



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2025 – 05:25 pm BST

PDB ID : 9R3J / pdb_00009r3j
Title : Crystal structure of human MAO B in complex with (E)-3-(benzo[d][1,3]dioxol-5-yl)-1-(3-(trifluoromethyl)phenyl)prop-2-en-1-one (chalcone inhibitor, 4e)
Authors : Marchese, S.; Binda, C.
Deposited on : 2025-05-05
Resolution : 1.70 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

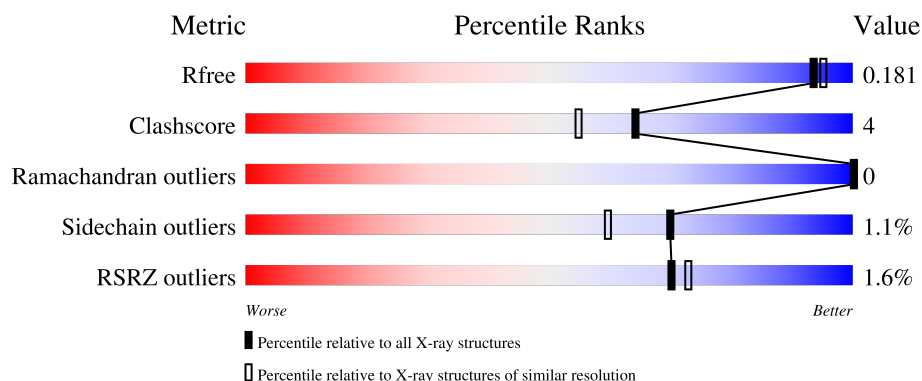
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.70 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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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 $\leq 5\%$. 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	AAA	519	
1	BBB	519	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9010 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.

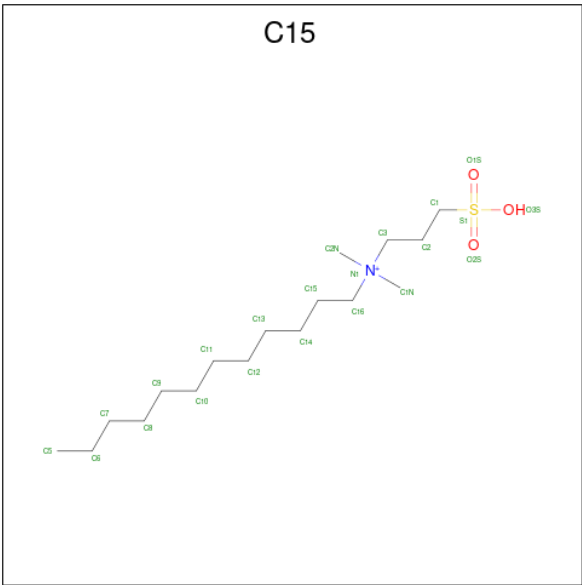
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	500	Total	C	N	O	S	0	3	0
			3996	2556	685	731	24			
1	BBB	495	Total	C	N	O	S	0	2	0
			3957	2529	680	724	24			

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



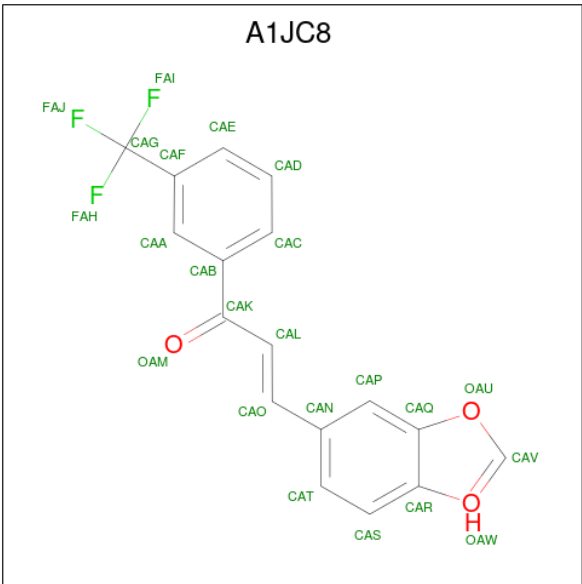
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	BBB	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is N-DODECYL-N,N-DIMETHYL-3-AMMONIO-1-PROPANESULFONATE (CCD ID: 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 ({E})-3-(1,3-benzodioxol-5-yl)-1-[3-(trifluoromethyl)phenyl]prop-2-en-1-one (CCD ID: A1JC8) (formula: C₁₇H₁₁F₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	F	O	0	0
			23	17	3	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	BBB	1	Total	C	F	O	0	0
			23	17	3	3		

