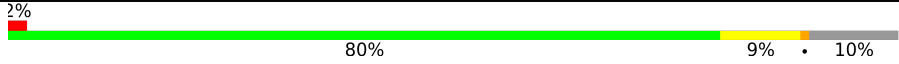
The reported resolution of this entry is 2.56 Å.

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))
$R_{free}$	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	560	
1	B	560	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8323 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.

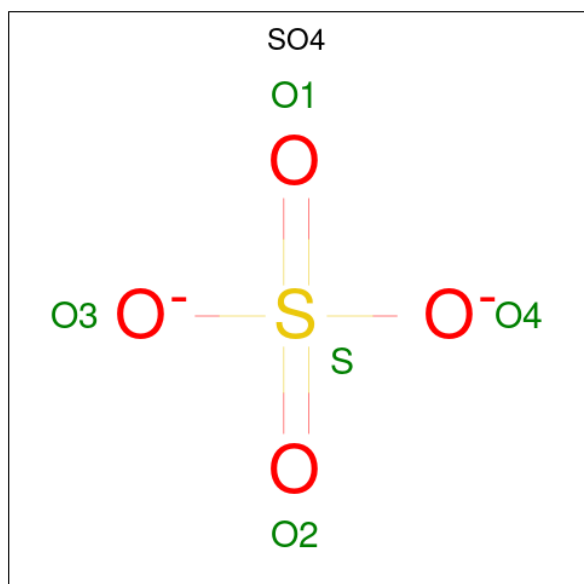
- Molecule 1 is a protein called Berberine bridge enzyme-like A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			3956	2551	653	729	23			
1	B	503	Total	C	N	O	S	0	0	0
			3957	2551	651	732	23			

There are 4 discrepancies between the modelled and reference sequences:

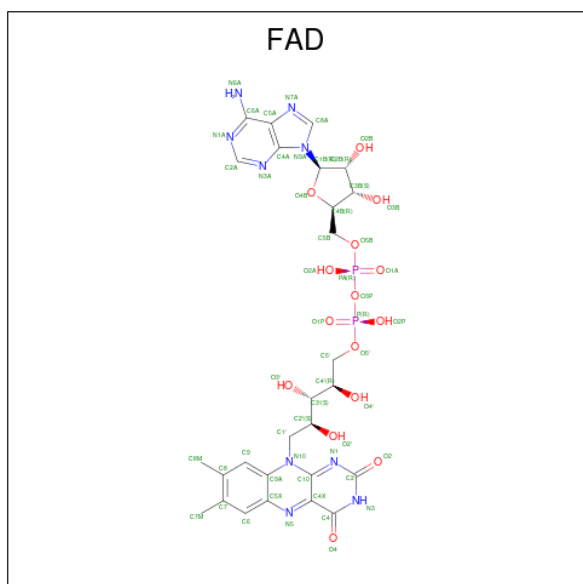
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP F1T160
A	1	GLY	-	expression tag	UNP F1T160
B	0	MET	-	initiating methionine	UNP F1T160
B	1	GLY	-	expression tag	UNP F1T160

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



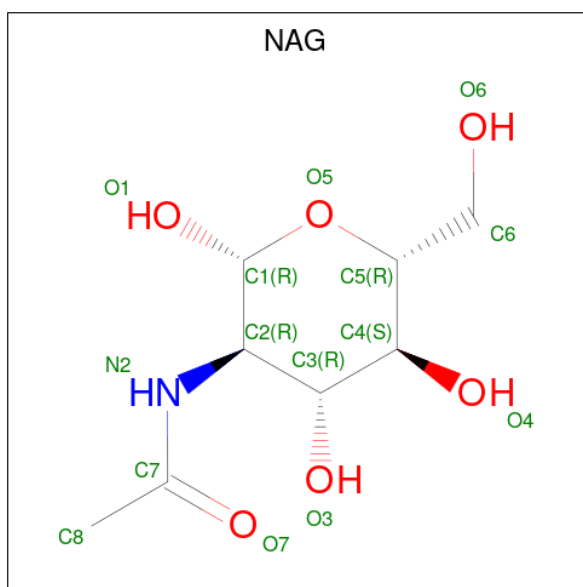
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



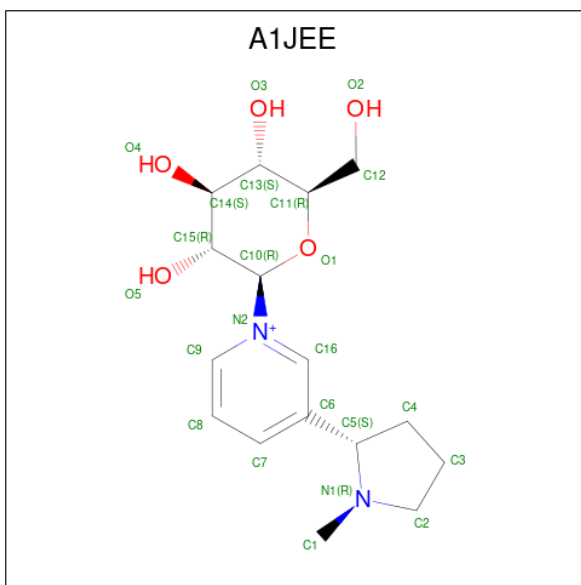
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $\text{C}_8\text{H}_{15}\text{NO}_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is (2 {R},3 {S},4 {S},5 {R},6 {R})-2-(hydroxymethyl)-6-[3-[(2 {S})-1-methylpyrrolidin-2-yl]pyridin-1-yl]oxane-3,4,5-triol (CCD ID: A1JEE) (formula: C<sub>16</sub>H<sub>25</sub>N<sub>2</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			23	16	2	5		
5	B	1	Total	C	N	O	0	0
			23	16	2	5		

