wwPDB X-ray Structure Validation Summary Report (i)

Mar 21, 2023 – 12:26 pm GMT

PDB ID	:	7ZW3
Title	:	Crystal Structure of human MAO B in complex with (Z)-N-benzyl-1-(8-hydroxyquinolin-2-yl)methanimine oxide (inhibitor 19)
Authors	:	Binda, C.; Gottinger, A.
Deposited on	:	2022-05-18
Resolution	:	2.00 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

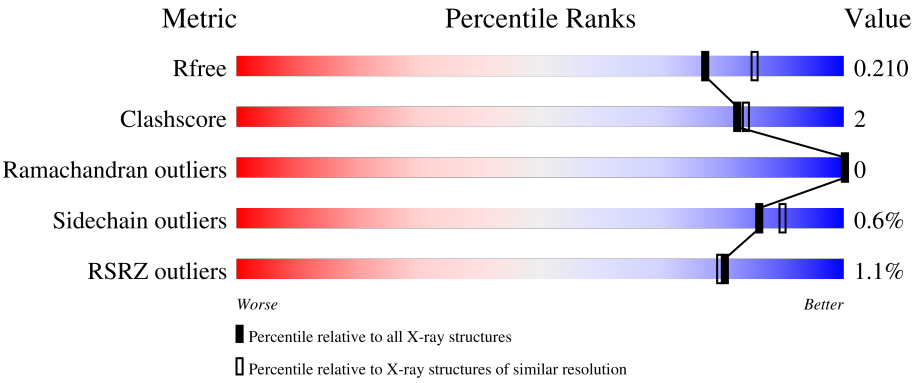
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

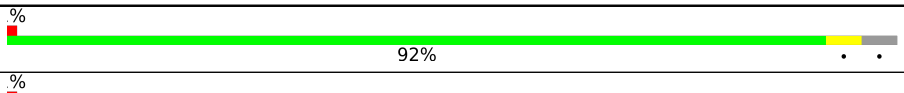
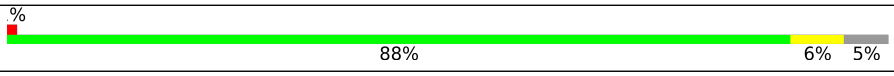
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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 <=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	AAA	520	
1	BBB	520	

2 Entry composition

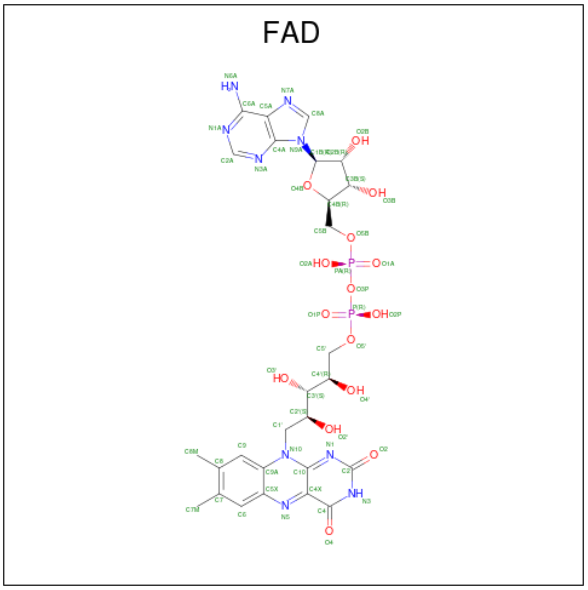
There are 5 unique types of molecules in this entry. The entry contains 8823 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Amine oxidase [flavin-containing] B.

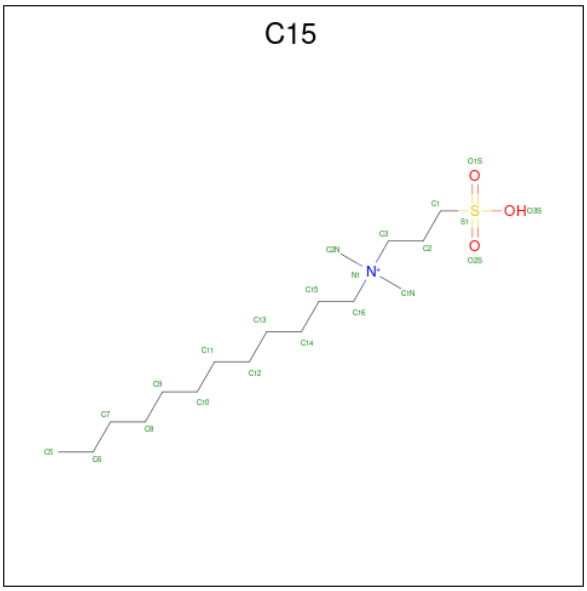
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	500	Total	C	N	O	S	0	6	0
			4006	2564	683	732	27			
1	BBB	495	Total	C	N	O	S	0	3	0
			3957	2530	677	724	26			

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



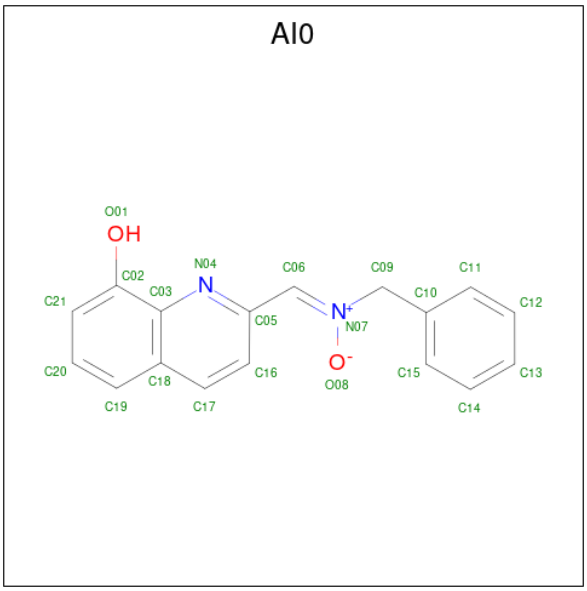
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	BBB	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is N-DODECYL-N,N-DIMETHYL-3-AMMONIO-1-PROPANESULFONATE (three-letter code: C15) (formula: $C_{17}H_{38}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	S	0	0
			15	10	1	3	1		
3	BBB	1	Total	C	N	O	S	0	0
			11	6	1	3	1		

- Molecule 4 is 1-(8-oxidanylquinolin-2-yl)-N-(phenylmethyl)methanimine oxide (three-letter code: AI0) (formula: $C_{17}H_{14}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	N	O	0	0
			21	17	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	BBB	1	Total	C	N	O	0	0
			21	17	2	2		

- Molecule 5 is water.

