wwPDB X-ray Structure Validation Summary Report (i)

Apr 21, 2024 – 11:34 pm BST

PDB ID	:	2VVL
Title	:	The structure of MAO-N-D3, a variant of monoamine oxidase from Aspergillus niger.
Authors	:	Atkin, K.E.; Hart, S.; Turkenburg, J.P.; Brzozowski, A.M.; Grogan, G.J.
Deposited on	:	2008-06-10
Resolution	:	2.45 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:

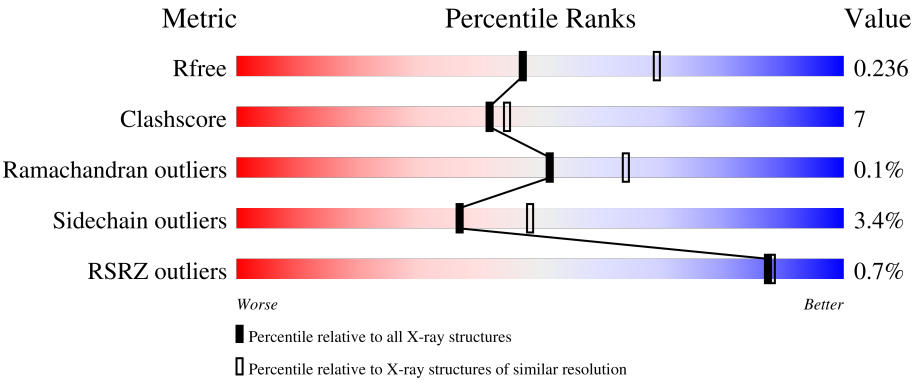
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	A	495	83% 12%
1	B	495	82% 12%
1	C	495	79% 15%
1	D	495	80% 14%
1	E	495	80% 15%

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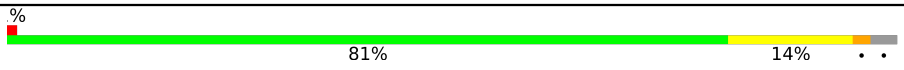
Mol	Chain	Length	Quality of chain
1	F	495	
1	H	495	
2	G	495	

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	FAD	A	600	X	-	-	-
3	FAD	B	600	X	-	-	-
3	FAD	C	600	X	-	-	-
3	FAD	D	600	X	-	-	-
3	FAD	E	600	X	-	-	-
3	FAD	F	600	X	-	-	-
3	FAD	G	600	X	-	-	-
3	FAD	H	600	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31496 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 MONOAMINE OXIDASE N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	29	1	0
			3782	2390	669	700	23			
1	B	476	Total	C	N	O	S	40	1	0
			3770	2382	667	698	23			
1	C	477	Total	C	N	O	S	43	1	0
			3778	2387	668	701	22			
1	D	478	Total	C	N	O	S	55	0	0
			3778	2387	666	702	23			
1	E	477	Total	C	N	O	S	50	1	0
			3777	2387	668	699	23			
1	F	478	Total	C	N	O	S	53	1	0
			3782	2389	669	702	22			
1	H	478	Total	C	N	O	S	60	1	0
			3785	2393	669	700	23			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	MET	ILE	engineered mutation	UNP P46882
A	336	SER	ASN	engineered mutation	UNP P46882
B	246	MET	ILE	engineered mutation	UNP P46882
B	336	SER	ASN	engineered mutation	UNP P46882
C	246	MET	ILE	engineered mutation	UNP P46882
C	336	SER	ASN	engineered mutation	UNP P46882
D	246	MET	ILE	engineered mutation	UNP P46882
D	336	SER	ASN	engineered mutation	UNP P46882
E	246	MET	ILE	engineered mutation	UNP P46882
E	336	SER	ASN	engineered mutation	UNP P46882
F	246	MET	ILE	engineered mutation	UNP P46882
F	336	SER	ASN	engineered mutation	UNP P46882
H	246	MET	ILE	engineered mutation	UNP P46882
H	336	SER	ASN	engineered mutation	UNP P46882
A	300	VAL	ALA	conflict	UNP P46882

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Chain	Residue	Modelled	Actual	Comment	Reference
A	304	VAL	LEU	conflict	UNP P46882
A	450	GLY	ARG	conflict	UNP P46882
B	300	VAL	ALA	conflict	UNP P46882
B	304	VAL	LEU	conflict	UNP P46882
B	450	GLY	ARG	conflict	UNP P46882
C	300	VAL	ALA	conflict	UNP P46882
C	304	VAL	LEU	conflict	UNP P46882
C	450	GLY	ARG	conflict	UNP P46882
D	300	VAL	ALA	conflict	UNP P46882
D	304	VAL	LEU	conflict	UNP P46882
D	450	GLY	ARG	conflict	UNP P46882
E	300	VAL	ALA	conflict	UNP P46882
E	304	VAL	LEU	conflict	UNP P46882
E	450	GLY	ARG	conflict	UNP P46882
F	300	VAL	ALA	conflict	UNP P46882
F	304	VAL	LEU	conflict	UNP P46882
F	450	GLY	ARG	conflict	UNP P46882
H	300	VAL	ALA	conflict	UNP P46882
H	304	VAL	LEU	conflict	UNP P46882
H	450	GLY	ARG	conflict	UNP P46882