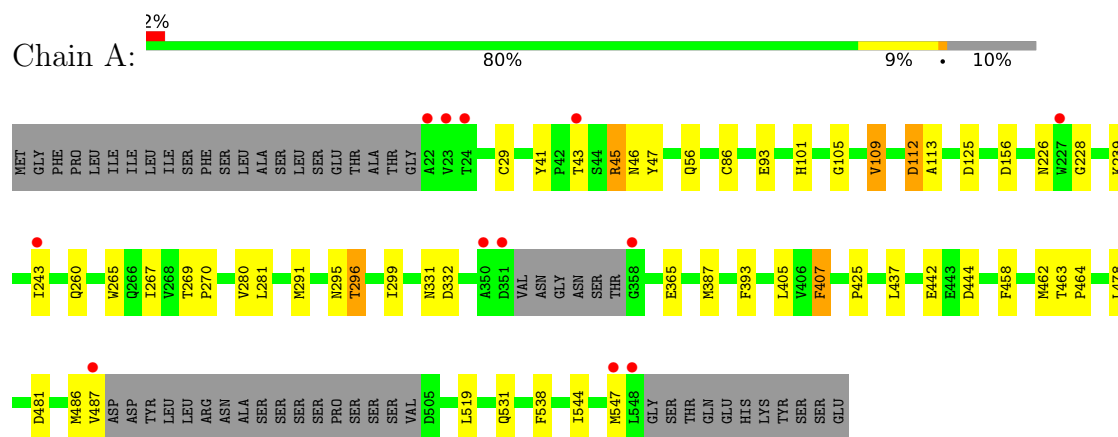
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	72	Total	O	0	0
			72	72		
6	B	69	Total	O	0	0
			69	69		

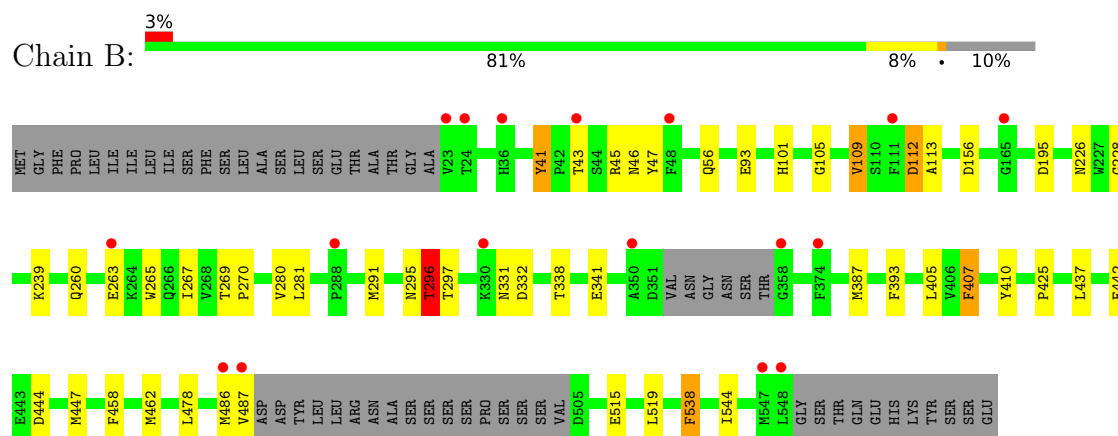
### 3 Residue-property plots [i](#)

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: Berberine bridge enzyme-like A



#### • Molecule 1: Berberine bridge enzyme-like A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.26Å 122.88Å 148.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.48 – 2.56 74.48 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.48-2.56) 99.8 (74.48-2.56)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.213 , 0.269 0.217 , 0.270	Depositor DCC
$R_{free}$ test set	2536 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.2	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8323	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: A1JEE, NAG, FAD, SO4

