



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 01:28 am BST

PDB ID : 2BXS
Title : Human Monoamine Oxidase A in complex with Clorgyline, Crystal Form B
Authors : De Colibus, L.; Binda, C.; Edmondson, D.E.; Mattevi, A.
Deposited on : 2005-07-27
Resolution : 3.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

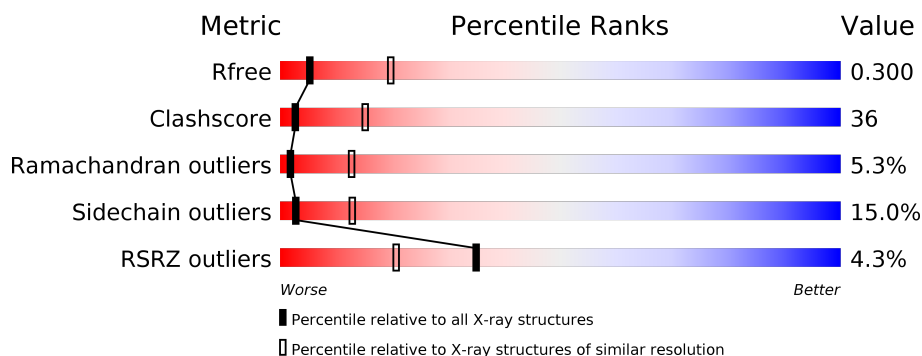
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	527	
1	B	527	

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
3	MLG	A	601	X	-	-	-
3	MLG	B	601	X	-	-	-

2 Entry composition [i](#)

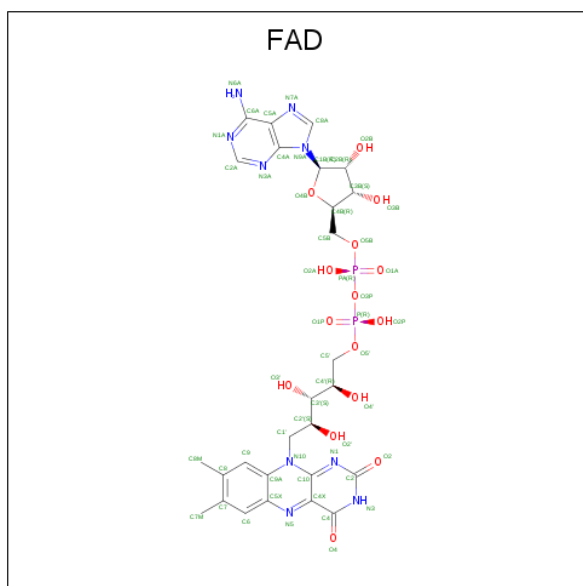
There are 3 unique types of molecules in this entry. The entry contains 7900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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] A.

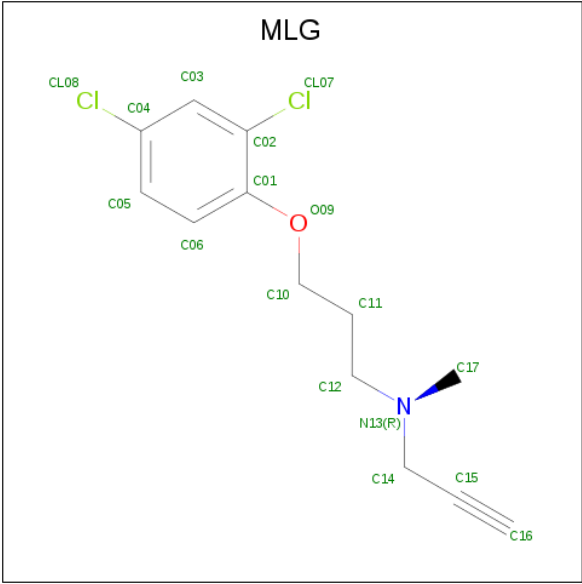
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3880	2482	660	717	21			
1	B	490	Total	C	N	O	S	0	0	0
			3880	2482	660	717	21			

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



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

- Molecule 3 is N-[3-(2,4-DICHLOROPHENOXY)PROPYL]-N-METHYL-N-PROP-2-YNYL AMINE (three-letter code: MLG) (formula: $C_{13}H_{15}Cl_2NO$).