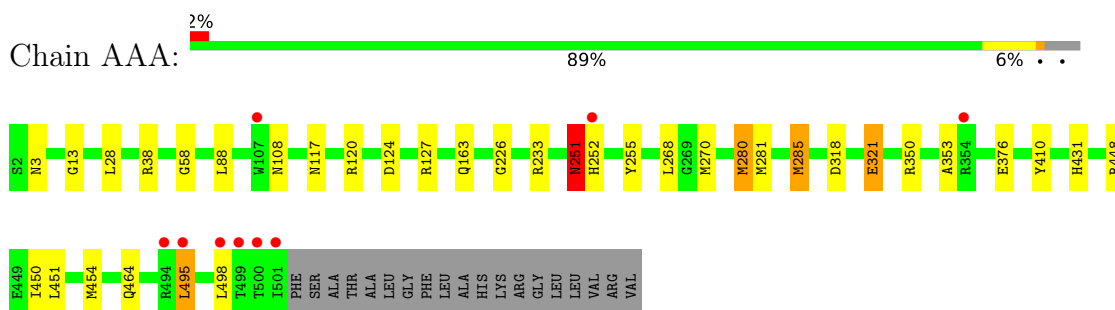
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	426	Total	O	0	0
			426	426		
5	BBB	453	Total	O	0	0
			453	453		

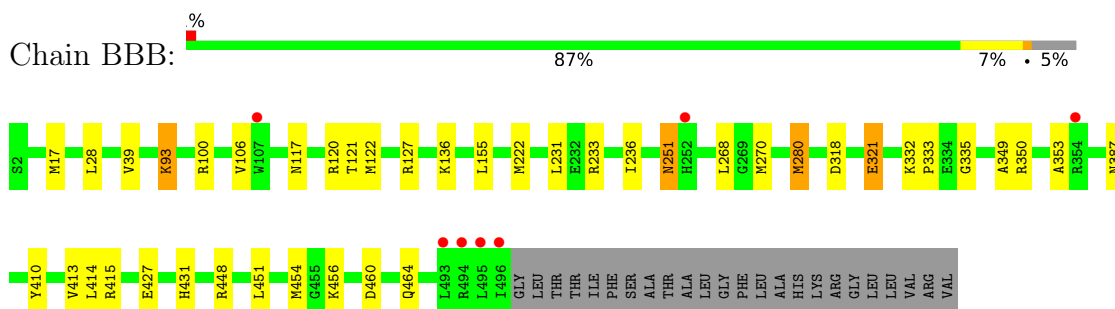
3 Residue-property plots [i](#)

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.30Å 222.29Å 86.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.27 – 1.70 47.27 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.27-1.70) 99.9 (47.27-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.150 , 0.172 0.162 , 0.181	Depositor DCC
R_{free} test set	3453 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.012 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9010	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: A1JC8, C15, 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	1.08	5/4102 (0.1%)	1.21	4/5567 (0.1%)
1	BBB	1.08	1/4060 (0.0%)	1.22	12/5509 (0.2%)
All	All	1.08	6/8162 (0.1%)	1.21	16/11076 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	226	GLY	C-O	5.77	1.31	1.24
1	AAA	252	HIS	CE1-NE2	5.64	1.38	1.32
1	AAA	38	ARG	C-O	5.56	1.30	1.23
1	AAA	13	GLY	C-O	5.55	1.28	1.23
1	AAA	376	GLU	CD-OE2	5.51	1.35	1.25

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	285	MET	CG-SD-CE	-9.20	80.65	100.90
1	AAA	127	ARG	CG-CD-NE	-6.74	97.16	112.00
1	AAA	124	ASP	CA-CB-CG	5.83	118.43	112.60
1	BBB	415	ARG	CB-CA-C	5.78	120.32	111.02
1	BBB	414	LEU	CA-C-N	-5.66	113.68	122.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3996	0	4010	34	0
1	BBB	3957	0	3960	35	0
2	AAA	53	0	29	1	0
2	BBB	53	0	29	0	0
3	AAA	15	0	21	0	0
3	BBB	11	0	13	0	0
4	AAA	23	0	0	0	0
4	BBB	23	0	0	0	0
5	AAA	426	0	0	3	0
5	BBB	453	0	0	6	0
All	All	9010	0	8062	61	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 4.

The worst 5 of 61 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:280:MET:CE	5:BBB:1026:HOH:O	2.25	0.83
1:BBB:28:LEU:HD11	1:BBB:454:MET:HE1	1.66	0.76
1:AAA:28:LEU:HD11	1:AAA:454:MET:HE1	1.66	0.76
1:BBB:117:ASN:HD22	1:BBB:120:ARG:HH21	1.36	0.71
1:AAA:431:HIS:CD2	5:AAA:1012:HOH:O	2.44	0.71

There are no symmetry-related clashes.