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	0.59	0/4058	1.09	14/5503 (0.3%)
1	B	0.59	0/4059	1.07	9/5505 (0.2%)
All	All	0.59	0/8117	1.08	23/11008 (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	A	0	1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ASP	CA-CB-CG	7.86	120.46	112.60
1	A	332	ASP	CA-CB-CG	7.49	120.09	112.60
1	B	296	THR	N-CA-C	-6.47	105.52	113.41
1	A	112	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	112	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	93	GLU	N-CA-CB	5.75	118.43	109.97
1	B	281	LEU	N-CA-CB	-5.57	102.03	110.77
1	A	296	THR	N-CA-C	-5.53	106.53	113.72
1	A	407	PHE	CA-CB-CG	5.48	119.28	113.80
1	A	442	GLU	CB-CG-CD	5.43	121.83	112.60
1	A	281	LEU	N-CA-CB	-5.33	102.41	110.77
1	B	407	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	442	GLU	CB-CA-C	5.29	119.27	110.81
1	B	93	GLU	N-CA-CB	5.24	117.67	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	531	GLN	N-CA-CB	5.16	118.28	110.28
1	A	125	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	538	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	444	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	41	TYR	N-CA-CB	-5.11	103.85	110.03
1	A	481	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	365	GLU	CB-CG-CD	5.03	121.15	112.60
1	B	442	GLU	CB-CA-C	5.01	118.83	110.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	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	3956	0	3849	23	0
1	B	3957	0	3847	27	0
2	A	5	0	0	0	0
3	A	53	0	31	3	0
3	B	53	0	31	3	0
4	A	56	0	52	1	0
4	B	56	0	52	0	0
5	A	23	0	0	0	0
5	B	23	0	0	0	0
6	A	72	0	0	0	0
6	B	69	0	0	2	0
All	All	8323	0	7862	48	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 (48) 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:101:HIS:ND1	3:A:602:FAD:HM82	1.20	1.44
1:A:101:HIS:ND1	3:A:602:FAD:C8M	2.16	1.08
1:A:267:ILE:HD11	1:B:267:ILE:HD11	1.50	0.91
1:B:101:HIS:ND1	3:B:601:FAD:C8M	2.54	0.70
1:B:101:HIS:ND1	3:B:601:FAD:HM83	2.05	0.70
1:B:263:GLU:OE2	1:B:387:MET:HE2	1.93	0.69
1:A:226:ASN:HD21	1:A:544:ILE:H	1.40	0.68
1:B:226:ASN:HD21	1:B:544:ILE:H	1.39	0.68
1:A:299:ILE:HG13	4:A:603:NAG:HN2	1.69	0.58
1:A:101:HIS:CG	3:A:602:FAD:HM82	2.23	0.56
1:A:112:ASP:O	1:A:113:ALA:HB3	2.08	0.54
1:A:265:TRP:NE1	1:A:269:THR:HG21	2.23	0.54
1:B:112:ASP:O	1:B:113:ALA:HB3	2.07	0.53
1:B:269:THR:OG1	1:B:270:PRO:HD3	2.08	0.53
1:B:265:TRP:CD1	1:B:269:THR:HG21	2.44	0.52
1:B:296:THR:HG22	1:B:297:THR:HG23	1.91	0.52
1:B:228:GLY:HA2	1:B:538:PHE:CE2	2.45	0.52
1:A:260:GLN:HA	1:A:387:MET:HE1	1.92	0.51
1:B:265:TRP:NE1	1:B:269:THR:HG21	2.25	0.51
1:A:265:TRP:CD1	1:A:269:THR:HG21	2.46	0.51
1:A:105:GLY:O	1:A:109:VAL:HG12	2.10	0.51
1:B:105:GLY:O	1:B:109:VAL:HG12	2.11	0.50
1:A:458:PHE:O	1:A:462:MET:HG2	2.10	0.50
1:A:269:THR:OG1	1:A:270:PRO:HD3	2.11	0.50
1:A:228:GLY:HA2	1:A:538:PHE:CE2	2.46	0.50
1:B:260:GLN:HA	1:B:387:MET:HE1	1.93	0.50
1:A:267:ILE:CD1	1:B:267:ILE:HD11	2.34	0.49
1:B:56:GLN:HA	1:B:56:GLN:OE1	2.13	0.48
1:B:515:GLU:HB2	6:B:702:HOH:O	2.12	0.48
1:A:393:PHE:CD1	1:A:462:MET:HE2	2.50	0.47
1:B:291:MET:HE2	1:B:291:MET:HB3	1.78	0.47
1:B:265:TRP:CH2	1:B:407:PHE:HB3	2.50	0.46
1:A:291:MET:HE2	1:A:291:MET:HB3	1.80	0.46
1:A:29:CYS:HG	1:A:86:CYS:HG	0.48	0.46
1:B:393:PHE:CD1	1:B:462:MET:HE2	2.51	0.45
1:B:458:PHE:O	1:B:462:MET:HG2	2.16	0.45
1:B:444:ASP:O	1:B:447:MET:HG2	2.17	0.45
1:A:56:GLN:HA	1:A:56:GLN:OE1	2.16	0.45
1:B:425:PRO:HB2	1:B:519:LEU:HD12	1.97	0.45
1:A:41:TYR:HB2	1:A:47:TYR:CZ	2.53	0.44
1:B:41:TYR:HB2	1:B:47:TYR:CZ	2.53	0.43
1:A:463:THR:HB	1:A:464:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:TYR:HB3	6:B:714:HOH:O	2.19	0.43
1:B:393:PHE:CE1	1:B:462:MET:HE2	2.53	0.43
1:A:265:TRP:CH2	1:A:407:PHE:HB3	2.54	0.43
1:A:425:PRO:HB2	1:A:519:LEU:HD12	2.00	0.43
1:B:338:THR:HG1	1:B:341:GLU:HG3	1.84	0.41
1:B:101:HIS:HB3	3:B:601:FAD:HM81	2.03	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	498/560 (89%)	477 (96%)	21 (4%)	0	100	100
1	B	497/560 (89%)	474 (95%)	23 (5%)	0	100	100
All	All	995/1120 (89%)	951 (96%)	44 (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	419/475 (88%)	403 (96%)	16 (4%)	29	42
1	B	421/475 (89%)	405 (96%)	16 (4%)	29	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	840/950 (88%)	808 (96%)	32 (4%)	29	42

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	45	ARG
1	A	46	ASN
1	A	109	VAL
1	A	239	LYS
1	A	243	ILE
1	A	280	VAL
1	A	295	ASN
1	A	296	THR
1	A	331	ASN
1	A	405	LEU
1	A	437	LEU
1	A	478	LEU
1	A	486	MET
1	A	487	VAL
1	A	547	MET
1	B	43	THR
1	B	45	ARG
1	B	46	ASN
1	B	109	VAL
1	B	156	ASP
1	B	239	LYS
1	B	280	VAL
1	B	295	ASN
1	B	296	THR
1	B	331	ASN
1	B	332	ASP
1	B	405	LEU
1	B	437	LEU
1	B	478	LEU
1	B	486	MET
1	B	487	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	36	HIS
1	A	46	ASN
1	A	226	ASN
1	A	435	GLN
1	B	34	ASN
1	B	36	HIS
1	B	46	ASN
1	B	226	ASN
1	B	271	ASN
1	B	435	GLN
1	B	531	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

13 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	$\# Z  > 2$
4	NAG	B	604	1	14,14,15	0.43	0	17,19,21	0.32	0
4	NAG	B	602	1	14,14,15	0.41	0	17,19,21	1.05	2 (11%)
4	NAG	B	603	1	14,14,15	0.42	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	A	602	-	56,58,58	0.50	0	81,89,89	0.70	0
4	NAG	A	603	1	14,14,15	0.46	0	17,19,21	1.59	1 (5%)
2	SO4	A	601	-	4,4,4	0.30	0	6,6,6	0.14	0
5	A1JEE	A	607	-	23,25,25	0.96	1 (4%)	32,36,36	1.15	6 (18%)
4	NAG	A	605	1	14,14,15	0.44	0	17,19,21	0.65	0
4	NAG	A	606	1	14,14,15	0.40	0	17,19,21	0.55	0
3	FAD	B	601	-	56,58,58	0.50	0	81,89,89	0.75	2 (2%)
4	NAG	B	605	1	14,14,15	0.42	0	17,19,21	0.37	0
5	A1JEE	B	606	-	23,25,25	0.80	1 (4%)	32,36,36	0.98	3 (9%)
4	NAG	A	604	1	14,14,15	0.38	0	17,19,21	1.04	1 (5%)