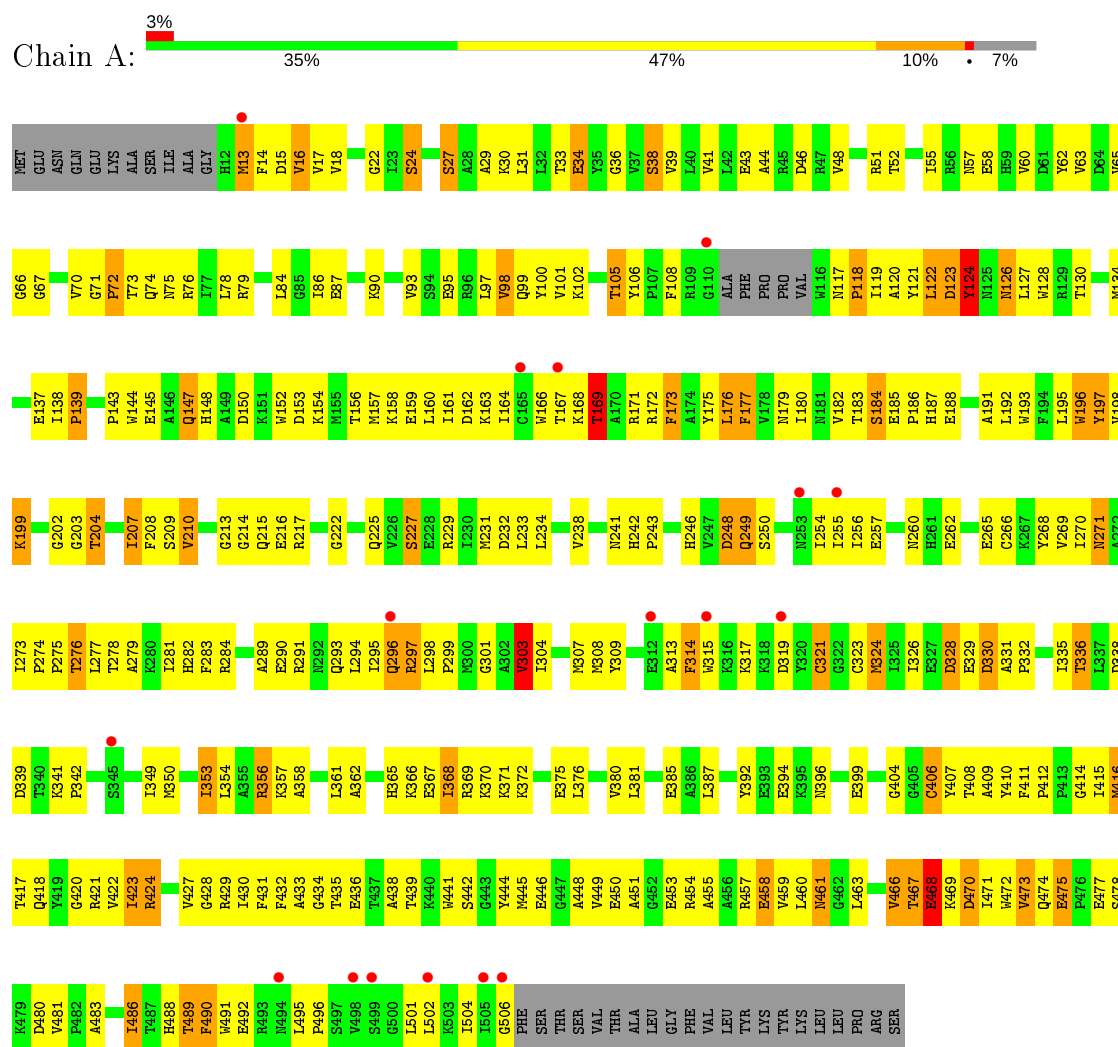


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		
3	B	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		

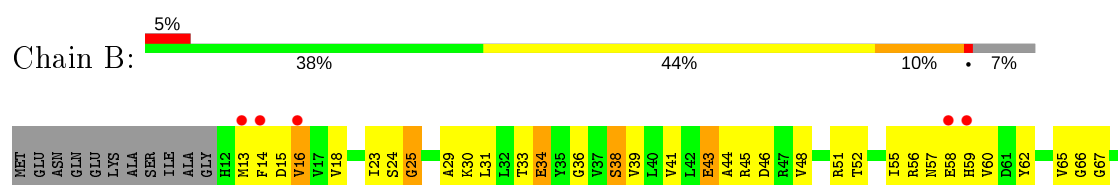
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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] A



• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] A



I504	V427	I349	P275	E137	V70
I505	G428	M350	T276	I138	G71
PHE	R429	L277	T278	P139	P72
SER	I430	I353	A279	P143	T73
THR	F431	L354	K280	I207	Q74
THR	F432	R355	I281	F208	N75
SER	A433	R356	H282	E145	R76
VAL	G434	K357	F283	A146	I77
THR	T435	A358	R284	Q147	
THR	E436			H148	
LEU		A362	R291	W152	L84
LEU	W441		N292	D153	G85
GLY	S442	H365	Q293	K154	I86
PHE	G443	K366	L294	M155	E87
VAL	G444	E367	I295	T156	T88
LEU	W445	I368	Q296	K157	Y89
TYR	M446	R369	R297	E159	K90
LYS	E447	K370	L298	L160	
LYS	A448	K371	P299	G222	V91
LEU		K372	M300	Q225	N92
LEU	A451	I373	G301	E226	V93
LEU	G452	C374	A302	S227	S94
PRO	E453	E375	V303	K163	E95
ARG	R454	L376	I304	I164	R96
SER	A455			G165	L97
	A456	L381	M307	W166	V98
	R457	G382	N308	T167	Q99
	E458	S383	Y309	K168	Y100
	V459	Q384	E312	T169	V101
	L460	E385	A313	R171	K102
	M461	E386	F314	F172	
		L387	W315	A174	T105
	V466	E394	K316	Y175	Y106
	T467	K395	K317	L176	P107
	K468	N396	K318	F177	F108
	D470	W397	D319	W178	R109
	I471	C398	T320	N179	G110
	W472	E399	G322	I180	ALA
	V473	E400	C323	W181	PHE
	Q474		M324	V182	PRO
	E475	T408	I325	S184	PRO
		A409	I326	E185	VAL
		Y410	E327	P186	W116
		F411	D328	H187	N117
	T487	P412	E261	E188	P118
	H488	G414	A331	S190	I119
	T489	I415	P332	L192	A120
	F490	M416	I335	W193	Y121
	W491	Q418	Y419	F194	L122
	E492	G420	R421	L195	D123
		P496	V422	W196	Y124
			I423	Y197	M125
			R424	V198	N126
				K199	L127
				I273	T130
				L274	I131
					D132
					M133
					M134
					G135
					K136