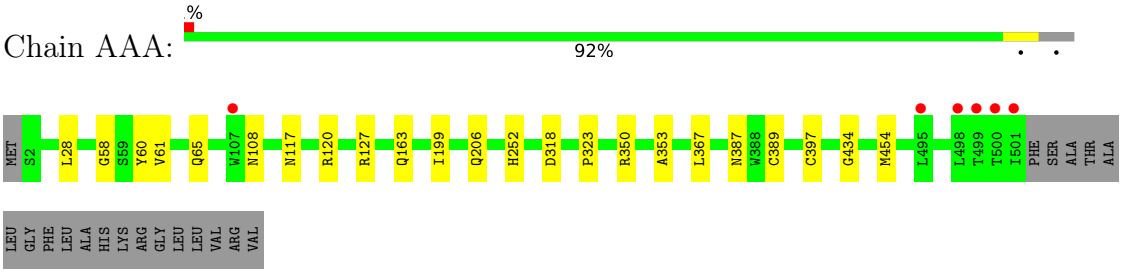
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	326	Total	O	0	0
			326	326		
5	BBB	360	Total	O	0	0
			360	360		

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.

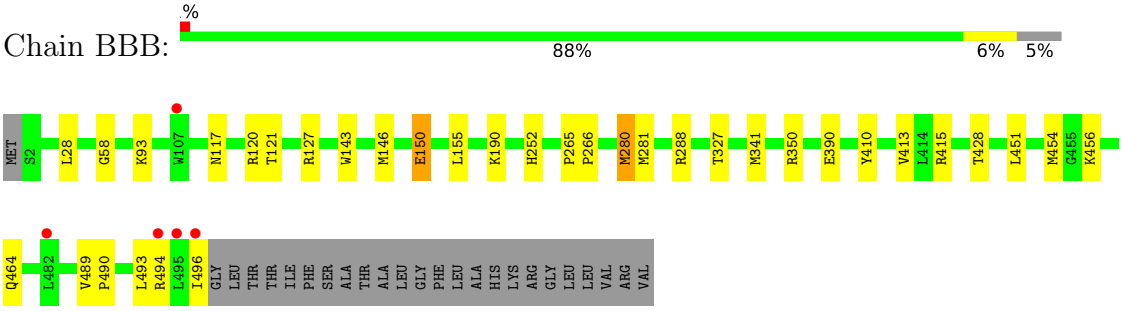
• Molecule 1: Amine oxidase [flavin-containing] B

Chain AAA:



• Molecule 1: Amine oxidase [flavin-containing] B

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	131.64Å 222.40Å 86.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.34 – 2.00 47.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.34-2.00) 99.2 (47.34-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.166 , 0.204 0.176 , 0.210	Depositor DCC
R_{free} test set	2205 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.015 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8823	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: C15, AI0, 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	AAA	0.74	0/4121	0.82	1/5592 (0.0%)
1	BBB	0.74	1/4063 (0.0%)	0.83	2/5513 (0.0%)
All	All	0.74	1/8184 (0.0%)	0.83	3/11105 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	150	GLU	CD-OE2	5.73	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	127	ARG	CG-CD-NE	-6.82	97.47	111.80
1	BBB	127	ARG	CG-CD-NE	-6.44	98.28	111.80
1	BBB	288	ARG	NE-CZ-NH2	-5.90	117.35	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	4006	0	4026	19	0
1	BBB	3957	0	3961	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AAA	53	0	29	2	0
2	BBB	53	0	29	1	0
3	AAA	15	0	21	0	0
3	BBB	11	0	13	0	0
4	AAA	21	0	0	1	0
4	BBB	21	0	0	0	0
5	AAA	326	0	0	1	3
5	BBB	360	0	0	3	0
All	All	8823	0	8079	40	3

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 2.

The worst 5 of 40 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:AAA:353:ALA:HB1	1:BBB:280:MET:HE1	1.78	0.66
1:BBB:117:ASN:HD22	1:BBB:120:ARG:HH21	1.44	0.64
1:BBB:451:LEU:HA	1:BBB:454:MET:HE2	1.81	0.62
1:BBB:150:GLU:OE1	5:BBB:701:HOH:O	2.16	0.61
1:AAA:28:LEU:HD11	1:AAA:454:MET:HE1	1.83	0.60

All (3) 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)
5:AAA:1019:HOH:O	5:AAA:1019:HOH:O[3_655]	1.03	1.17
5:AAA:1003:HOH:O	5:AAA:1003:HOH:O[3_655]	1.31	0.89
5:AAA:941:HOH:O	5:AAA:941:HOH:O[3_655]	1.52	0.68

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	AAA	504/520 (97%)	487 (97%)	17 (3%)	0	100	100
1	BBB	496/520 (95%)	482 (97%)	14 (3%)	0	100	100
All	All	1000/1040 (96%)	969 (97%)	31 (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	AAA	435/444 (98%)	433 (100%)	2 (0%)	88	92
1	BBB	428/444 (96%)	425 (99%)	3 (1%)	84	88
All	All	863/888 (97%)	858 (99%)	5 (1%)	86	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	350	ARG
1	AAA	397	CYS
1	BBB	190	LYS
1	BBB	280	MET
1	BBB	350	ARG

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 (i)