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
4	NAG	B	604	1	-	4/6/23/26	0/1/1/1
4	NAG	B	602	1	-	6/6/23/26	0/1/1/1
4	NAG	B	603	1	-	4/6/23/26	0/1/1/1
3	FAD	A	602	-	-	6/34/50/50	0/6/6/6
4	NAG	A	603	1	-	6/6/23/26	0/1/1/1
5	A1JEE	A	607	-	-	4/6/40/40	0/3/3/3
4	NAG	A	605	1	-	4/6/23/26	0/1/1/1
4	NAG	A	606	1	-	3/6/23/26	0/1/1/1
3	FAD	B	601	-	-	8/34/50/50	0/6/6/6
4	NAG	B	605	1	-	0/6/23/26	0/1/1/1
5	A1JEE	B	606	-	-	4/6/40/40	0/3/3/3
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	607	A1JEE	C16-N2	3.40	1.39	1.35
5	B	606	A1JEE	C16-N2	2.72	1.38	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAG	O5-C1-C2	5.80	120.45	111.29
4	B	602	NAG	O5-C1-C2	2.94	115.93	111.29
4	A	604	NAG	C2-N2-C7	2.91	127.04	122.90
5	B	606	A1JEE	O3-C13-C14	-2.90	103.66	110.35
5	A	607	A1JEE	C11-O1-C10	2.82	113.64	108.81
3	B	601	FAD	O2P-P-O1P	2.72	125.68	112.24
3	B	601	FAD	C1'-C2'-C3'	2.33	116.29	109.79
5	A	607	A1JEE	C14-C15-C10	2.25	112.64	109.13
5	A	607	A1JEE	C9-N2-C16	-2.24	119.93	121.97
5	A	607	A1JEE	O4-C14-C13	-2.24	105.17	110.35
5	A	607	A1JEE	O3-C13-C14	-2.21	105.25	110.35
5	A	607	A1JEE	O3-C13-C11	2.20	114.77	109.30
4	B	602	NAG	C1-C2-N2	-2.20	106.74	110.49
5	B	606	A1JEE	C14-C15-C10	2.13	112.45	109.13
5	B	606	A1JEE	C9-N2-C16	-2.12	120.04	121.97

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	FAD	O3'-C3'-C4'-C5'
4	A	603	NAG	C8-C7-N2-C2
4	A	603	NAG	O7-C7-N2-C2
4	A	605	NAG	O7-C7-N2-C2
4	A	606	NAG	C8-C7-N2-C2
4	A	606	NAG	O7-C7-N2-C2
4	B	602	NAG	C8-C7-N2-C2
4	B	602	NAG	O7-C7-N2-C2
5	A	607	A1JEE	N1-C5-C6-C16
5	B	606	A1JEE	N1-C5-C6-C16
4	A	605	NAG	C8-C7-N2-C2
4	B	604	NAG	C8-C7-N2-C2
4	B	604	NAG	O7-C7-N2-C2
4	B	602	NAG	O5-C5-C6-O6
4	A	603	NAG	O5-C5-C6-O6
4	B	603	NAG	O5-C5-C6-O6
4	B	602	NAG	C4-C5-C6-O6
4	A	603	NAG	C1-C2-N2-C7
4	A	606	NAG	C1-C2-N2-C7
4	B	602	NAG	C1-C2-N2-C7
4	B	603	NAG	C4-C5-C6-O6
4	B	604	NAG	O5-C5-C6-O6
4	A	603	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	603	NAG	C8-C7-N2-C2
4	B	603	NAG	O7-C7-N2-C2
4	B	604	NAG	C4-C5-C6-O6
3	B	601	FAD	C2'-C3'-C4'-C5'
3	A	602	FAD	O3'-C3'-C4'-O4'
3	B	601	FAD	O3'-C3'-C4'-O4'
3	A	602	FAD	C2'-C3'-C4'-O4'
3	B	601	FAD	C2'-C3'-C4'-O4'
3	A	602	FAD	C2'-C3'-C4'-C5'
3	A	602	FAD	O3'-C3'-C4'-C5'
5	A	607	A1JEE	C4-C5-C6-C16
5	B	606	A1JEE	C4-C5-C6-C16
3	B	601	FAD	P-O3P-PA-O5B
4	A	605	NAG	C4-C5-C6-O6
5	B	606	A1JEE	N1-C5-C6-C7
5	A	607	A1JEE	N1-C5-C6-C7
4	A	605	NAG	O5-C5-C6-O6
3	A	602	FAD	PA-O3P-P-O1P
4	A	603	NAG	C3-C2-N2-C7
4	B	602	NAG	C3-C2-N2-C7
3	B	601	FAD	PA-O3P-P-O1P
5	B	606	A1JEE	C4-C5-C6-C7
3	B	601	FAD	O4B-C4B-C5B-O5B
5	A	607	A1JEE	C4-C5-C6-C7
3	B	601	FAD	PA-O3P-P-O2P
3	A	602	FAD	O4'-C4'-C5'-O5'