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.37Å 152.08Å 82.20Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	15.00 – 3.15 59.26 – 3.15	Depositor EDS
% Data completeness (in resolution range)	90.5 (15.00-3.15) 90.4 (59.26-3.15)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.268 , 0.330 0.253 , 0.300	Depositor DCC
R_{free} test set	1502 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 106.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	7900	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.51% 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: MLG, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	0/3973	0.84	1/5389 (0.0%)
1	B	0.81	1/3973 (0.0%)	0.82	2/5389 (0.0%)
All	All	0.82	1/7946 (0.0%)	0.83	3/10778 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	441	TRP	CB-CG	-5.02	1.41	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	ILE	CB-CA-C	5.56	122.73	111.60
1	B	353	ILE	N-CA-C	-5.09	97.26	111.00
1	A	303	VAL	CB-CA-C	-5.07	101.77	111.40

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	A	3880	0	3828	285	0
1	B	3880	0	3828	275	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	29	0	0
2	B	53	0	29	2	0
3	A	17	0	15	6	0
3	B	17	0	15	4	0
All	All	7900	0	7744	563	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 36.

The worst 5 of 563 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:B:408:THR:HG23	1:B:409:ALA:O	1.50	1.11
1:A:304:ILE:HB	1:A:353:ILE:CG2	1.90	1.02
1:A:304:ILE:HB	1:A:353:ILE:HG23	1.39	1.02
1:A:408:THR:HG23	1:A:409:ALA:O	1.59	1.01
1:B:422:VAL:O	1:B:424:ARG:N	1.96	0.99

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	486/527 (92%)	386 (79%)	73 (15%)	27 (6%)	2	12
1	B	486/527 (92%)	389 (80%)	72 (15%)	25 (5%)	2	13
All	All	972/1054 (92%)	775 (80%)	145 (15%)	52 (5%)	2	13

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	THR
1	A	204	THR
1	A	209	SER
1	A	314	PHE
1	A	366	LYS

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	A	412/450 (92%)	346 (84%)	66 (16%)	2	10
1	B	412/450 (92%)	354 (86%)	58 (14%)	3	15
All	All	824/900 (92%)	700 (85%)	124 (15%)	3	13

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	458	GLU
1	B	43	GLU
1	B	435	THR
1	A	461	ASN
1	A	475	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	GLN
1	B	133	ASN
1	B	365	HIS
1	A	494	ASN
1	B	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	A	600	1,3	51,58,58	1.36	9 (17%)	60,89,89	2.18	18 (30%)
3	MLG	A	601	2	16,17,17	2.79	4 (25%)	20,21,21	7.25	8 (40%)
2	FAD	B	600	1,3	51,58,58	1.61	7 (13%)	60,89,89	2.22	21 (35%)
3	MLG	B	601	2	16,17,17	2.49	2 (12%)	20,21,21	7.52	9 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	1,3	-	6/30/50/50	0/6/6/6
3	MLG	A	601	2	1/1/1/1	5/9/10/10	0/1/1/1
3	MLG	B	601	2	1/1/1/1	4/9/10/10	0/1/1/1
2	FAD	B	600	1,3	-	5/30/50/50	0/6/6/6

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	MLG	C14-C15	-7.88	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	MLG	C14-C15	-6.96	1.38	1.47
3	B	601	MLG	C15-C16	6.35	1.37	1.18
3	A	601	MLG	C15-C16	6.20	1.36	1.18
2	B	600	FAD	C2A-N3A	5.33	1.40	1.32

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	MLG	C14-C15-C16	-31.22	125.30	177.67
3	B	601	MLG	C14-C15-C16	-31.13	125.45	177.67
3	B	601	MLG	C01-C02-CL07	-6.87	111.36	119.43
2	A	600	FAD	C1'-N10-C10	6.35	124.09	118.41
2	B	600	FAD	C9A-C5X-N5	-5.69	113.46	122.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	MLG	N13
3	B	601	MLG	N13

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C2'-C1'-N10-C10
2	A	600	FAD	O3'-C3'-C4'-O4'
2	A	600	FAD	O3'-C3'-C4'-C5'
3	A	601	MLG	C15-C14-N13-C17
3	B	601	MLG	C10-C11-C12-N13