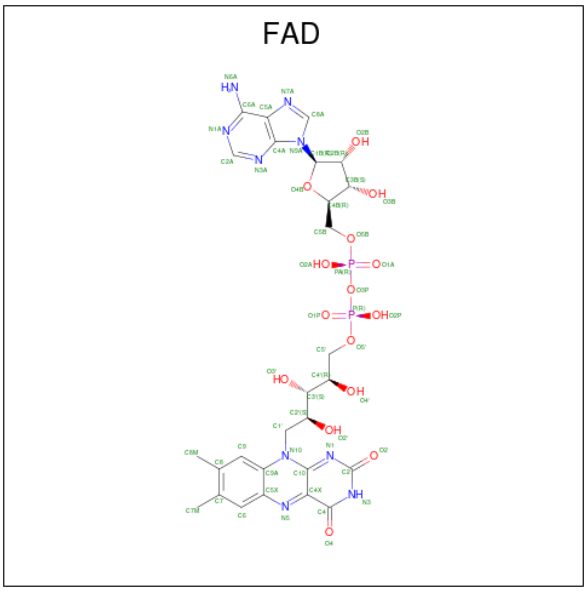
- Molecule 2 is a protein called MONOAMINE OXIDASE N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	478	3785	2392	669	701	23	46	1	0

There are 6 discrepancies between the modelled and reference sequences:

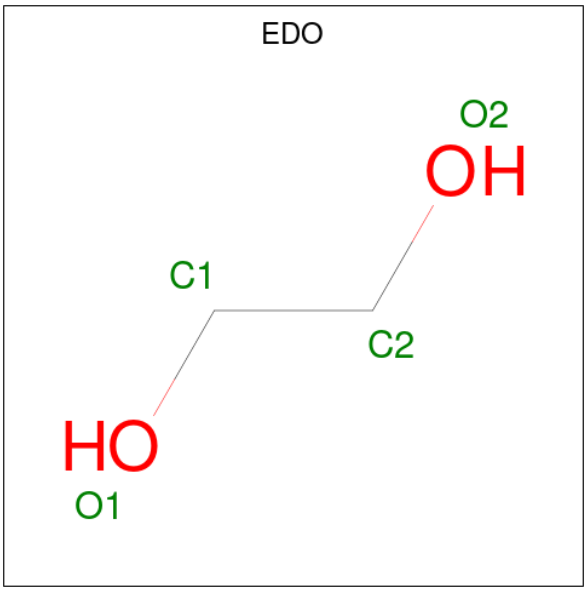
Chain	Residue	Modelled	Actual	Comment	Reference
G	246	MET	ILE	engineered mutation	UNP P46882
G	336	SER	ASN	engineered mutation	UNP P46882
G	20	THR	PRO	conflict	UNP P46882
G	300	VAL	ALA	conflict	UNP P46882
G	304	VAL	LEU	conflict	UNP P46882
G	450	GLY	ARG	conflict	UNP P46882

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	118	Total O 118 118	0	0
5	B	134	Total O 134 134	0	0
5	C	95	Total O 95 95	0	0
5	D	102	Total O 102 102	0	0
5	E	122	Total O 122 122	0	0

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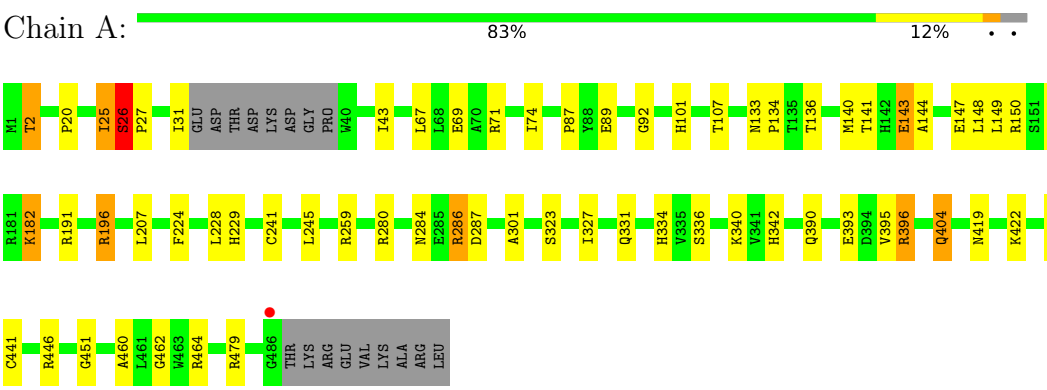
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	103	Total O 103 103	0	0
5	G	53	Total O 53 53	0	0
5	H	80	Total O 80 80	0	0

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.