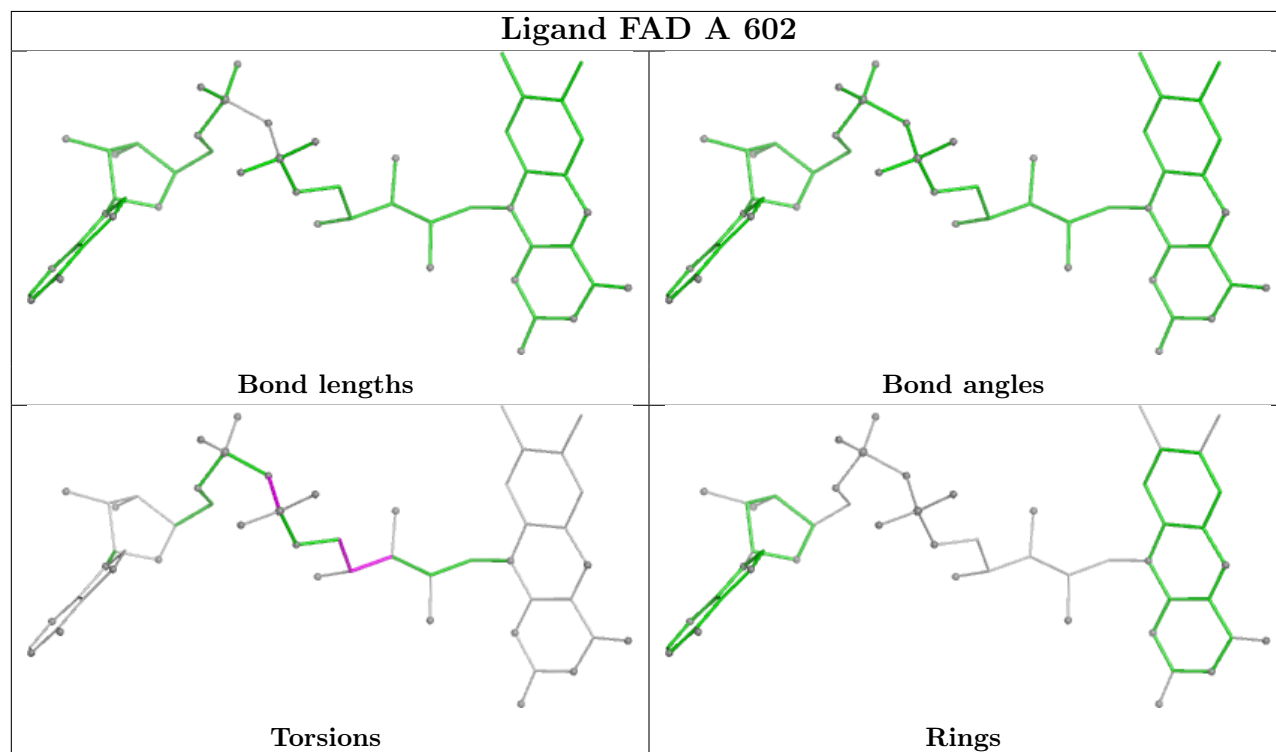
There are no ring outliers.

3 monomers are involved in 7 short contacts:

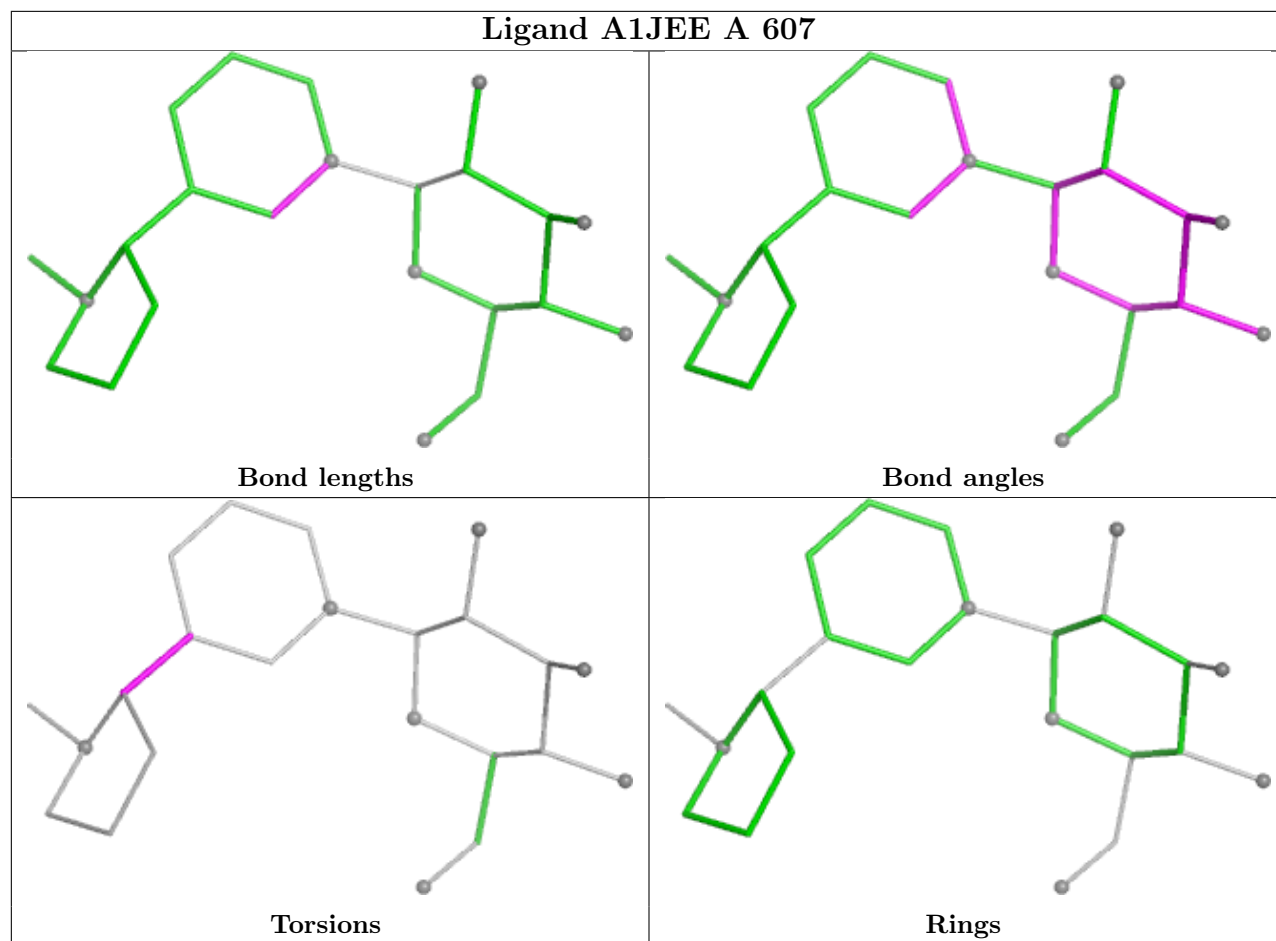
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	FAD	3	0
4	A	603	NAG	1	0
3	B	601	FAD	3	0