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	AAA	501/519 (96%)	490 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	495/519 (95%)	483 (98%)	12 (2%)	0	100	100
All	All	996/1038 (96%)	973 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	432/443 (98%)	426 (99%)	6 (1%)	62	49
1	BBB	427/443 (96%)	424 (99%)	3 (1%)	81	75
All	All	859/886 (97%)	850 (99%)	9 (1%)	70	64

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	251	ASN
1	BBB	280	MET
1	AAA	350	ARG
1	AAA	495	LEU
1	AAA	498	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	C15	AAA	602	-	14,14,21	0.76	1 (7%)	18,19,26	0.70	0
3	C15	BBB	602	-	10,10,21	0.99	1 (10%)	14,15,26	1.19	1 (7%)
2	FAD	AAA	601	1	53,58,58	1.11	4 (7%)	68,89,89	1.66	14 (20%)
2	FAD	BBB	601	1	53,58,58	1.37	8 (15%)	68,89,89	1.73	14 (20%)
4	A1JC8	BBB	603	-	19,25,25	2.25	9 (47%)	26,36,36	1.83	5 (19%)
4	A1JC8	AAA	603	-	19,25,25	2.16	7 (36%)	26,36,36	1.86	7 (26%)

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
3	C15	AAA	602	-	-	1/14/14/21	-
3	C15	BBB	602	-	-	4/8/8/21	-
2	FAD	AAA	601	1	-	1/30/50/50	0/6/6/6
2	FAD	BBB	601	1	-	1/30/50/50	0/6/6/6
4	A1JC8	BBB	603	-	-	0/15/21/21	0/3/3/3
4	A1JC8	AAA	603	-	-	0/15/21/21	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	603	A1JC8	FAH-CAG	-6.02	1.10	1.32
4	BBB	603	A1JC8	CAB-CAK	-4.87	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	603	A1JC8	CAB-CAK	-4.47	1.42	1.49
2	BBB	601	FAD	C4X-N5	3.92	1.38	1.30
4	BBB	603	A1JC8	FAH-CAG	-3.70	1.19	1.32

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	601	FAD	C9A-C5X-N5	-5.31	116.67	122.43
2	AAA	601	FAD	C9A-C5X-N5	-4.73	117.29	122.43
4	BBB	603	A1JC8	CAA-CAF-CAG	4.48	125.64	119.58
4	AAA	603	A1JC8	FAI-CAG-CAF	-4.18	103.75	112.93
2	BBB	601	FAD	O4B-C1B-C2B	-4.09	100.94	106.93