6 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	AI0	BBB	603	-	22,23,23	0.90	1 (4%)	27,31,31	0.94	1 (3%)
2	FAD	AAA	601	1	53,58,58	1.08	3 (5%)	68,89,89	1.70	20 (29%)
3	C15	BBB	602	-	10,10,21	0.84	1 (10%)	14,15,26	0.97	0
4	AI0	AAA	603	-	22,23,23	0.94	1 (4%)	27,31,31	0.72	1 (3%)
2	FAD	BBB	601	1	53,58,58	1.14	5 (9%)	68,89,89	1.62	14 (20%)
3	C15	AAA	602	-	14,14,21	0.81	1 (7%)	18,19,26	0.79	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	AI0	BBB	603	-	-	3/7/8/8	0/3/3/3
2	FAD	AAA	601	1	-	4/30/50/50	0/6/6/6
3	C15	BBB	602	-	-	4/8/8/21	-
4	AI0	AAA	603	-	-	2/7/8/8	0/3/3/3
2	FAD	BBB	601	1	-	2/30/50/50	0/6/6/6
3	C15	AAA	602	-	-	2/14/14/21	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	603	AI0	C05-C06	3.26	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	601	FAD	C4X-N5	3.08	1.36	1.30
4	BBB	603	AI0	C05-C06	2.96	1.53	1.47
2	BBB	601	FAD	C10-N1	2.67	1.38	1.33
2	BBB	601	FAD	C2A-N3A	2.65	1.36	1.32

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	601	FAD	O4B-C1B-C2B	-4.49	100.36	106.93
2	BBB	601	FAD	N3A-C2A-N1A	-4.44	121.74	128.68
2	AAA	601	FAD	O4B-C1B-C2B	-3.92	101.20	106.93
4	BBB	603	AI0	C05-C06-N07	3.79	130.83	121.87
2	BBB	601	FAD	O4-C4-C4X	-3.66	116.88	126.60

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	601	FAD	C5B-O5B-PA-O2A
3	BBB	602	C15	C2-C1-S1-O1S
3	BBB	602	C15	C2-C1-S1-O2S
4	AAA	603	AI0	C10-C09-N07-O08
3	BBB	602	C15	S1-C1-C2-C3

There are no ring outliers.

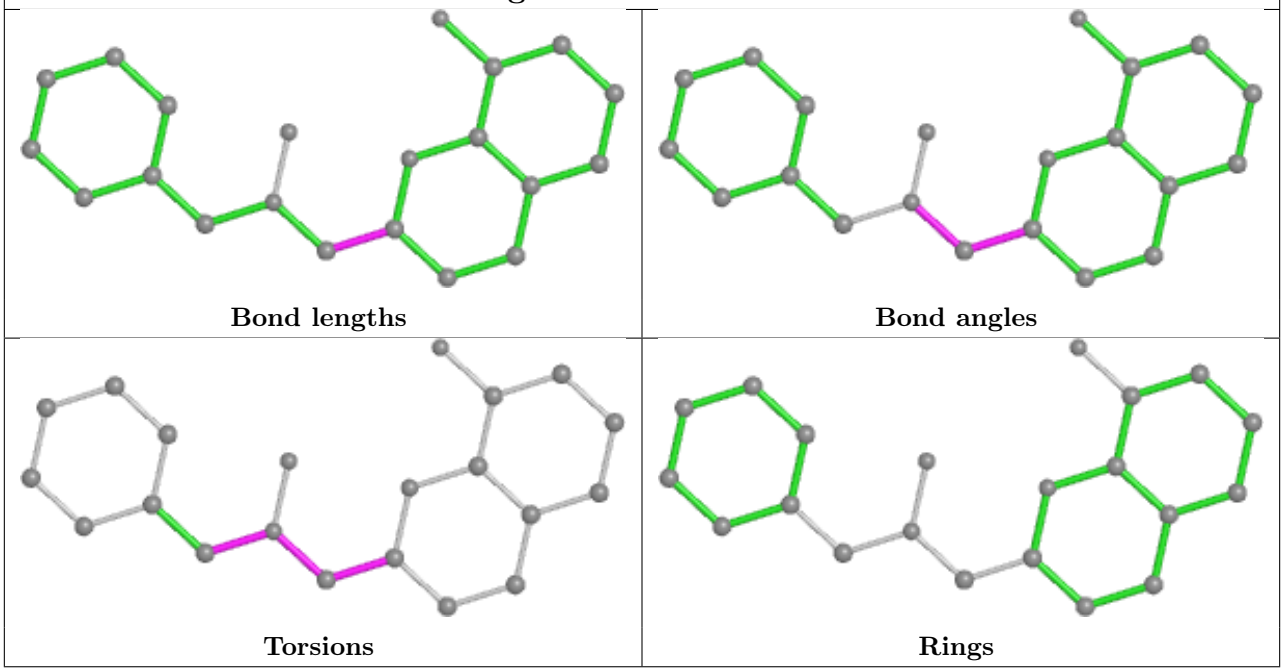
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	601	FAD	2	0
4	AAA	603	AI0	1	0
2	BBB	601	FAD	1	0