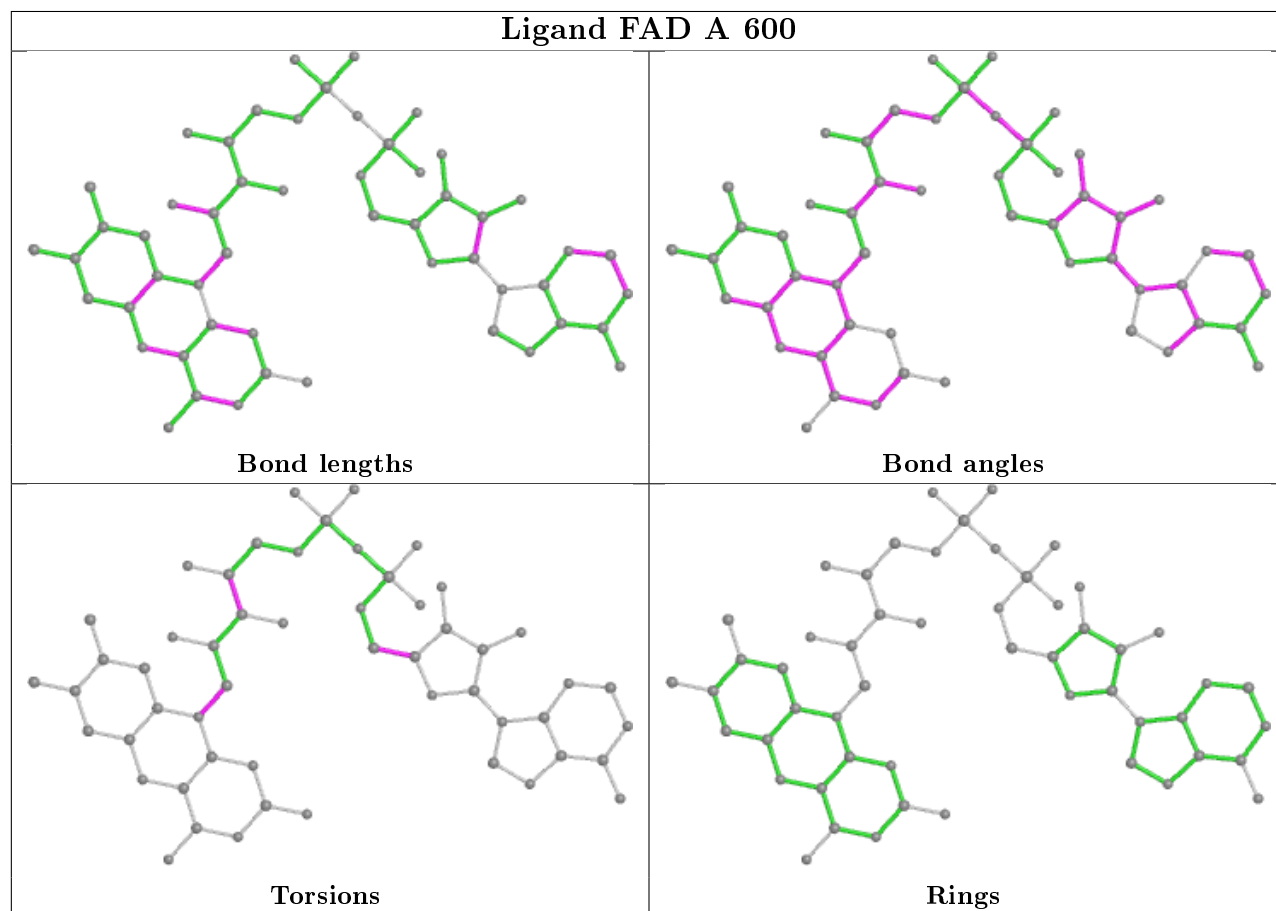
There are no ring outliers.

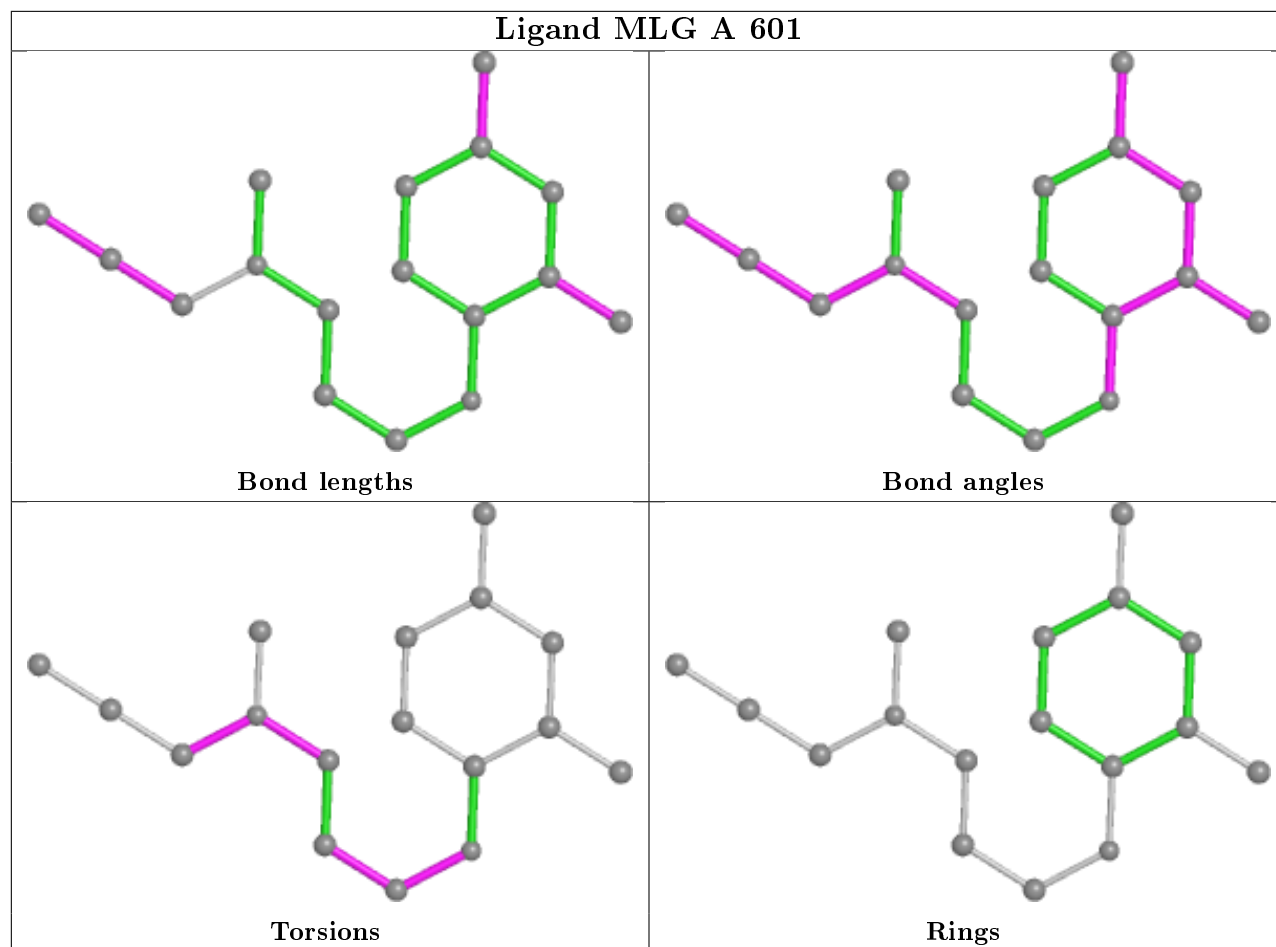
3 monomers are involved in 12 short contacts:

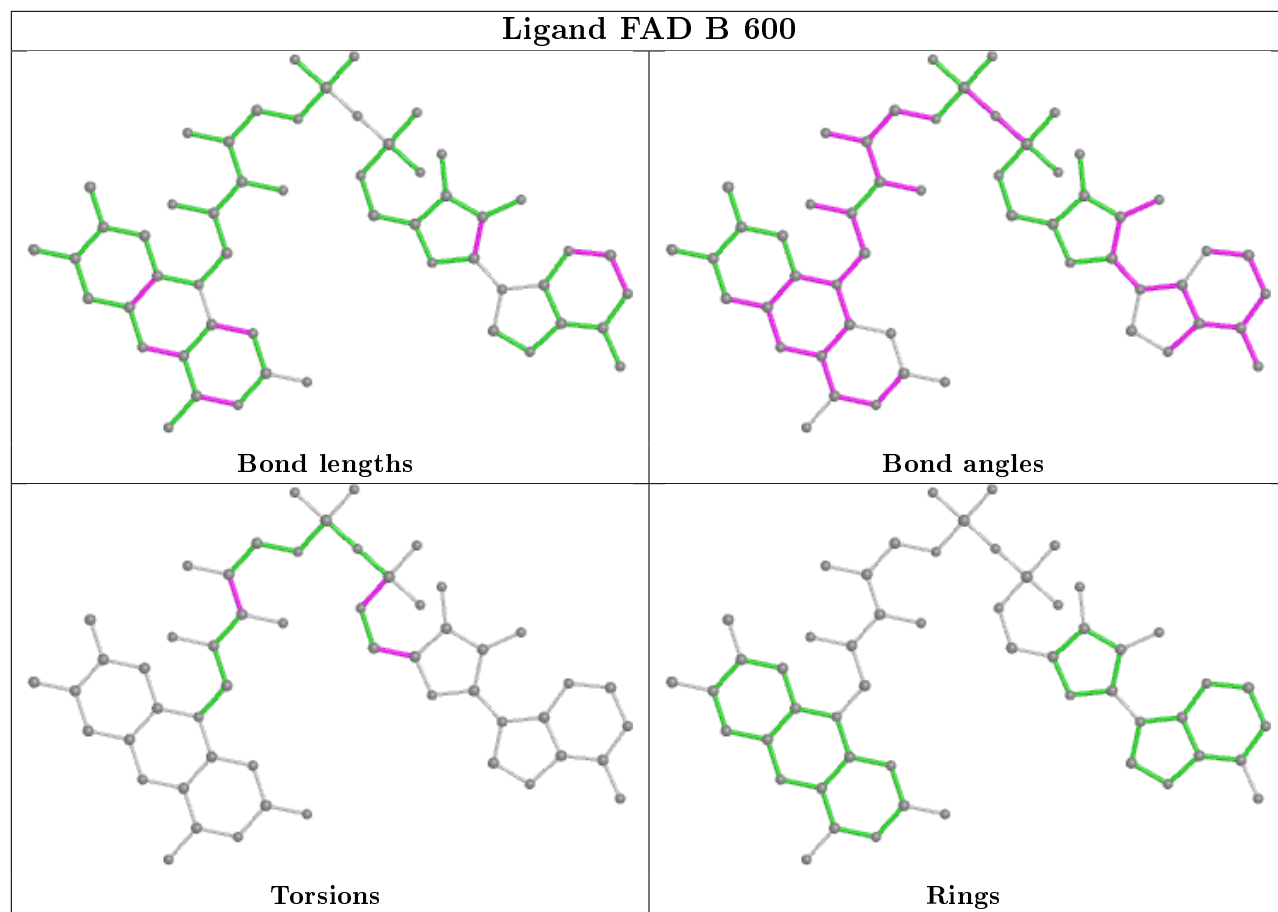
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	MLG	6	0
2	B	600	FAD	2	0
3	B	601	MLG	4	0