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

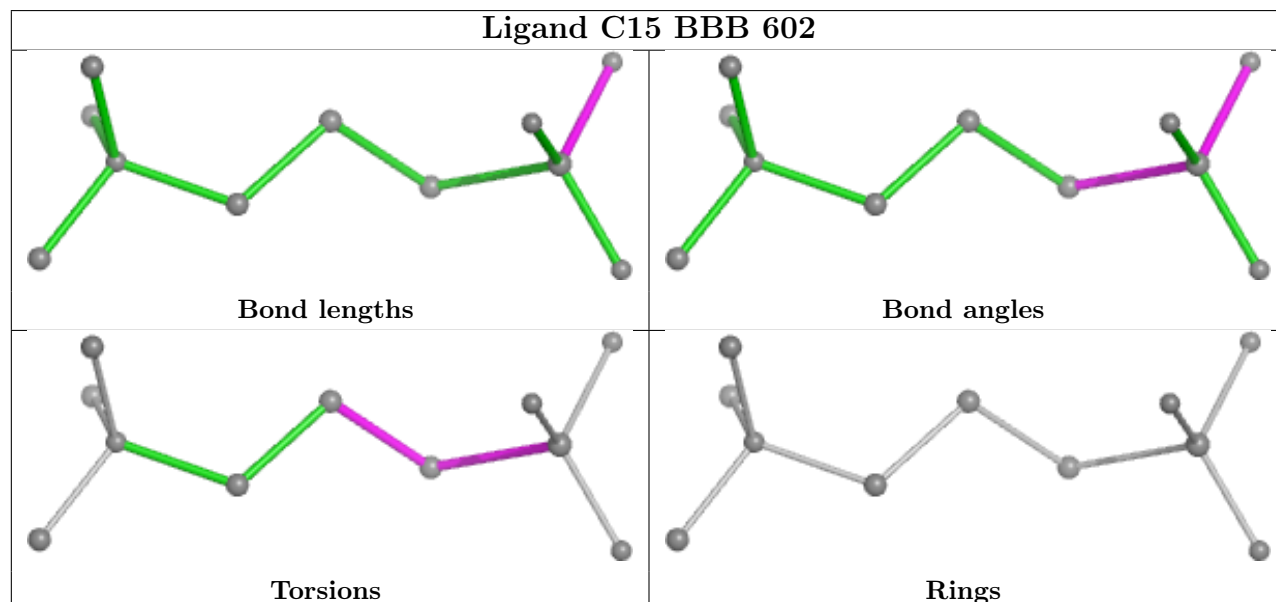
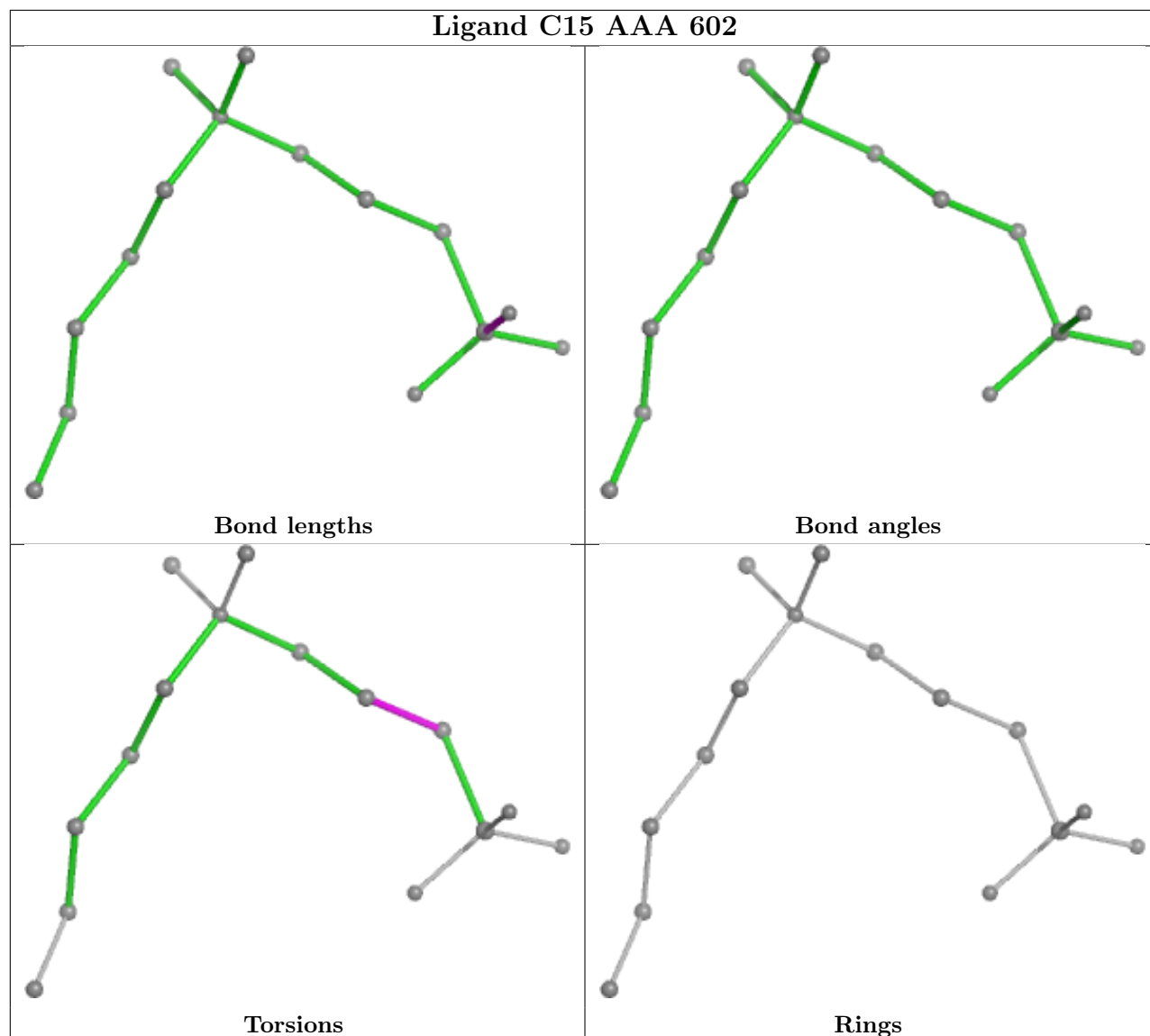
Mol	Chain	Res	Type	Atoms
3	BBB	602	C15	C2-C1-S1-O1S
3	BBB	602	C15	C2-C1-S1-O2S
3	AAA	602	C15	S1-C1-C2-C3
3	BBB	602	C15	S1-C1-C2-C3
3	BBB	602	C15	C2-C1-S1-O3S