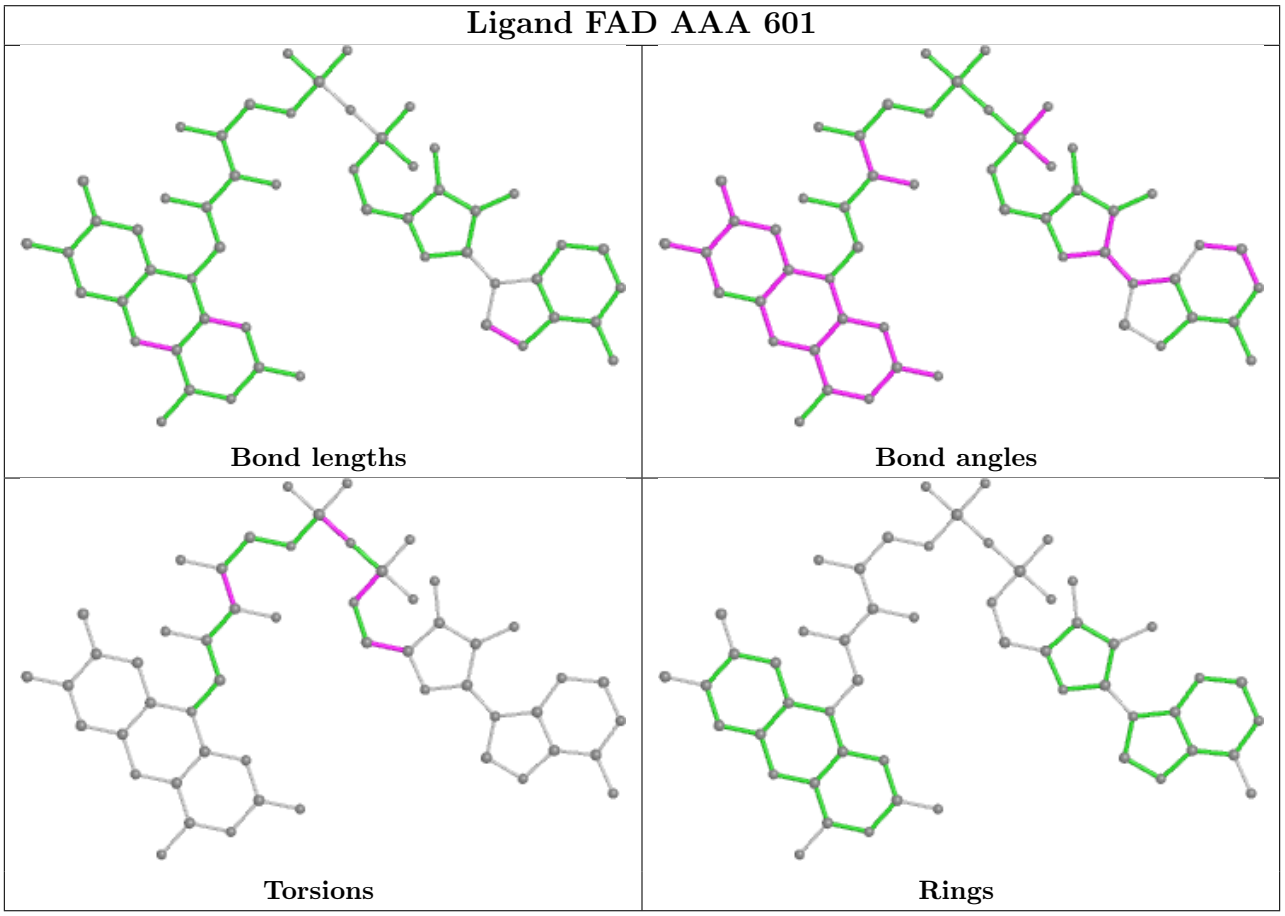
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