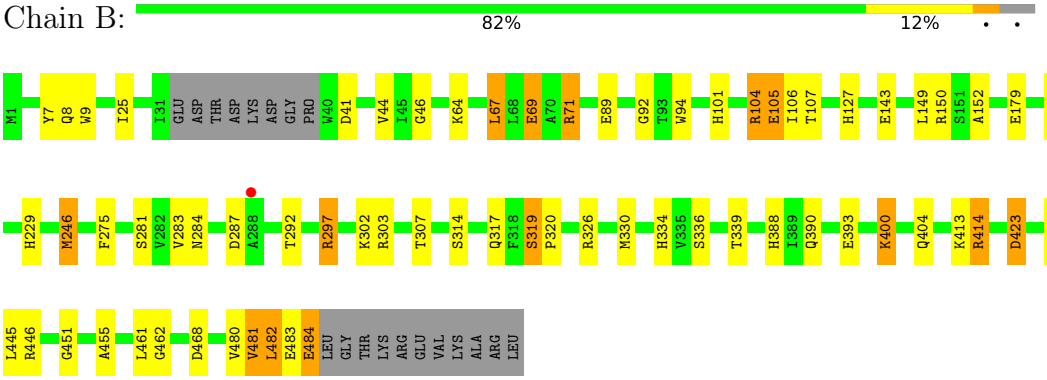
• Molecule 1: MONOAMINE OXIDASE N

Chain A:



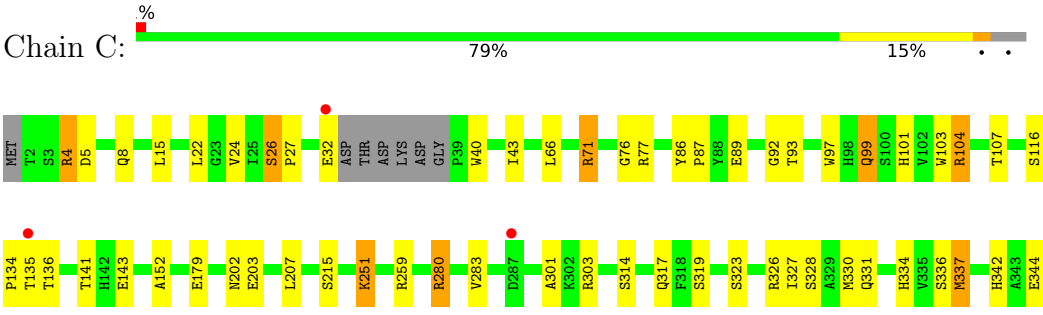
• Molecule 1: MONOAMINE OXIDASE N

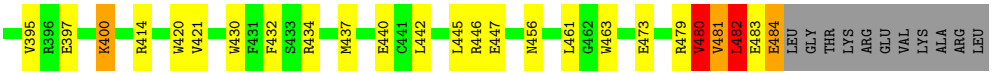
Chain B:



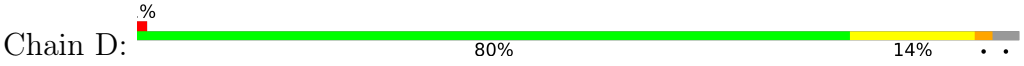
• Molecule 1: MONOAMINE OXIDASE N

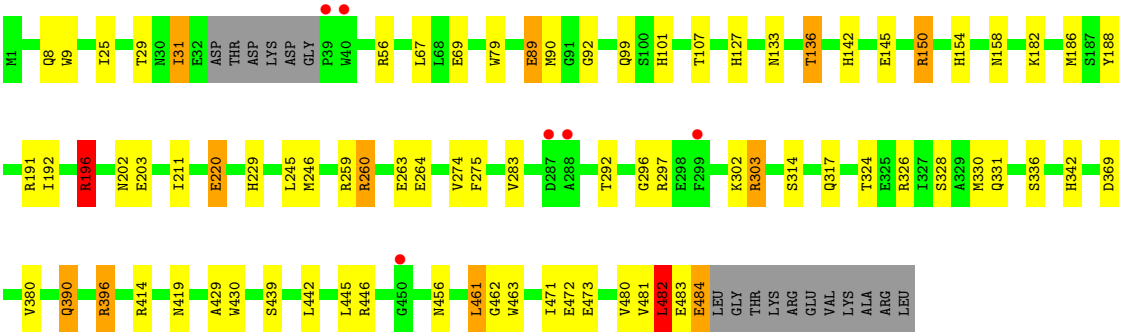
Chain C:



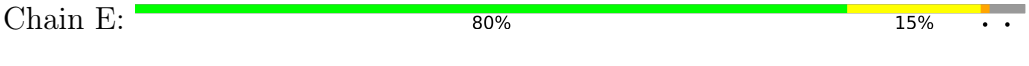


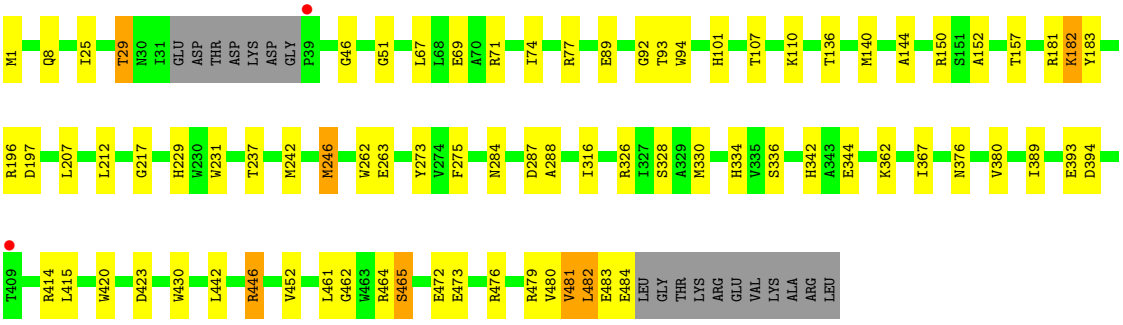
• Molecule 1: MONOAMINE OXIDASE N



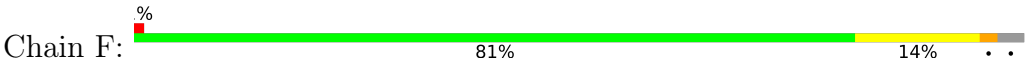


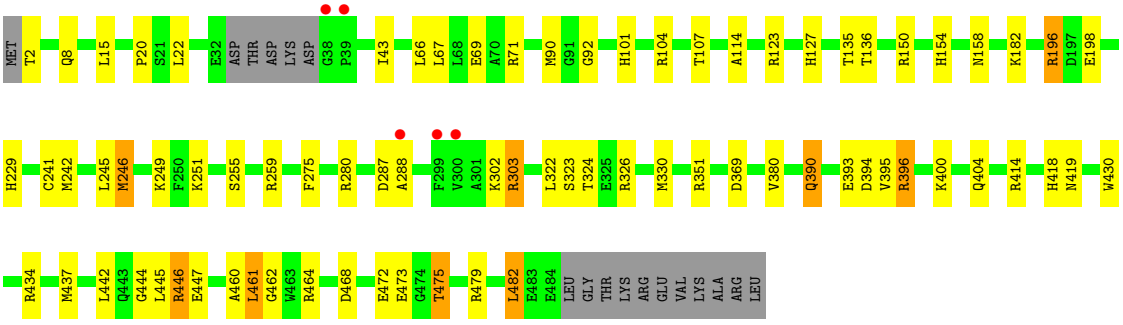
• Molecule 1: MONOAMINE OXIDASE N



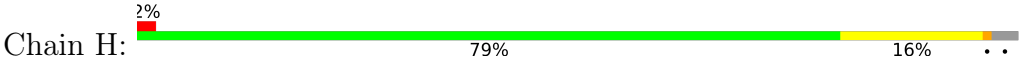


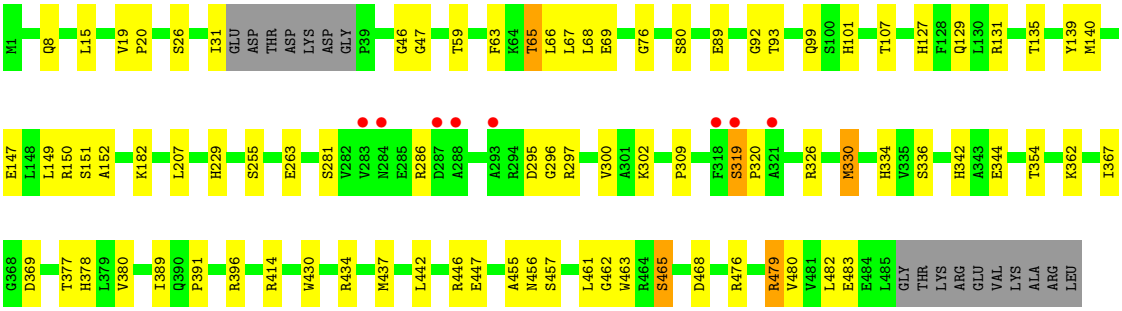
• Molecule 1: MONOAMINE OXIDASE N





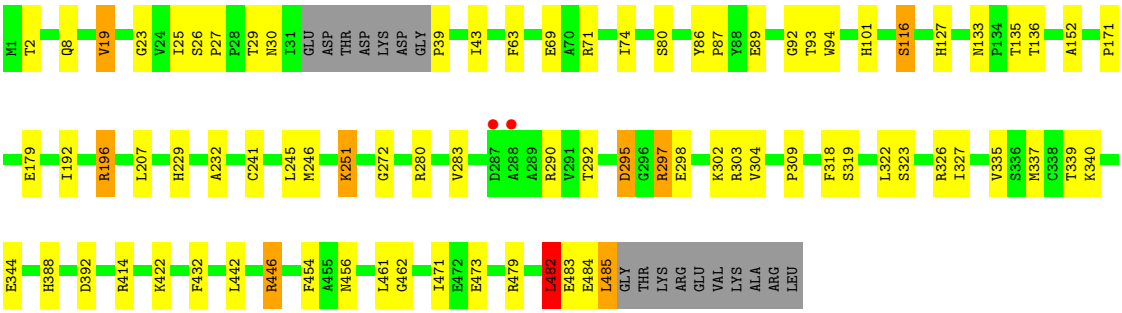
• Molecule 1: MONOAMINE OXIDASE N





• Molecule 2: MONOAMINE OXIDASE N

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.29Å 187.25Å 132.43Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	132.45 – 2.45 49.53 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (132.45-2.45) 97.2 (49.53-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.85 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.4.0065	Depositor
R, R_{free}	0.182 , 0.236 0.190 , 0.236	Depositor DCC
R_{free} test set	9016 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.148 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31496	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 3.22% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 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	0.95	6/3885 (0.2%)	0.82	4/5266 (0.1%)
1	B	0.97	8/3873 (0.2%)	0.92	17/5250 (0.3%)
1	C	0.89	7/3882 (0.2%)	0.87	10/5263 (0.2%)
1	D	0.92	6/3879 (0.2%)	0.84	9/5259 (0.2%)
1	E	0.84	6/3881 (0.2%)	0.80	11/5261 (0.2%)
1	F	0.87	5/3886 (0.1%)	0.89	15/5269 (0.3%)
1	H	0.91	9/3889 (0.2%)	0.79	9/5272 (0.2%)
2	G	0.91	6/3888 (0.2%)	0.80	8/5270 (0.2%)
All	All	0.91	53/31063 (0.2%)	0.84	83/42110 (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	4
1	B	0	2
1	C	0	2
1	D	0	2
1	F	0	1
1	H	0	1
All	All	0	12

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	483	GLU	C-N	-13.38	1.03	1.34
1	C	4	ARG	C-N	-9.81	1.11	1.34
1	H	455	ALA	C-N	-9.05	1.13	1.34
1	H	67	LEU	C-N	-9.02	1.13	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	ARG	C-N	-8.99	1.13	1.34

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	136	THR	O-C-N	-16.38	96.49	122.70
1	B	297	ARG	O-C-N	16.17	148.58	122.70
1	F	150[A]	ARG	NE-CZ-NH1	-13.08	113.76	120.30
1	F	150[B]	ARG	NE-CZ-NH1	-13.08	113.76	120.30
1	F	150[A]	ARG	NE-CZ-NH2	12.14	126.37	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ARG	Mainchain
1	A	25	ILE	Peptide
1	A	26	SER	Peptide