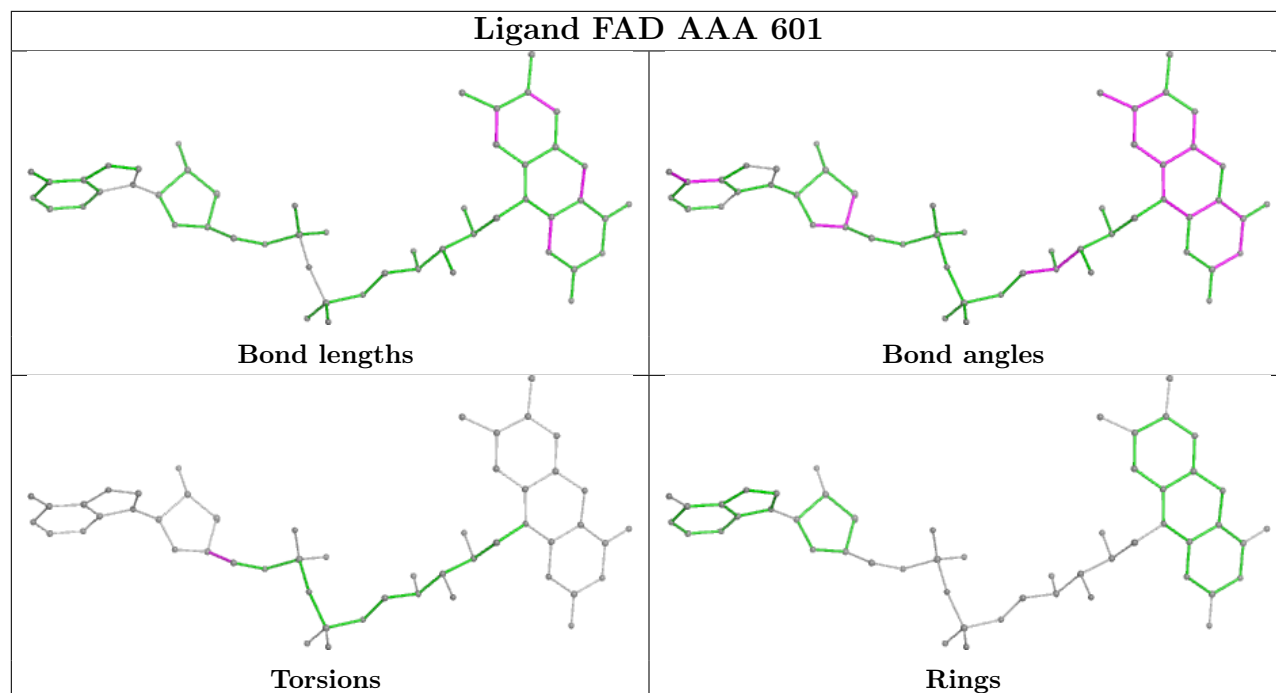
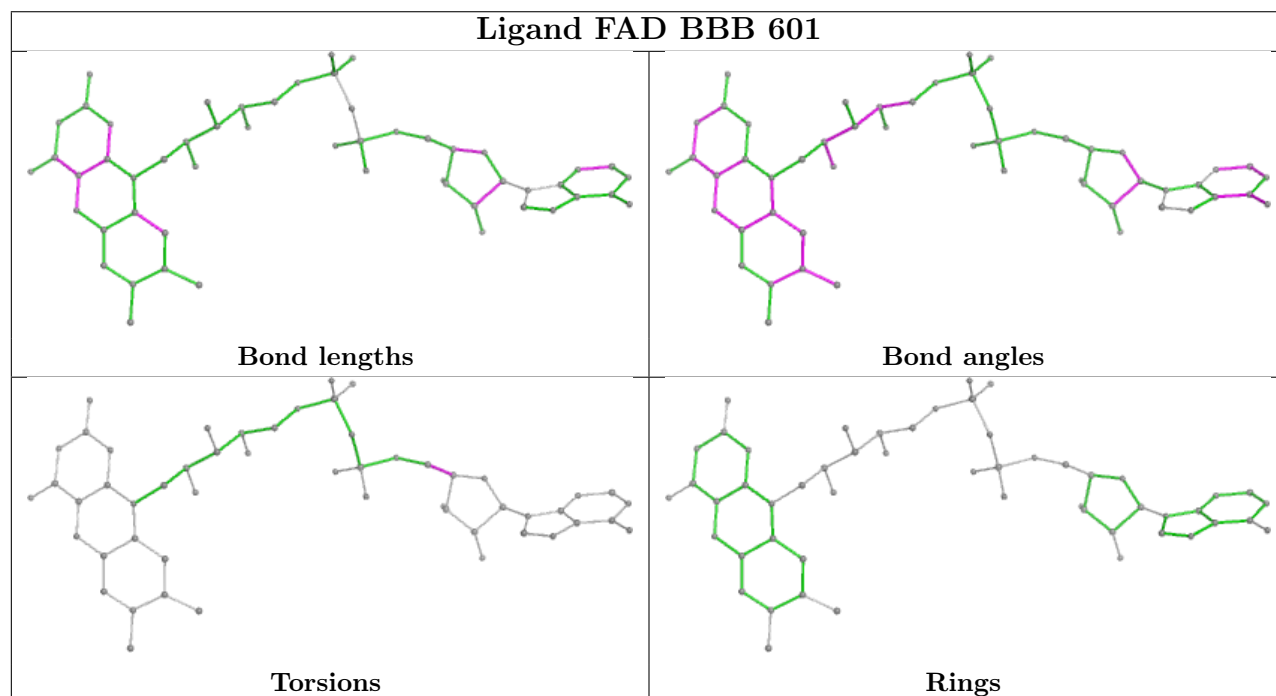
There are no ring outliers.