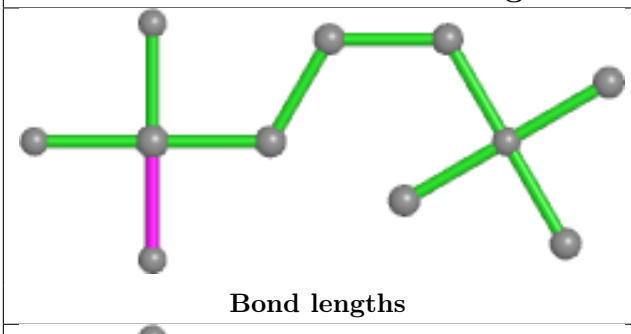
Ligand AI0 BBB 603



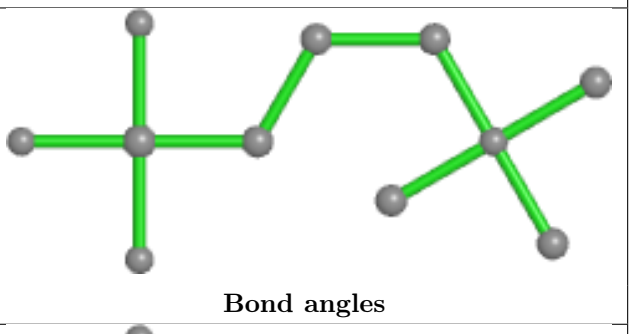
Ligand FAD AAA 601



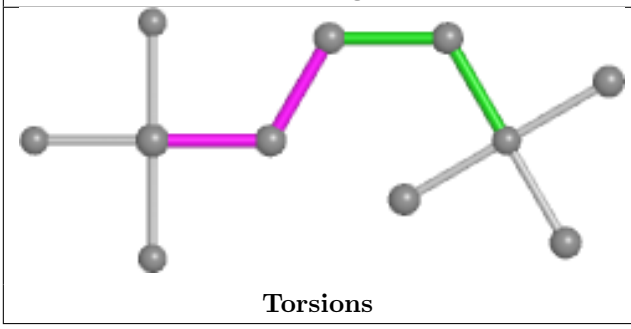
Ligand C15 BBB 602



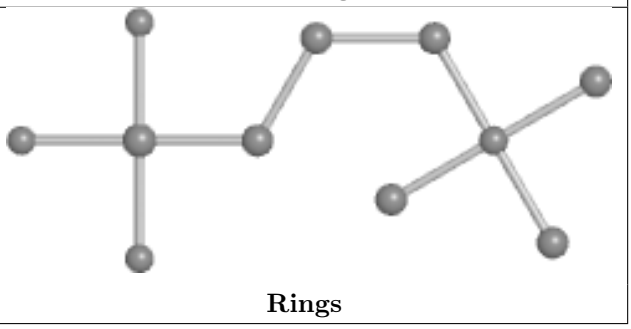
Bond lengths



Bond angles

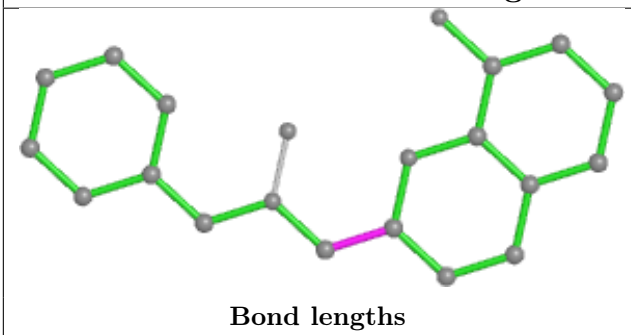


Torsions

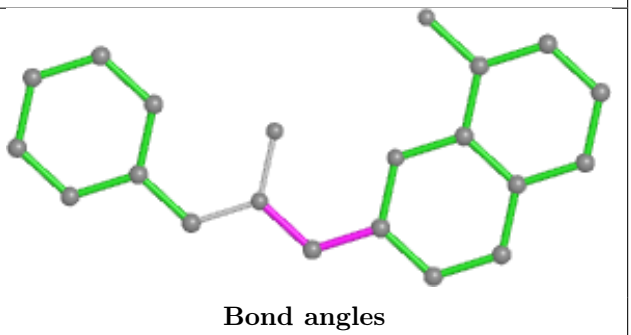


Rings

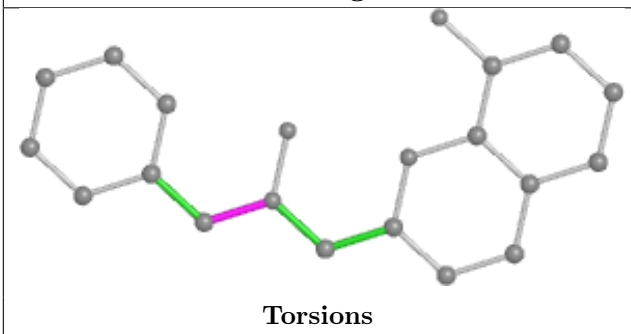
Ligand AI0 AAA 603



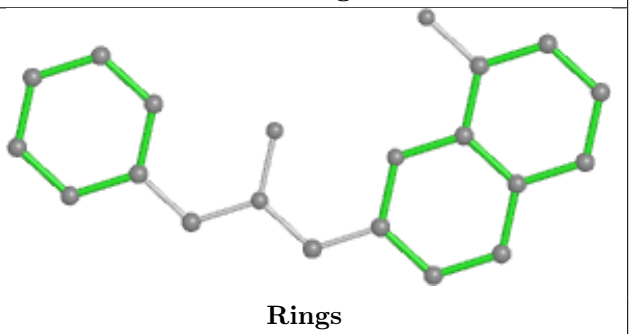
Bond lengths



Bond angles

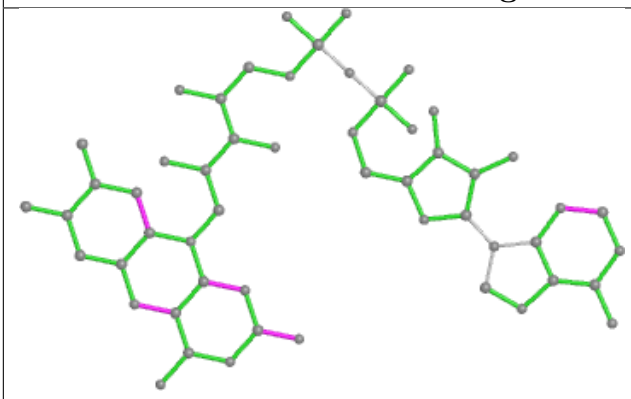


Torsions

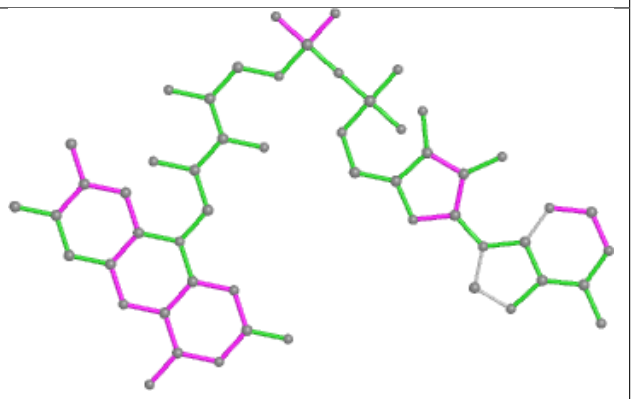


Rings

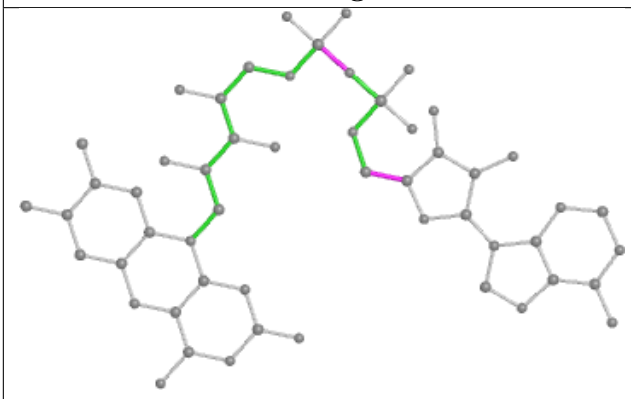
Ligand FAD BBB 601



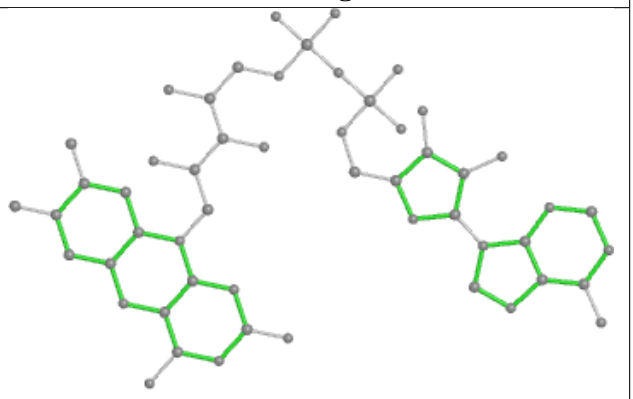
Bond lengths



Bond angles

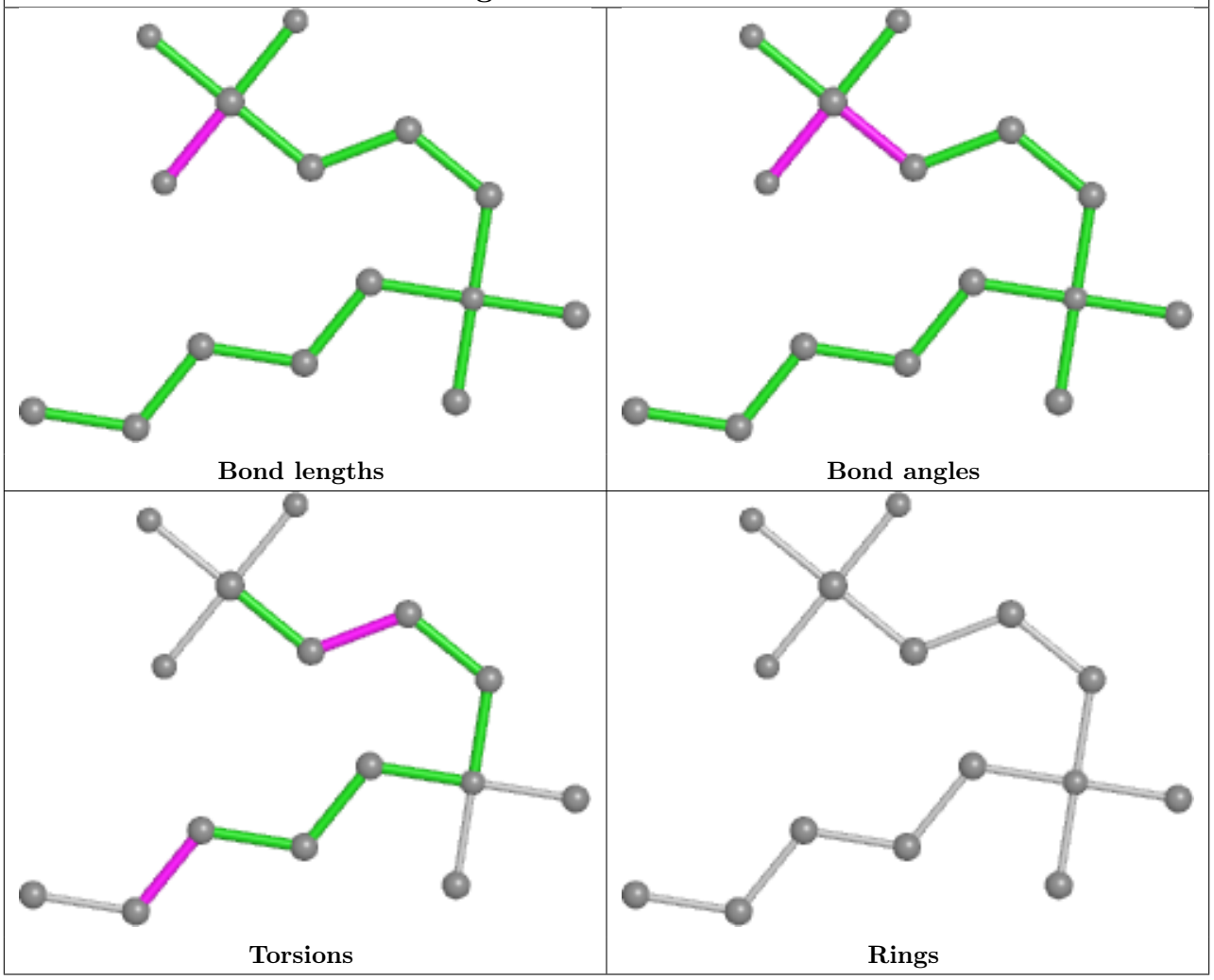


Torsions



Rings

Ligand C15 AAA 602