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

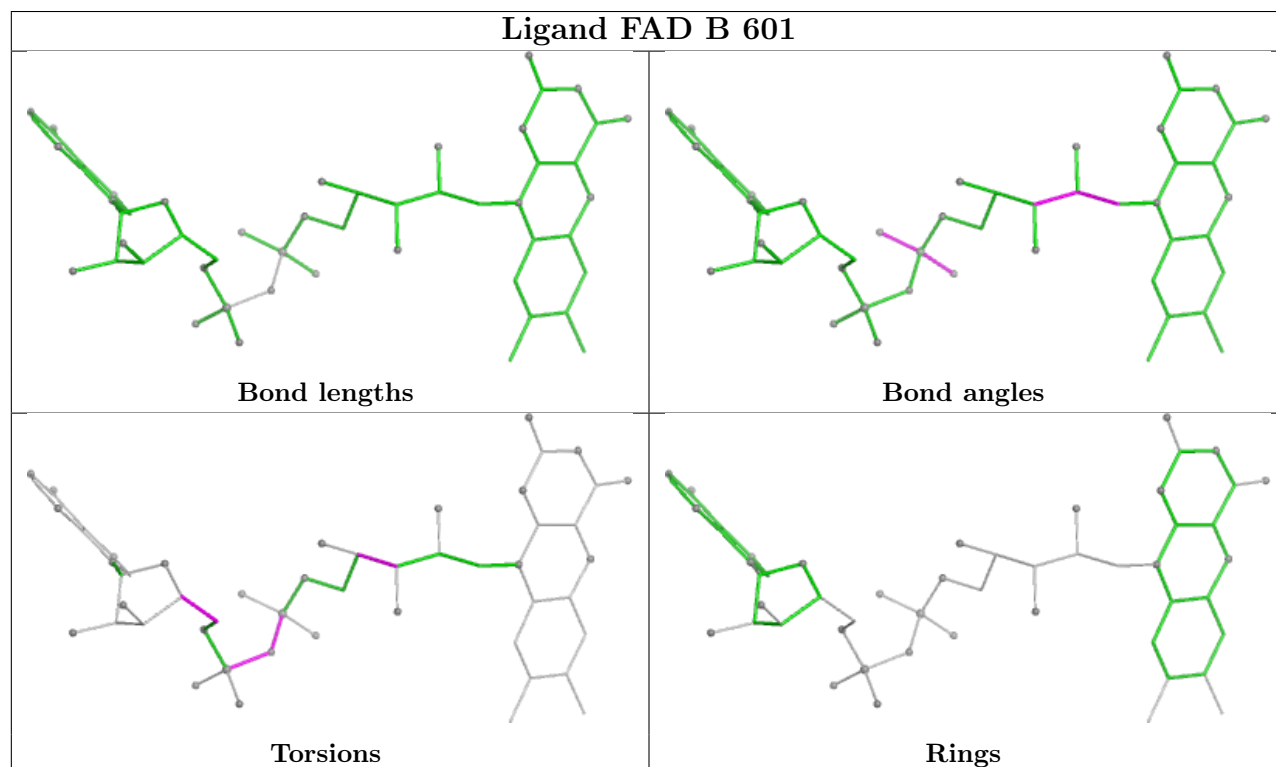
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