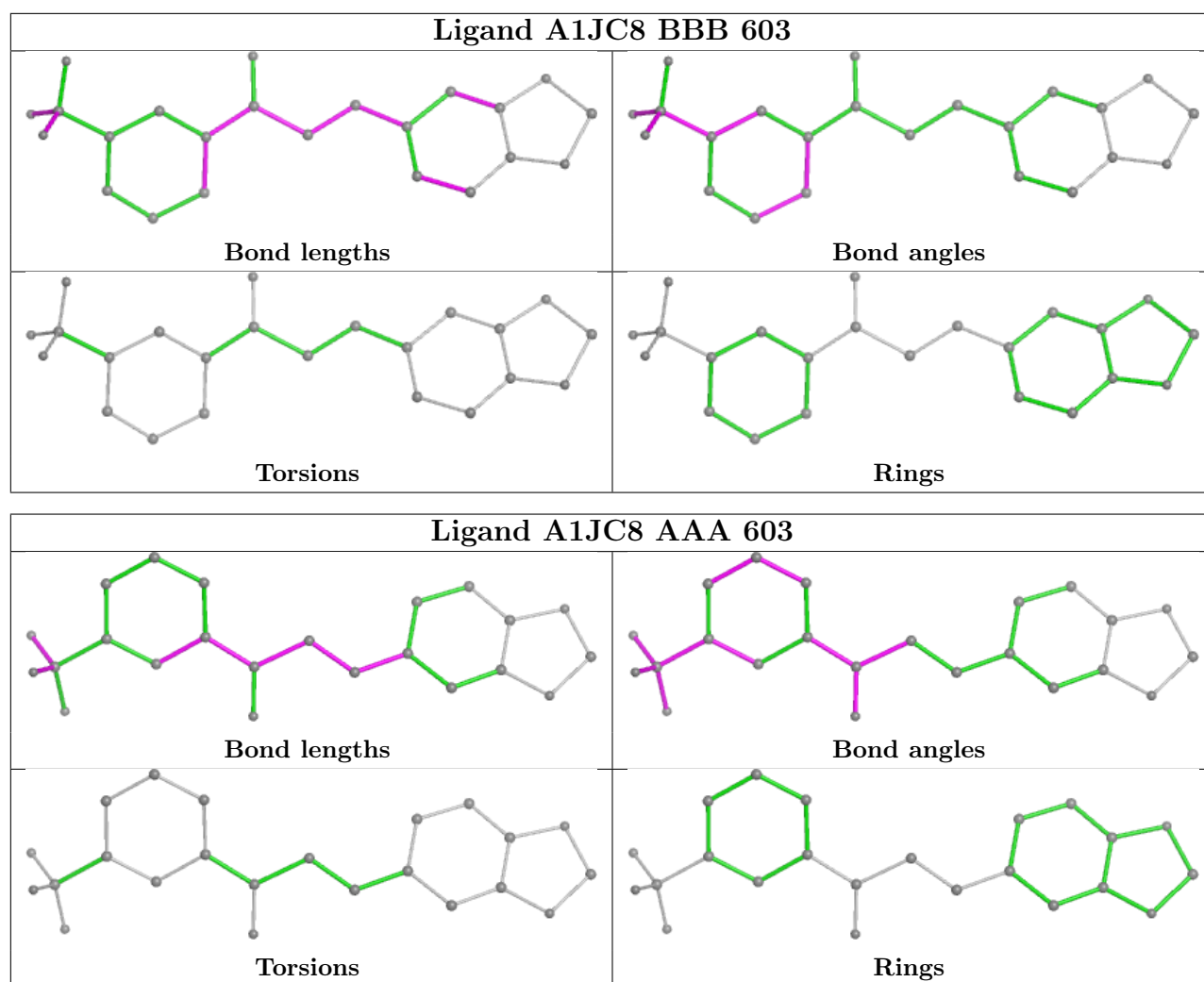
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	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 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 FAD AAA 601**Ligand FAD BBB 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 [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, 95th 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	500/519 (96%)	-0.33	9 (1%) 67 70	8, 17, 34, 69	3 (0%)
1	BBB	495/519 (95%)	-0.43	7 (1%) 73 76	9, 16, 32, 69	2 (0%)
All	All	995/1038 (95%)	-0.38	16 (1%) 70 73	8, 16, 33, 69	5 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	501	ILE	6.8
1	BBB	495	LEU	4.6
1	BBB	496	ILE	4.5
1	BBB	494	ARG	3.5
1	AAA	107	TRP	3.3

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](#)