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^{th} 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^2)	Q<0.9
1	AAA	500/520 (96%)	-0.38	6 (1%)	79	78	14, 21, 38, 73	0
1	BBB	495/520 (95%)	-0.43	5 (1%)	82	81	12, 19, 35, 75	0
All	All	995/1040 (95%)	-0.40	11 (1%)	80	79	12, 20, 37, 75	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	500	THR	4.9
1	AAA	501	ILE	4.3
1	AAA	498	LEU	3.8
1	AAA	495	LEU	3.0
1	BBB	494	ARG	2.9

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

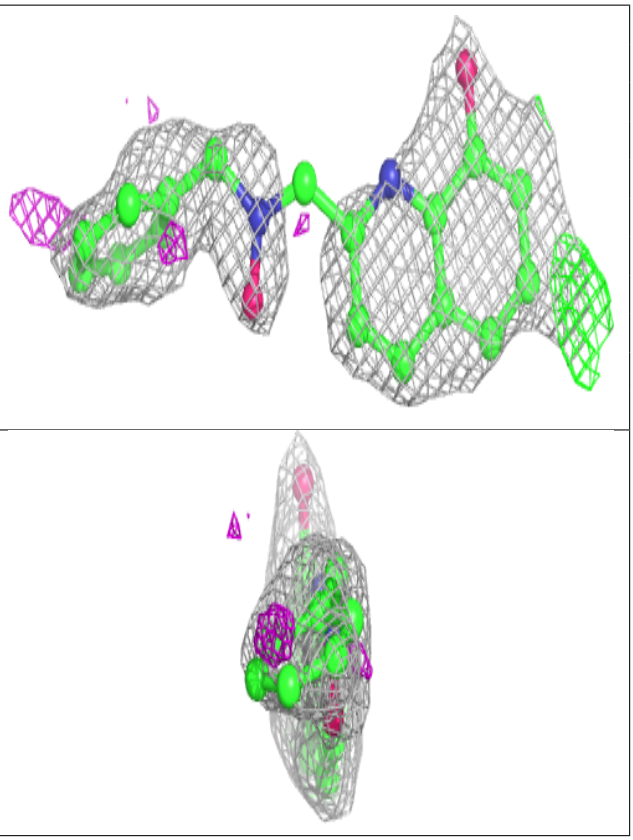
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	AI0	AAA	603	21/21	0.81	0.24	47,51,57,61	0
3	C15	BBB	602	11/22	0.84	0.18	40,45,75,78	0
4	AI0	BBB	603	21/21	0.85	0.19	39,47,56,68	0
3	C15	AAA	602	15/22	0.87	0.13	34,37,73,77	0
2	FAD	BBB	601	53/53	0.98	0.11	12,13,15,16	0
2	FAD	AAA	601	53/53	0.99	0.07	13,15,17,17	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.