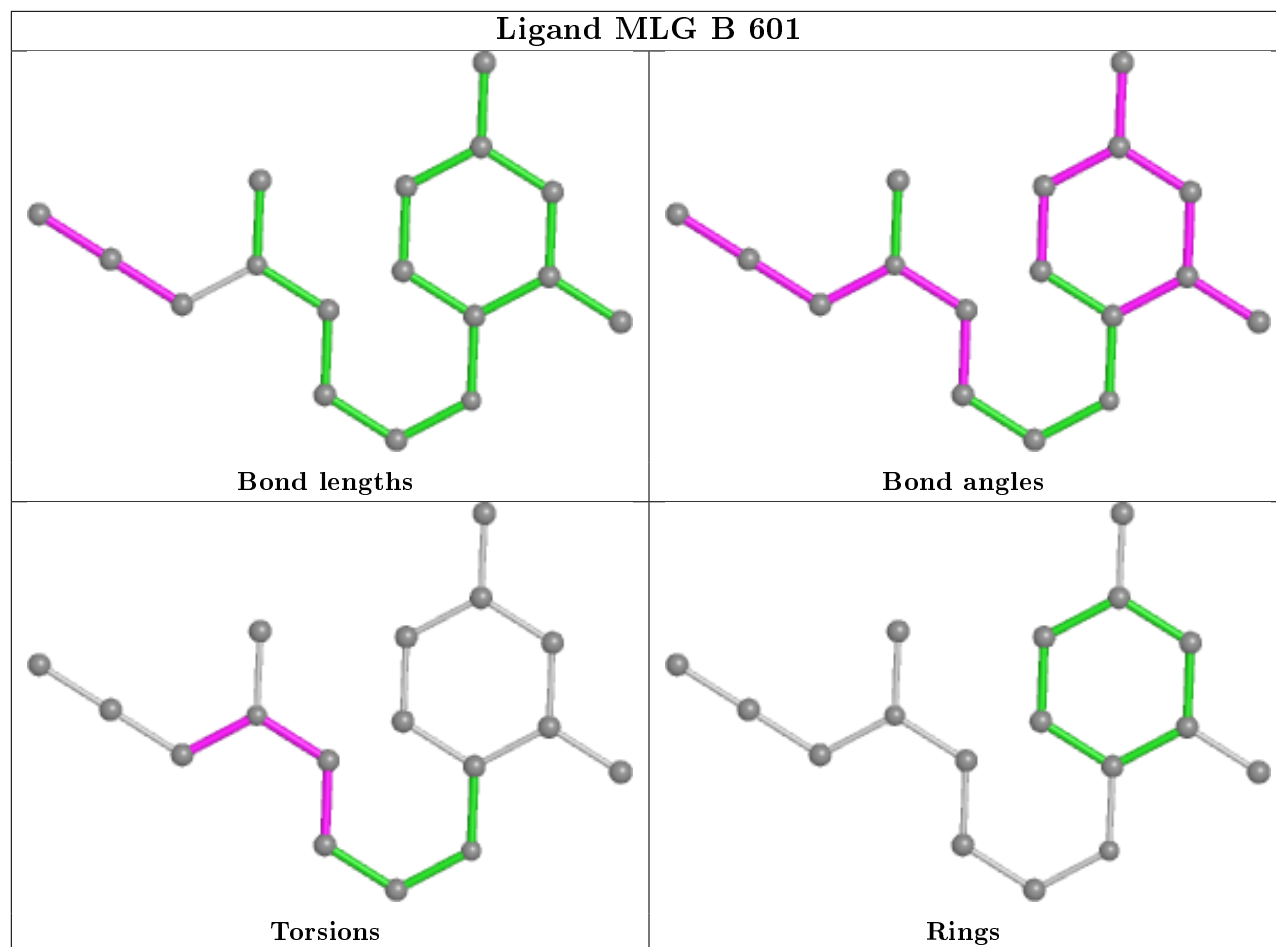
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	A	490/527 (92%)	0.09	17 (3%) 44 27	36, 38, 39, 41	0
1	B	490/527 (92%)	0.27	25 (5%) 28 15	36, 38, 39, 41	0
All	All	980/1054 (92%)	0.18	42 (4%) 35 21	36, 38, 39, 41	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	TRP	5.7
1	B	117	ASN	4.9
1	B	16	VAL	3.5
1	B	92	ASN	3.2
1	B	120	ALA	3.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