1	A	440	GLU	Mainchain
1	B	150[A]	ARG	Sidechain

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	3782	0	3629	42	0
1	B	3770	0	3615	57	0
1	C	3778	0	3613	65	0
1	D	3778	0	3616	50	0
1	E	3777	0	3623	54	0
1	F	3782	0	3617	49	0
1	H	3785	0	3630	52	0
2	G	3785	0	3633	47	0
3	A	53	0	30	5	0
3	B	53	0	30	4	0
3	C	53	0	30	5	0
3	D	53	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	53	0	31	4	0
3	F	53	0	30	4	0
3	G	53	0	31	5	0
3	H	53	0	30	4	0
4	A	4	0	6	0	0
4	C	8	0	12	1	0
4	D	4	0	6	0	0
4	F	4	0	6	0	0
4	G	8	0	12	3	0
5	A	118	0	0	1	0
5	B	134	0	0	1	0
5	C	95	0	0	0	0
5	D	102	0	0	2	0
5	E	122	0	0	1	0
5	F	103	0	0	1	0
5	G	53	0	0	0	0
5	H	80	0	0	1	0
All	All	31496	0	29260	414	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 7.

The worst 5 of 414 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:C:481:VAL:C	1:C:482:LEU:HD12	1.44	1.36
1:B:483:GLU:O	1:B:484:GLU:HG2	1.40	1.20
1:B:482:LEU:HD12	1:B:482:LEU:N	1.69	1.06
1:D:483:GLU:O	1:D:484:GLU:HB3	1.49	1.05
1:C:481:VAL:O	1:C:482:LEU:HD12	1.55	1.04

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	475/495 (96%)	454 (96%)	20 (4%)	1 (0%)	47 57
1	B	473/495 (96%)	457 (97%)	16 (3%)	0	100 100
1	C	474/495 (96%)	453 (96%)	19 (4%)	2 (0%)	34 41
1	D	474/495 (96%)	458 (97%)	16 (3%)	0	100 100
1	E	474/495 (96%)	451 (95%)	22 (5%)	1 (0%)	47 57
1	F	475/495 (96%)	456 (96%)	19 (4%)	0	100 100
1	H	475/495 (96%)	460 (97%)	15 (3%)	0	100 100
2	G	475/495 (96%)	449 (94%)	26 (6%)	0	100 100
All	All	3795/3960 (96%)	3638 (96%)	153 (4%)	4 (0%)	51 64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	E	481	VAL
1	C	481	VAL
1	C	179	GLU

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	400/414 (97%)	386 (96%)	14 (4%)	36 47
1	B	399/414 (96%)	390 (98%)	9 (2%)	50 63
1	C	400/414 (97%)	383 (96%)	17 (4%)	29 38
1	D	400/414 (97%)	384 (96%)	16 (4%)	31 41
1	E	400/414 (97%)	388 (97%)	12 (3%)	41 52
1	F	400/414 (97%)	387 (97%)	13 (3%)	38 49
1	H	401/414 (97%)	385 (96%)	16 (4%)	31 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	401/414 (97%)	387 (96%)	14 (4%)	36 47
All	All	3201/3312 (97%)	3090 (96%)	111 (4%)	37 47

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	29	THR
1	H	482	LEU
1	F	182	LYS
1	H	479[B]	ARG
1	H	149	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	8	GLN
1	H	404	GLN
1	F	8	GLN
1	H	342	HIS
1	H	101	HIS

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)