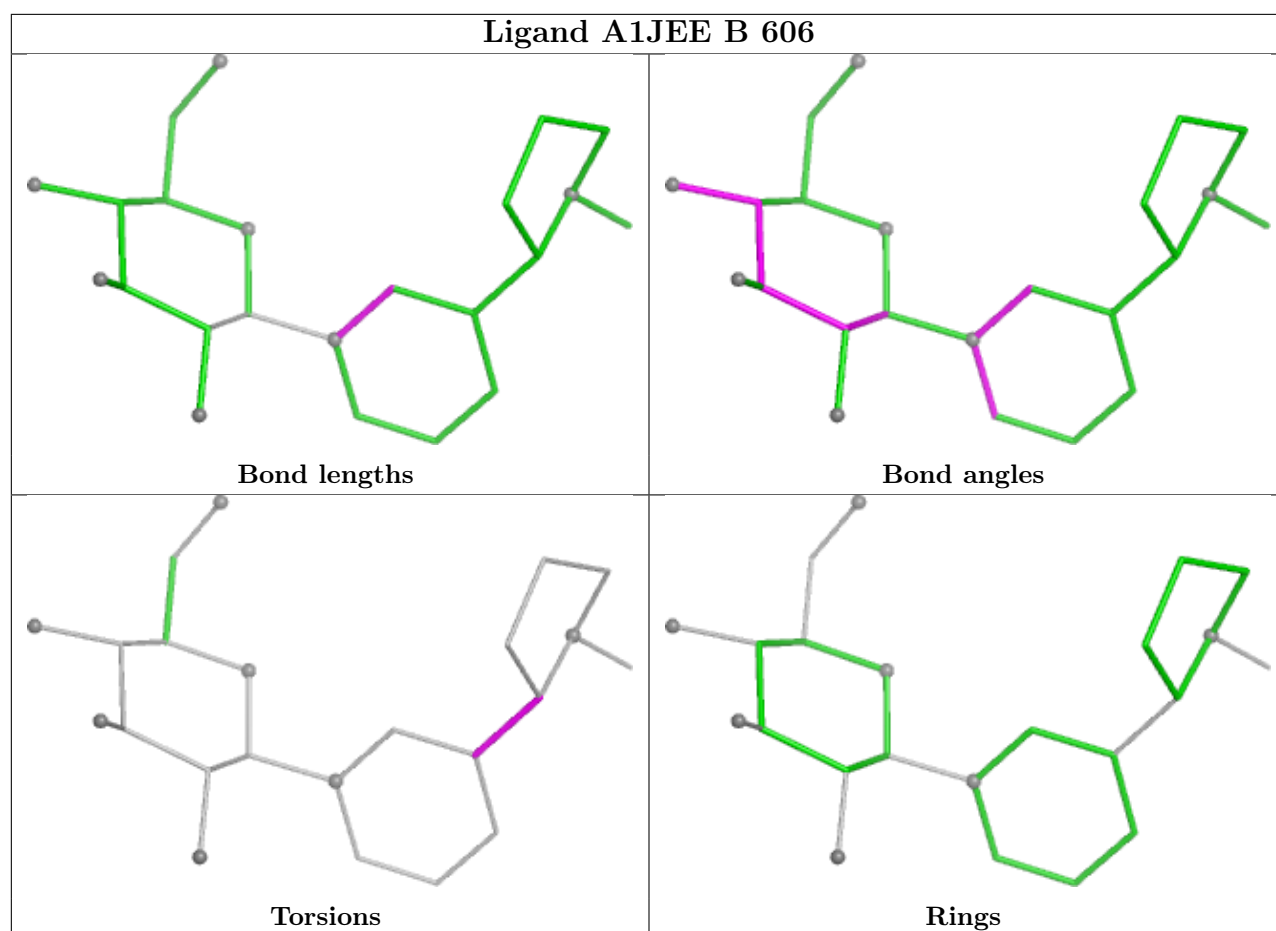


## Ligand A1JEE A 607



## Ligand FAD B 601





## 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	504/560 (90%)	0.33	12 (2%) 59 61	40, 55, 79, 126	0
1	B	503/560 (89%)	0.40	17 (3%) 48 49	41, 57, 83, 116	0
All	All	1007/1120 (89%)	0.36	29 (2%) 53 55	40, 56, 81, 126	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	LEU	7.1
1	A	351	ASP	6.9
1	B	548	LEU	5.7
1	A	487	VAL	4.1
1	B	23	VAL	3.8
1	B	487	VAL	3.8
1	B	358	GLY	3.7
1	A	22	ALA	3.5
1	A	43	THR	3.4
1	B	36	HIS	3.3
1	A	350	ALA	3.2
1	A	358	GLY	3.1
1	A	547	MET	2.8
1	B	486	MET	2.8
1	A	23	VAL	2.6
1	B	547	MET	2.5
1	B	24	THR	2.5
1	A	243	ILE	2.4
1	B	350	ALA	2.4
1	B	374	PHE	2.3
1	A	24	THR	2.3
1	B	43	THR	2.3
1	B	330	LYS	2.3
1	B	288	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	111	PHE	2.2
1	B	48	PHE	2.2
1	A	227	TRP	2.1
1	B	165	GLY	2.1
1	B	263	GLU	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

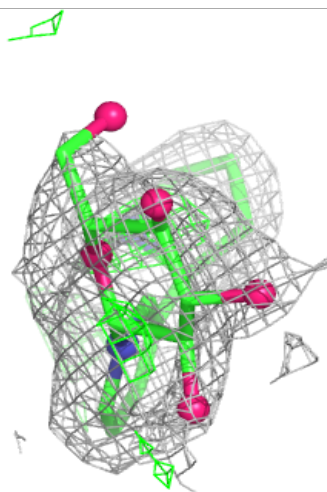
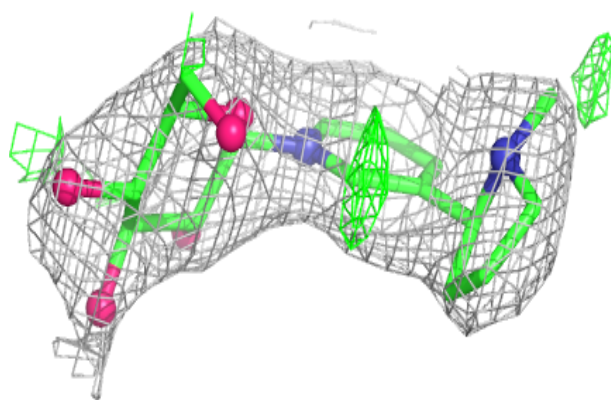
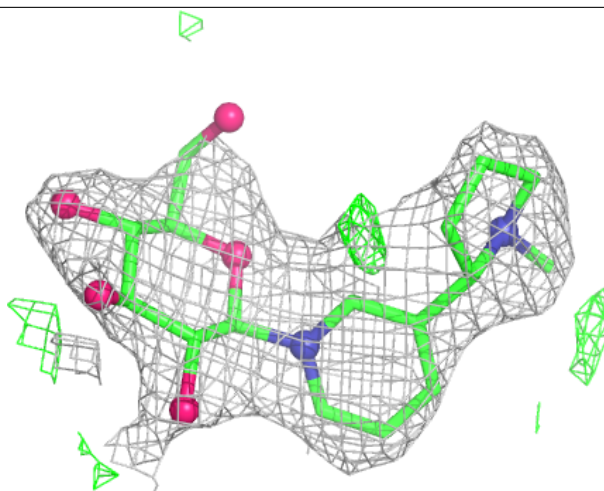
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	NAG	A	606	14/15	0.56	0.16	85,109,120,125	0
2	SO4	A	601	5/5	0.79	0.12	92,93,95,96	0
4	NAG	B	602	14/15	0.79	0.14	62,77,89,105	0
4	NAG	A	603	14/15	0.82	0.17	49,59,78,82	0
4	NAG	B	604	14/15	0.82	0.13	84,95,106,106	0
4	NAG	B	603	14/15	0.83	0.13	79,91,102,108	0
4	NAG	A	605	14/15	0.83	0.13	89,106,120,120	0
4	NAG	B	605	14/15	0.83	0.12	74,81,92,92	0
4	NAG	A	604	14/15	0.85	0.11	69,80,90,91	0
5	A1JEE	A	607	23/23	0.85	0.15	61,73,81,86	0
5	A1JEE	B	606	23/23	0.89	0.14	70,76,85,88	0
3	FAD	B	601	53/53	0.96	0.08	32,54,64,81	0
3	FAD	A	602	53/53	0.97	0.07	32,43,56,62	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.