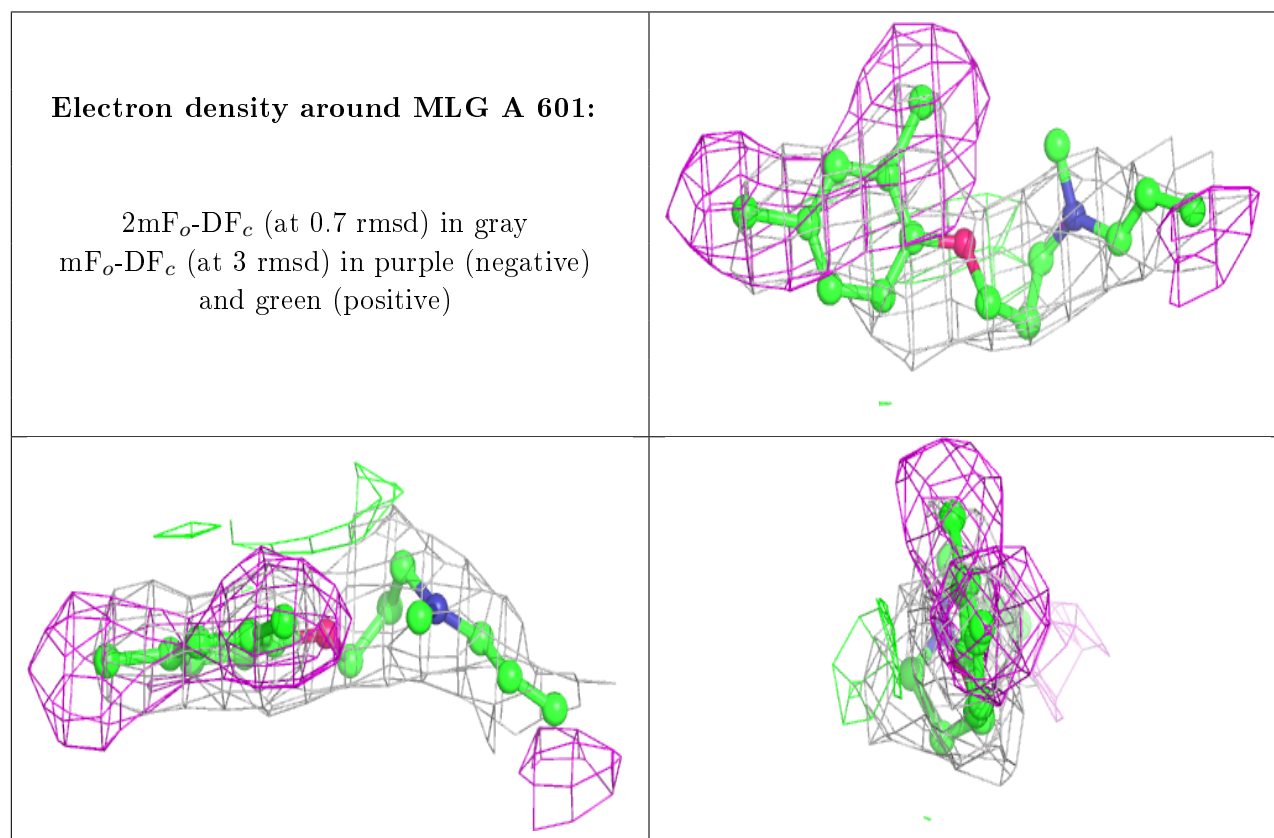
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

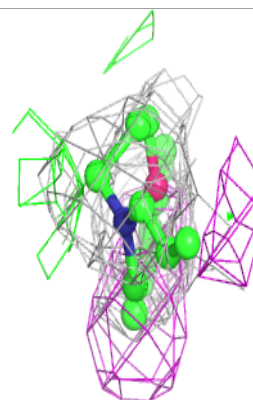
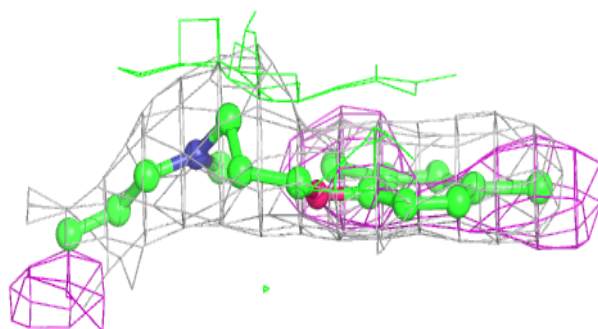
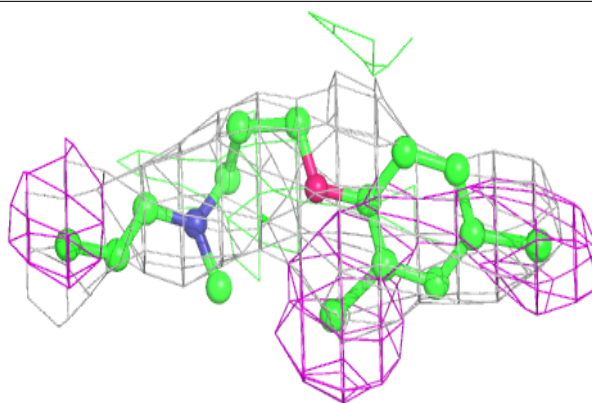
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MLG	A	601	17/17	0.82	0.36	44,54,62,65	0
3	MLG	B	601	17/17	0.83	0.40	46,56,63,64	0
2	FAD	B	600	53/53	0.96	0.17	25,32,40,43	0
2	FAD	A	600	53/53	0.97	0.14	26,32,37,43	0

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.