15 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	FAD	F	600	-	53,58,58	1.63	6 (11%)	68,89,89	2.21	19 (27%)
3	FAD	B	600	-	53,58,58	1.65	5 (9%)	68,89,89	2.64	20 (29%)
3	FAD	E	600	-	53,58,58	1.72	6 (11%)	68,89,89	2.35	21 (30%)
3	FAD	H	600	-	53,58,58	1.60	4 (7%)	68,89,89	2.26	22 (32%)
4	EDO	F	601	-	3,3,3	0.41	0	2,2,2	0.65	0
3	FAD	D	600	-	53,58,58	1.51	5 (9%)	68,89,89	2.30	17 (25%)
3	FAD	C	600	-	53,58,58	1.48	3 (5%)	68,89,89	2.27	18 (26%)
3	FAD	A	600	-	53,58,58	1.44	6 (11%)	68,89,89	2.42	19 (27%)
3	FAD	G	600	-	53,58,58	1.51	5 (9%)	68,89,89	2.36	19 (27%)
4	EDO	G	602	-	3,3,3	0.49	0	2,2,2	0.38	0
4	EDO	G	601	-	3,3,3	0.44	0	2,2,2	0.79	0
4	EDO	C	601	-	3,3,3	0.41	0	2,2,2	0.65	0
4	EDO	D	601	-	3,3,3	0.43	0	2,2,2	0.22	0
4	EDO	C	602	-	3,3,3	0.48	0	2,2,2	0.39	0
4	EDO	A	601	-	3,3,3	0.45	0	2,2,2	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	F	600	-	3/3/9/9	11/30/50/50	0/6/6/6
3	FAD	B	600	-	3/3/9/9	9/30/50/50	0/6/6/6
3	FAD	E	600	-	3/3/9/9	13/30/50/50	0/6/6/6
3	FAD	H	600	-	3/3/9/9	10/30/50/50	0/6/6/6
4	EDO	F	601	-	-	1/1/1/1	-
3	FAD	D	600	-	3/3/9/9	10/30/50/50	0/6/6/6
3	FAD	C	600	-	3/3/9/9	9/30/50/50	0/6/6/6
3	FAD	A	600	-	3/3/9/9	11/30/50/50	0/6/6/6
3	FAD	G	600	-	3/3/9/9	18/30/50/50	0/6/6/6
4	EDO	G	602	-	-	1/1/1/1	-
4	EDO	G	601	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	601	-	-	1/1/1/1	-
4	EDO	D	601	-	-	1/1/1/1	-
4	EDO	C	602	-	-	1/1/1/1	-
4	EDO	A	601	-	-	1/1/1/1	-

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	600	FAD	O4B-C1B	7.27	1.51	1.41
3	H	600	FAD	O4B-C1B	6.93	1.50	1.41
3	B	600	FAD	C4X-N5	6.87	1.44	1.30
3	F	600	FAD	C4X-N5	6.74	1.43	1.30
3	E	600	FAD	C4X-N5	6.52	1.43	1.30

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	600	FAD	C3B-C2B-C1B	-9.80	86.22	100.98
3	B	600	FAD	C3B-C2B-C1B	-9.41	86.82	100.98
3	A	600	FAD	C3B-C2B-C1B	-8.99	87.44	100.98
3	E	600	FAD	C3B-C2B-C1B	-8.97	87.47	100.98
3	A	600	FAD	C2B-C3B-C4B	-8.66	85.82	102.64

5 of 24 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	600	FAD	C3B
3	A	600	FAD	C4B
3	A	600	FAD	C2'
3	B	600	FAD	C3B
3	B	600	FAD	C4B

5 of 98 torsion outliers are listed below:

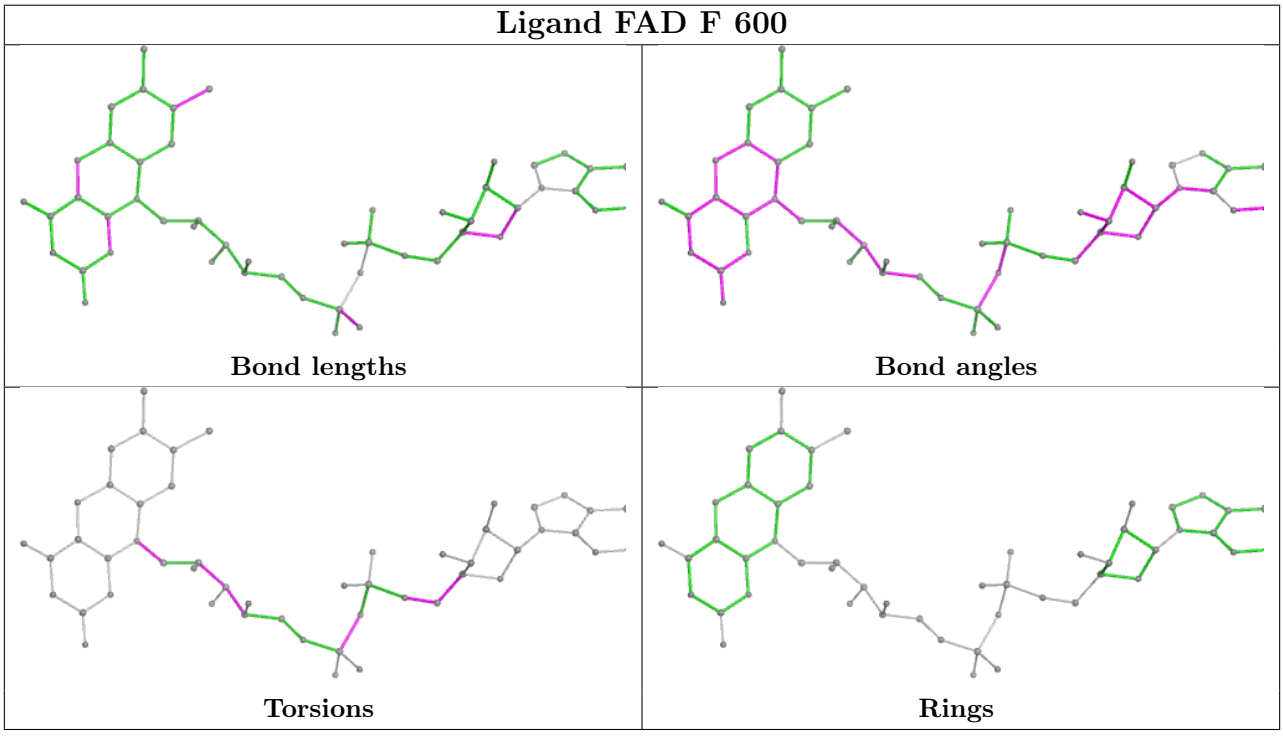
Mol	Chain	Res	Type	Atoms
3	A	600	FAD	C1'-C2'-C3'-O3'
3	A	600	FAD	C1'-C2'-C3'-C4'
3	A	600	FAD	O2'-C2'-C3'-O3'
3	A	600	FAD	O2'-C2'-C3'-C4'
3	A	600	FAD	PA-O3P-P-O5'

There are no ring outliers.

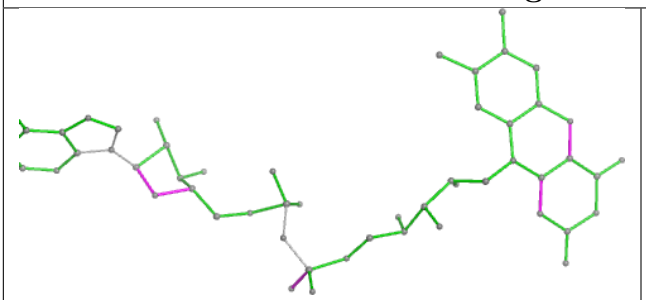
10 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	600	FAD	4	0
3	B	600	FAD	4	0
3	E	600	FAD	4	0
3	H	600	FAD	4	0
3	D	600	FAD	5	0
3	C	600	FAD	5	0
3	A	600	FAD	5	0
3	G	600	FAD	5	0
4	G	601	EDO	3	0
4	C	601	EDO	1	0

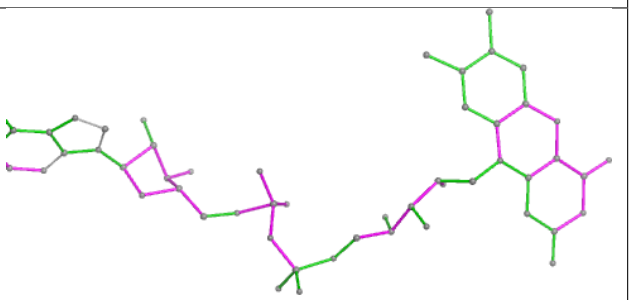
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