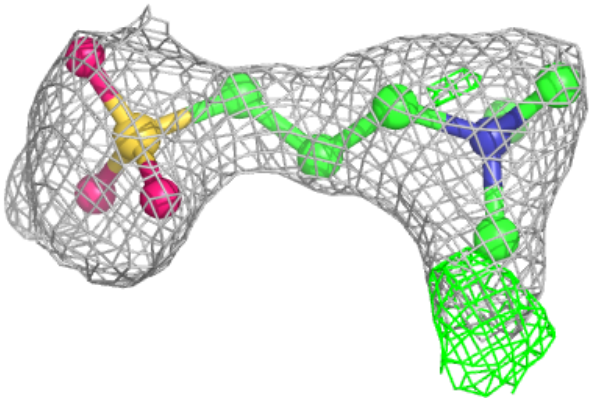
Electron density around AI0 AAA 603:

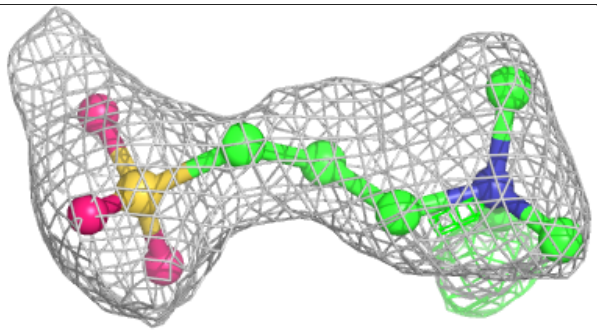
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

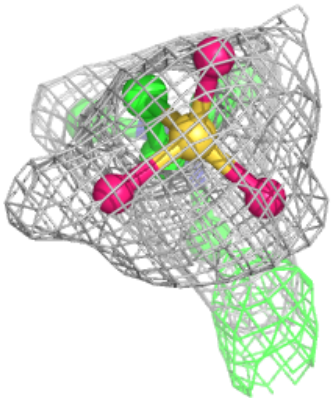


Electron density around C15 BBB 602:

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

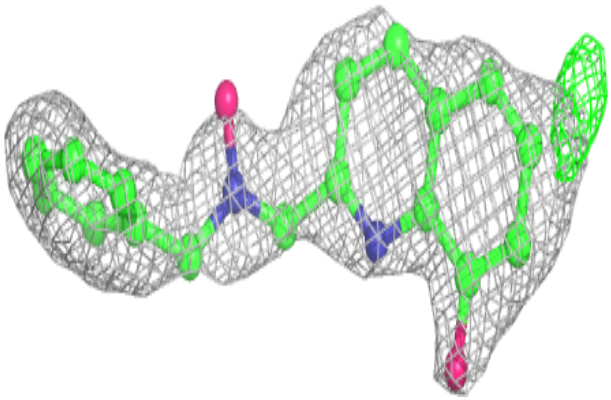


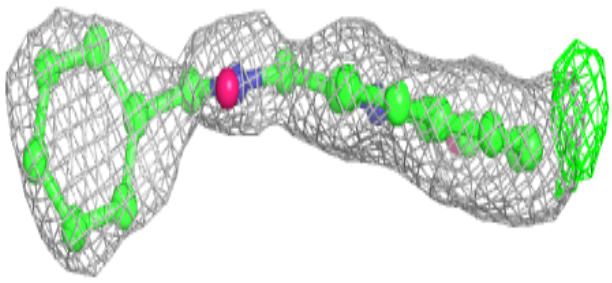


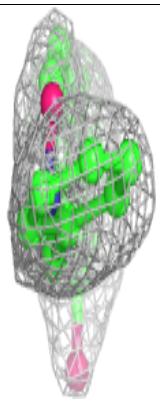


Electron density around AI0 BBB 603:

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

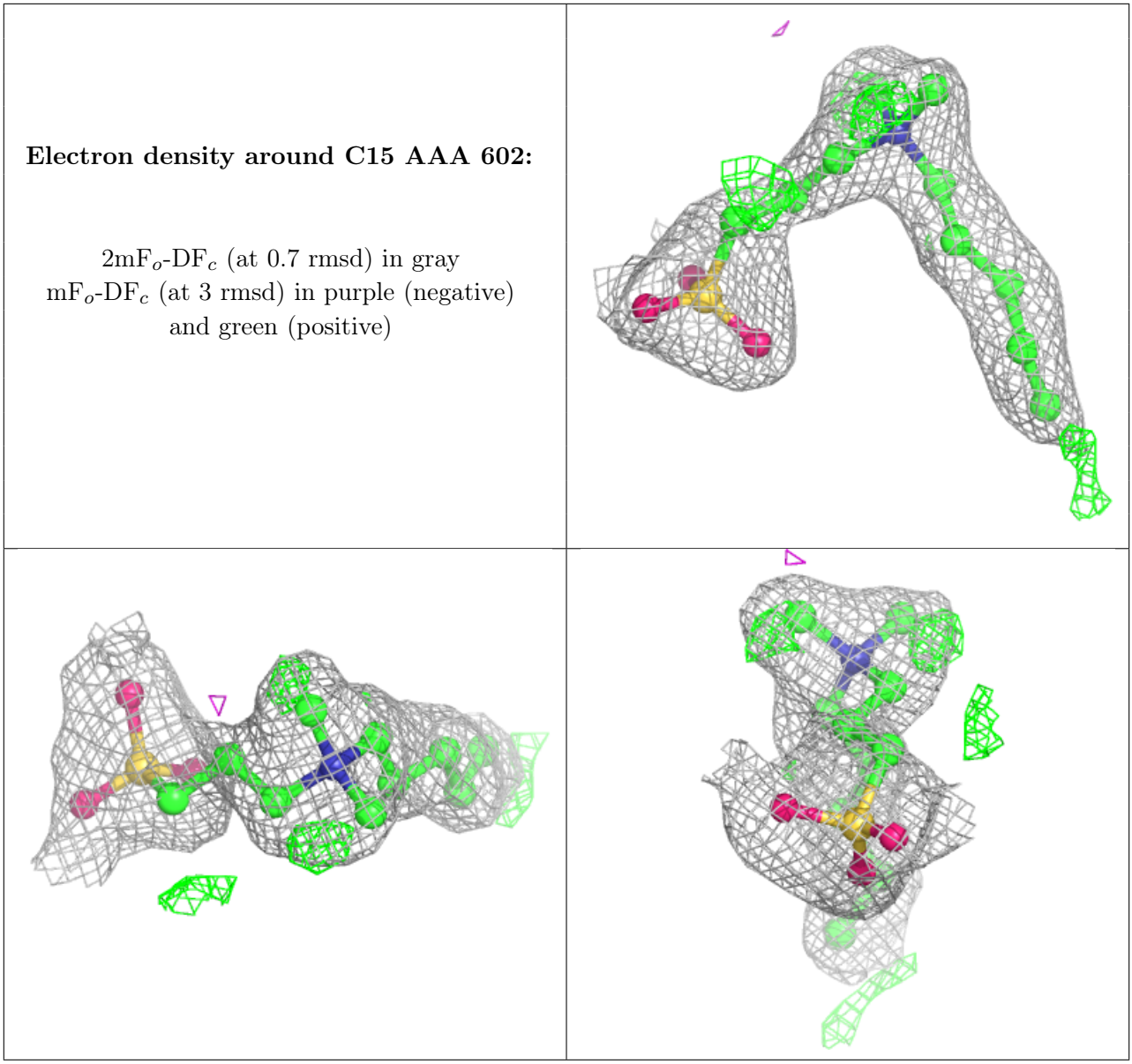






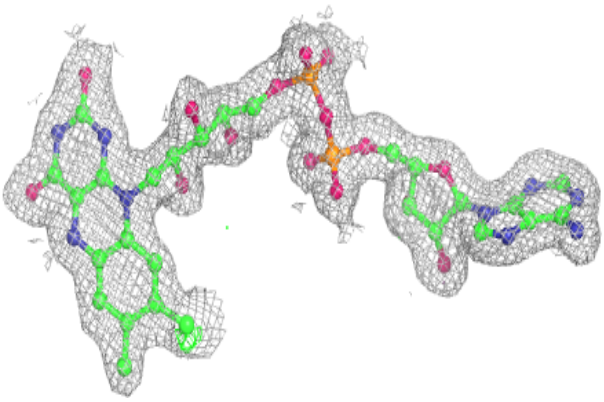
Electron density around C15 AAA 602:

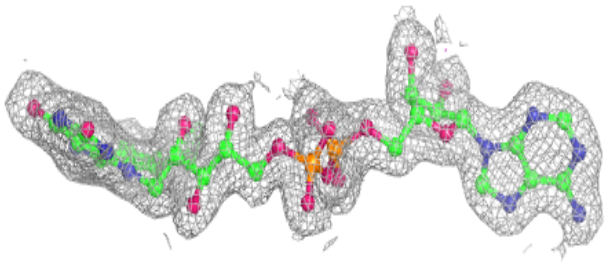
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

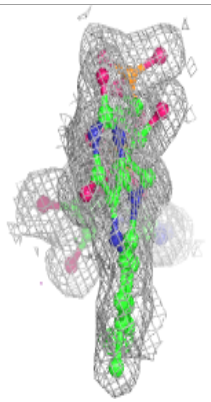


Electron density around FAD BBB 601:

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

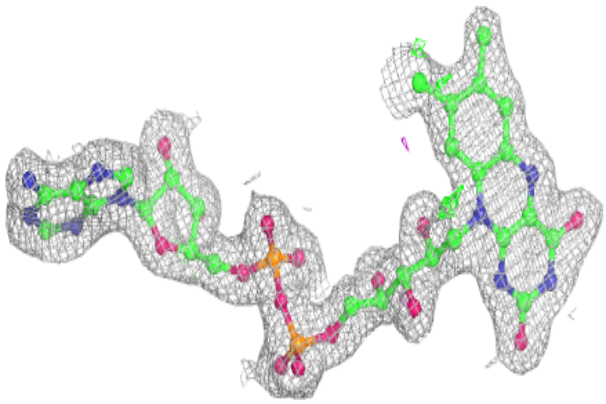


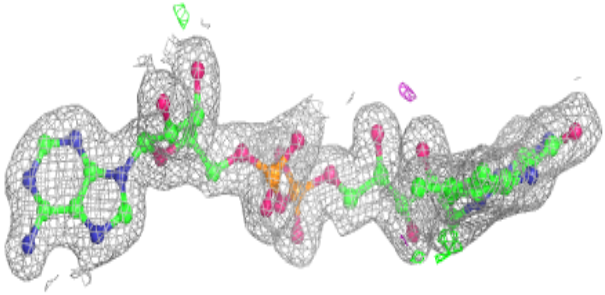


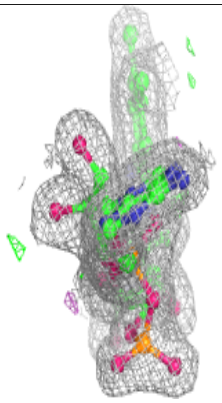


Electron density around FAD AAA 601:

$2mF_o$-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.