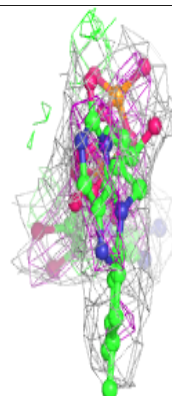
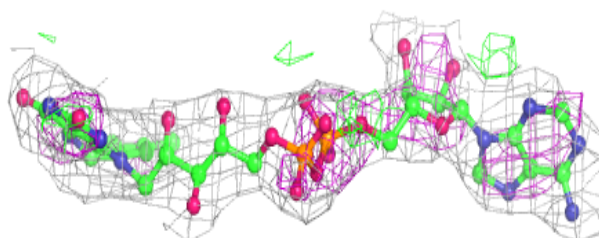
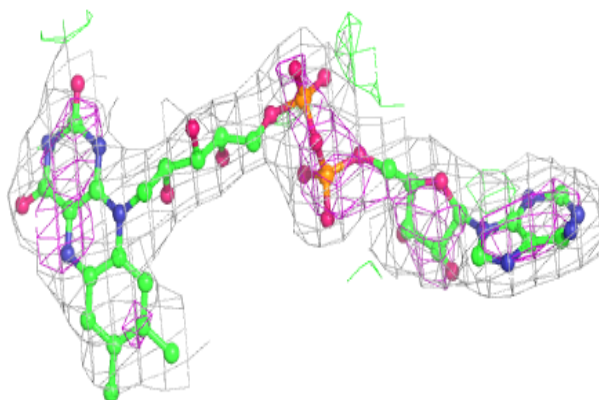


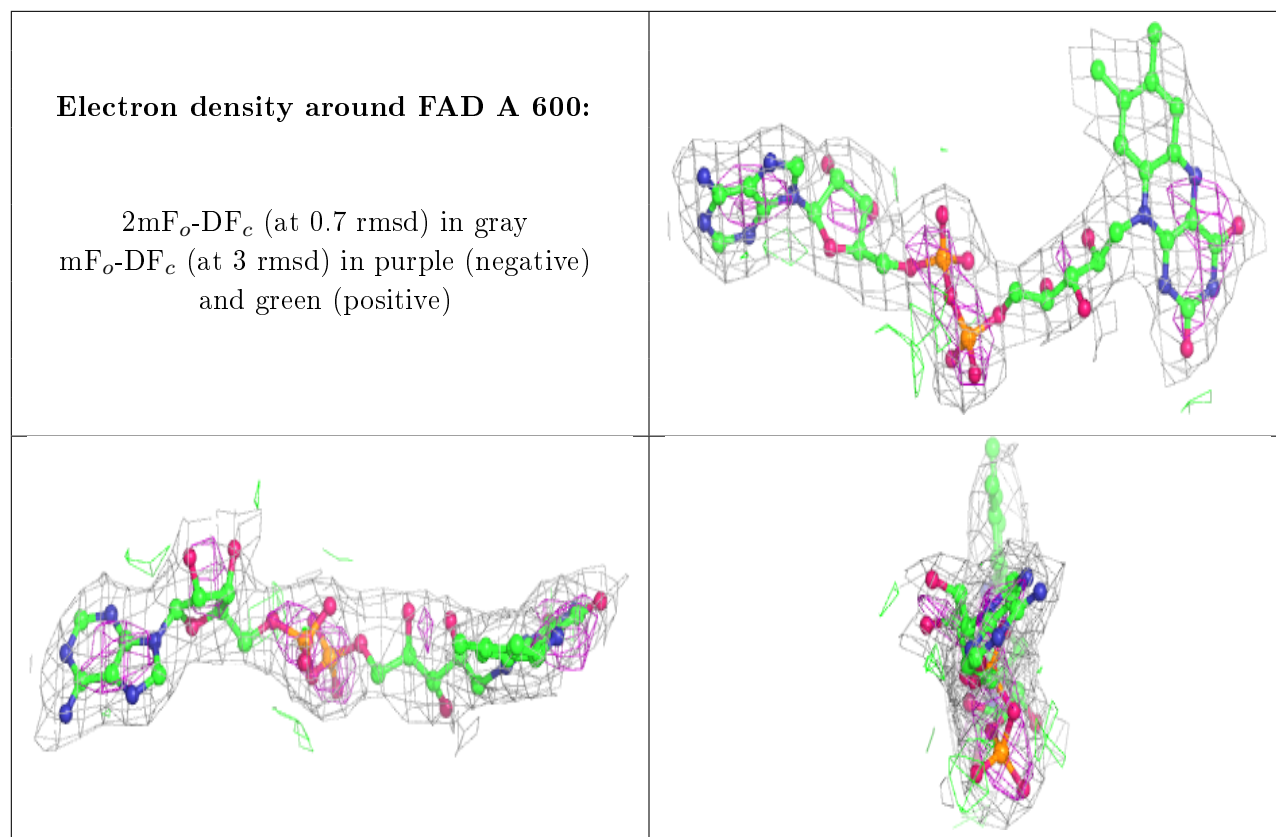
Electron density around MLG B 601:

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

**Electron density around FAD B 600:**

$2mF_o-DF_c$ (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.