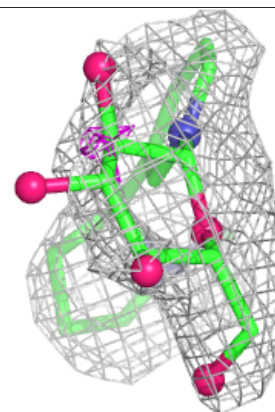
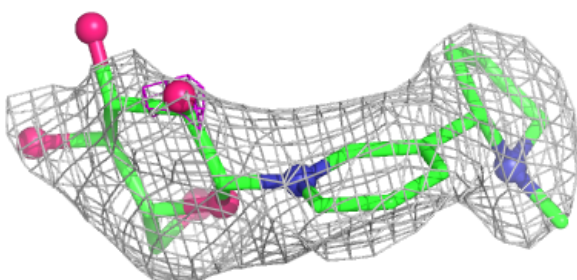
**Electron density around A1JEE A 607:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

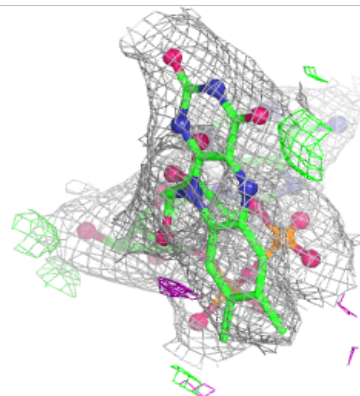
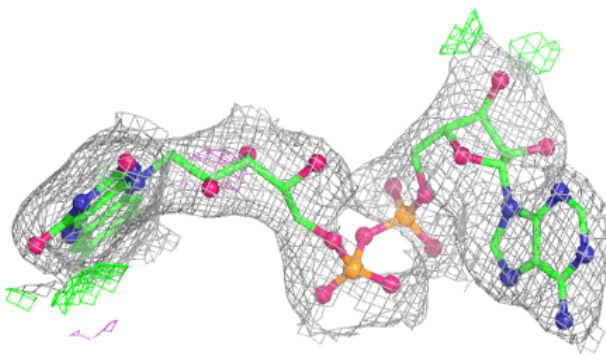
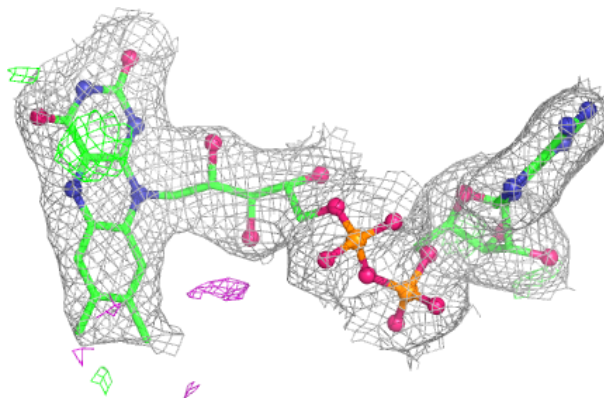


**Electron density around A1JEE B 606:**

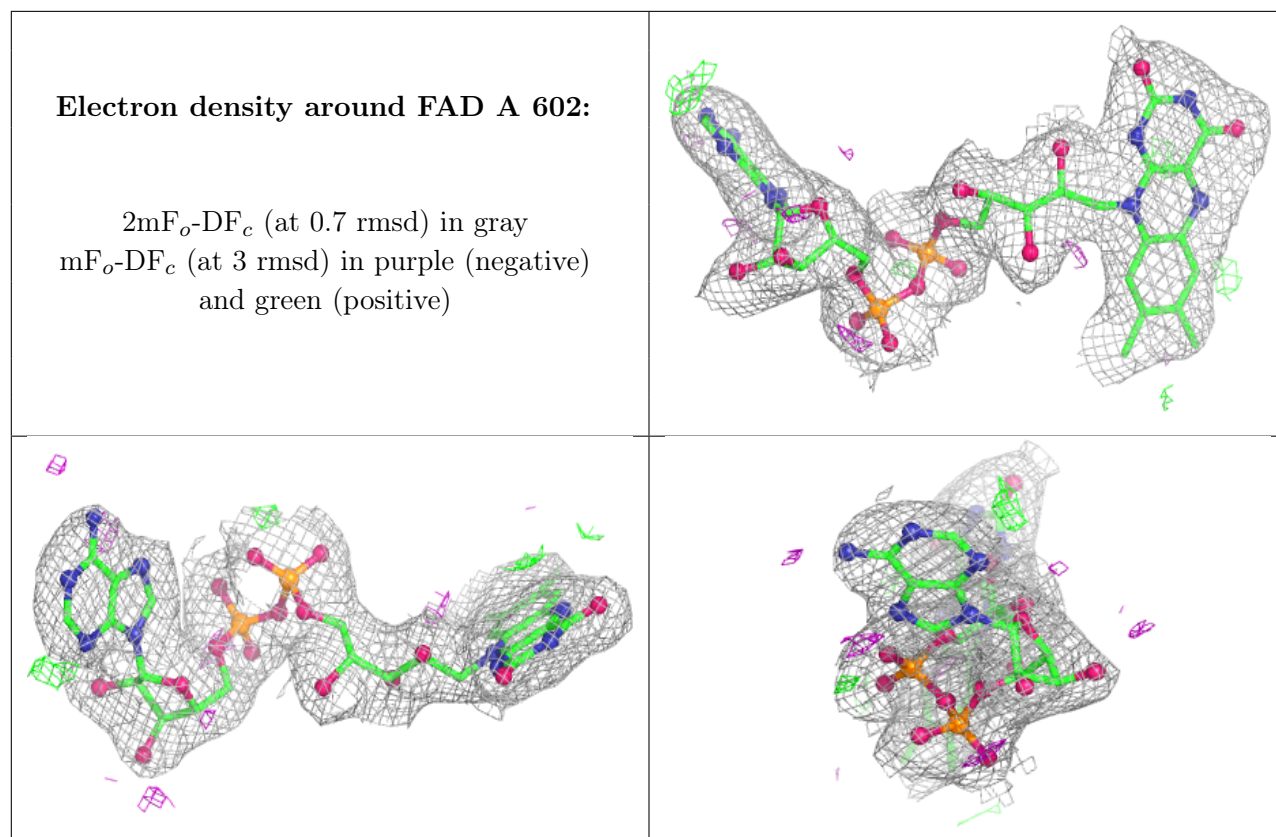
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FAD B 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.