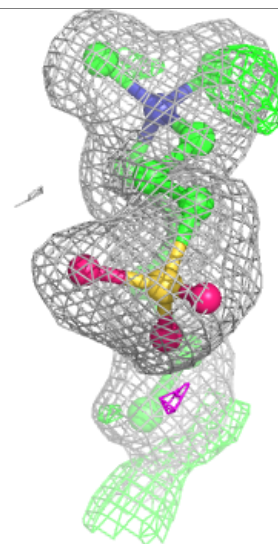
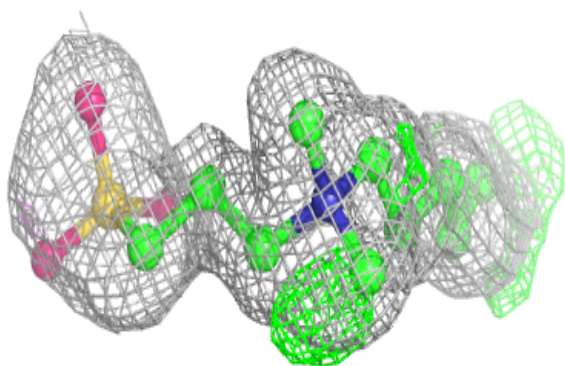
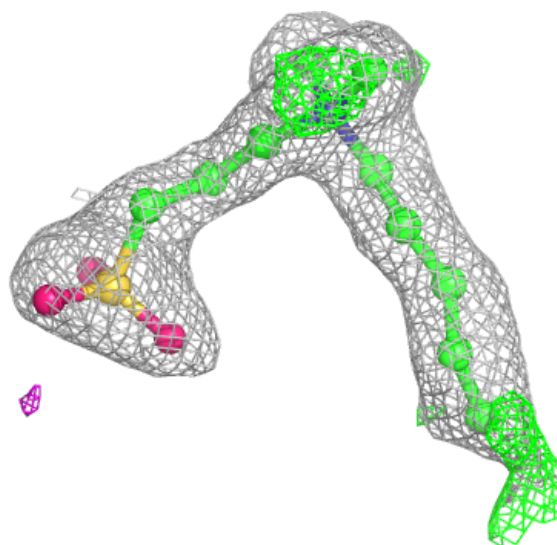
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	C15	AAA	602	15/22	0.81	0.15	27,36,58,65	0
3	C15	BBB	602	11/22	0.84	0.14	31,40,72,73	0
4	A1JC8	AAA	603	23/23	0.95	0.06	18,20,30,39	0
4	A1JC8	BBB	603	23/23	0.95	0.06	17,20,28,35	0
2	FAD	AAA	601	53/53	0.99	0.03	10,12,13,14	0
2	FAD	BBB	601	53/53	0.99	0.03	10,11,13,13	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.

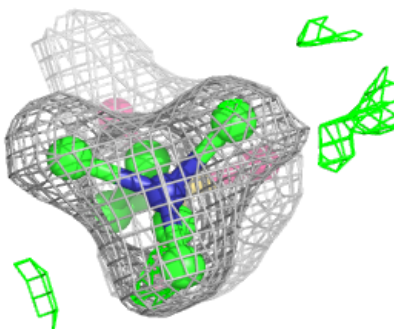
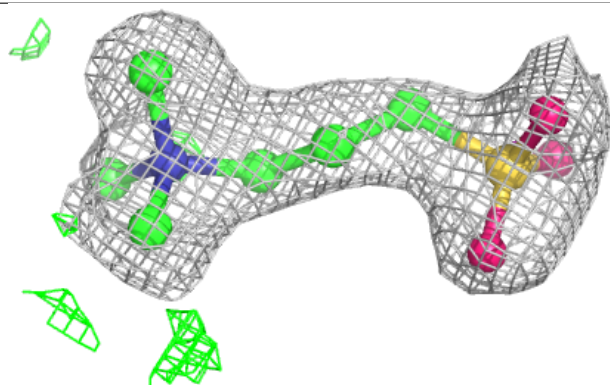
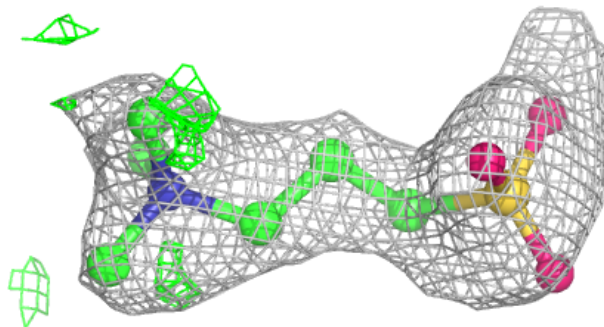
Electron density around C15 AAA 602:

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

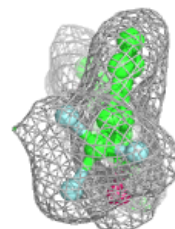
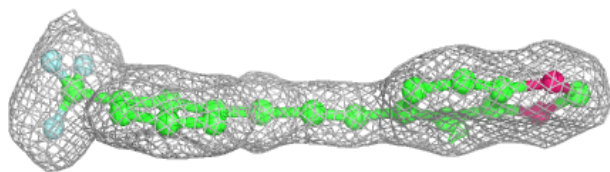
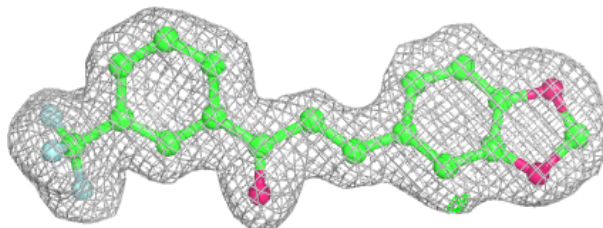


Electron density around C15 BBB 602:

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

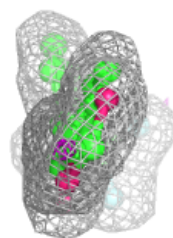
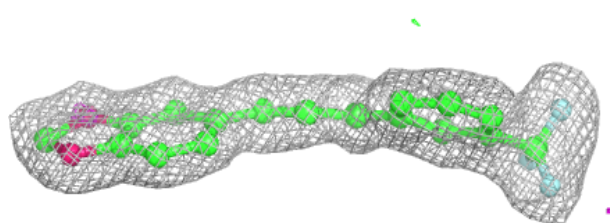
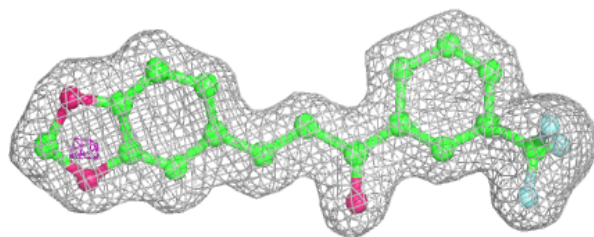
**Electron density around A1JC8 AAA 603:**

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

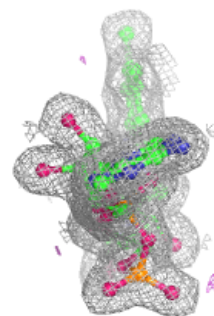
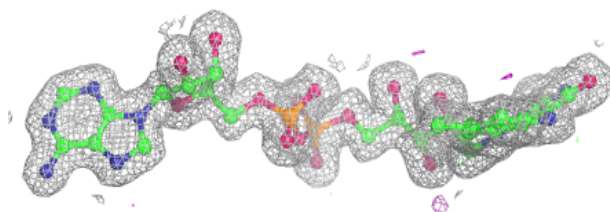
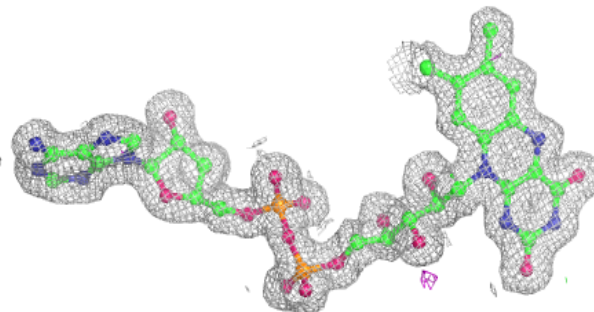


Electron density around A1JC8 BBB 603:

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

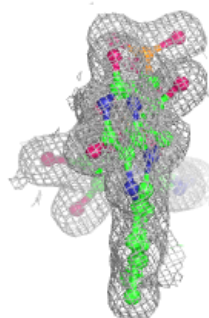
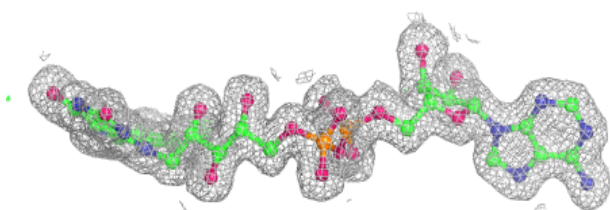
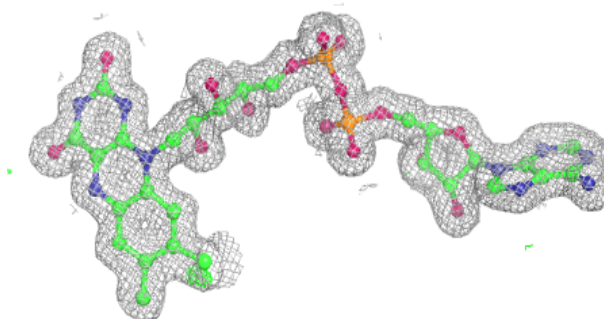
**Electron density around FAD AAA 601:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.