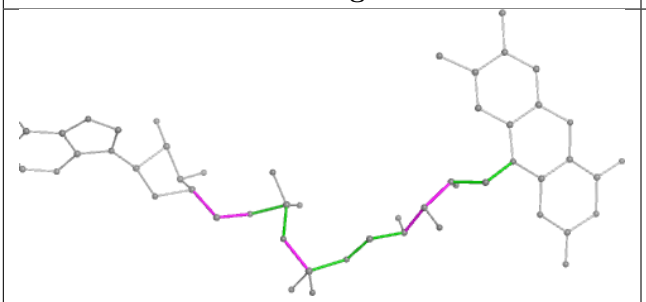
Ligand FAD B 600



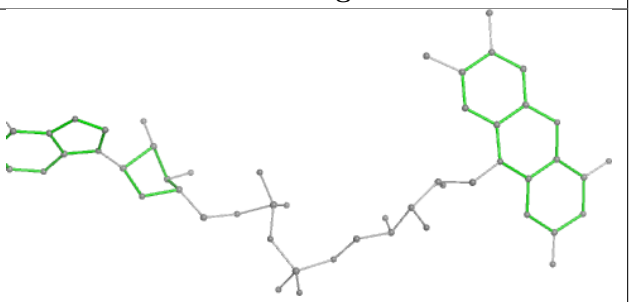
Bond lengths



Bond angles

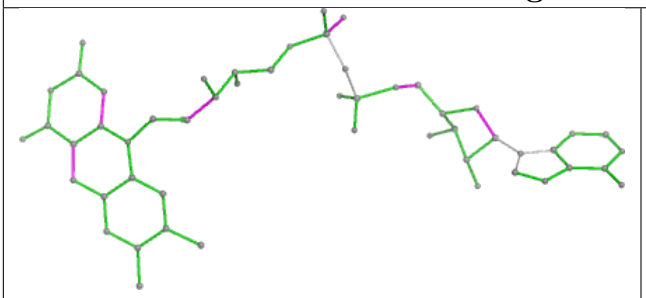


Torsions

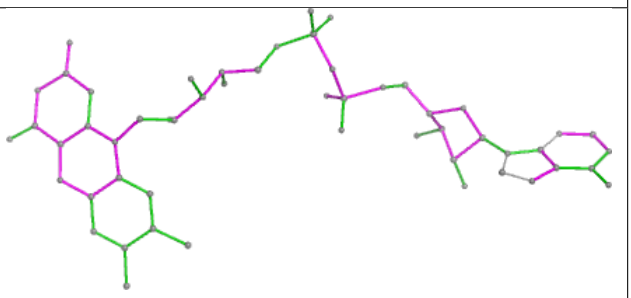


Rings

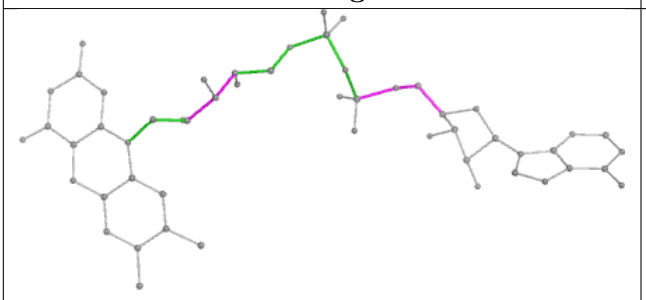
Ligand FAD E 600



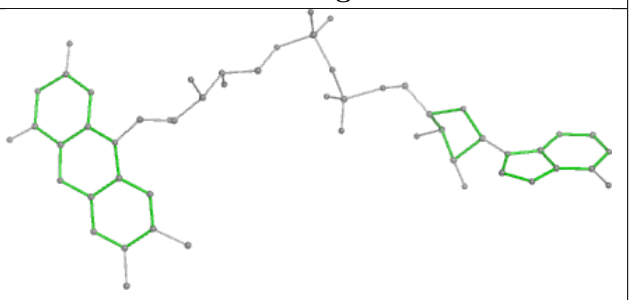
Bond lengths



Bond angles

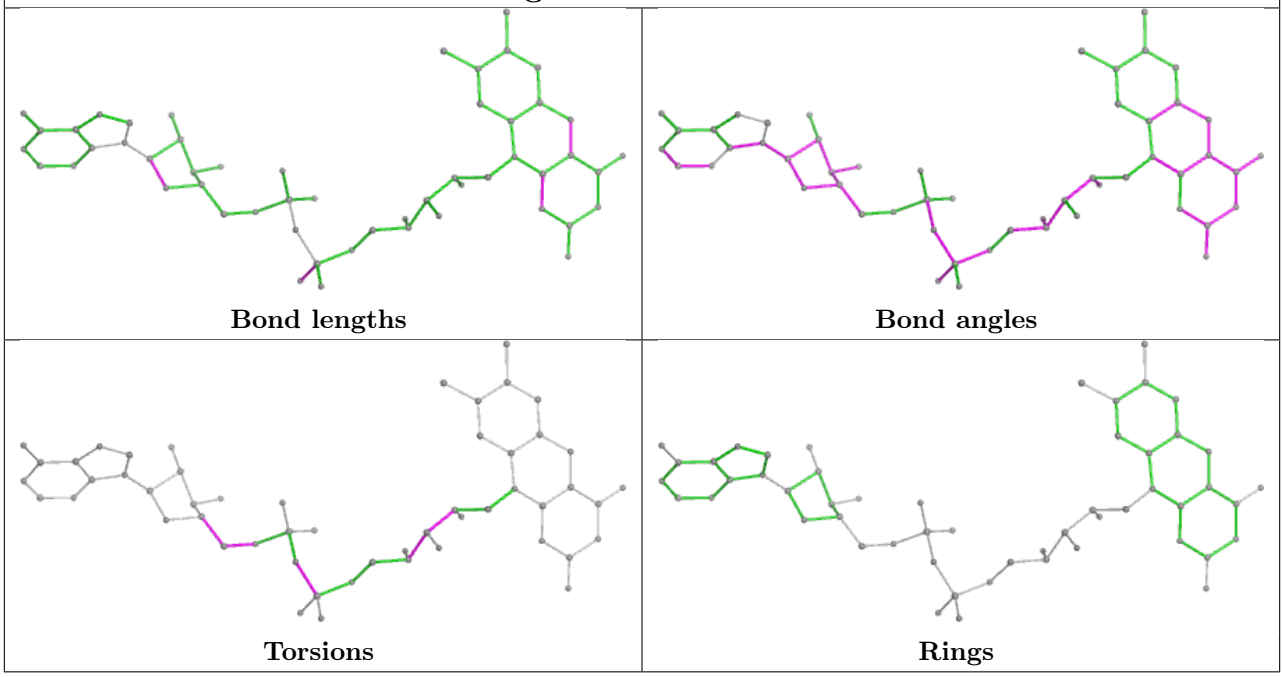


Torsions

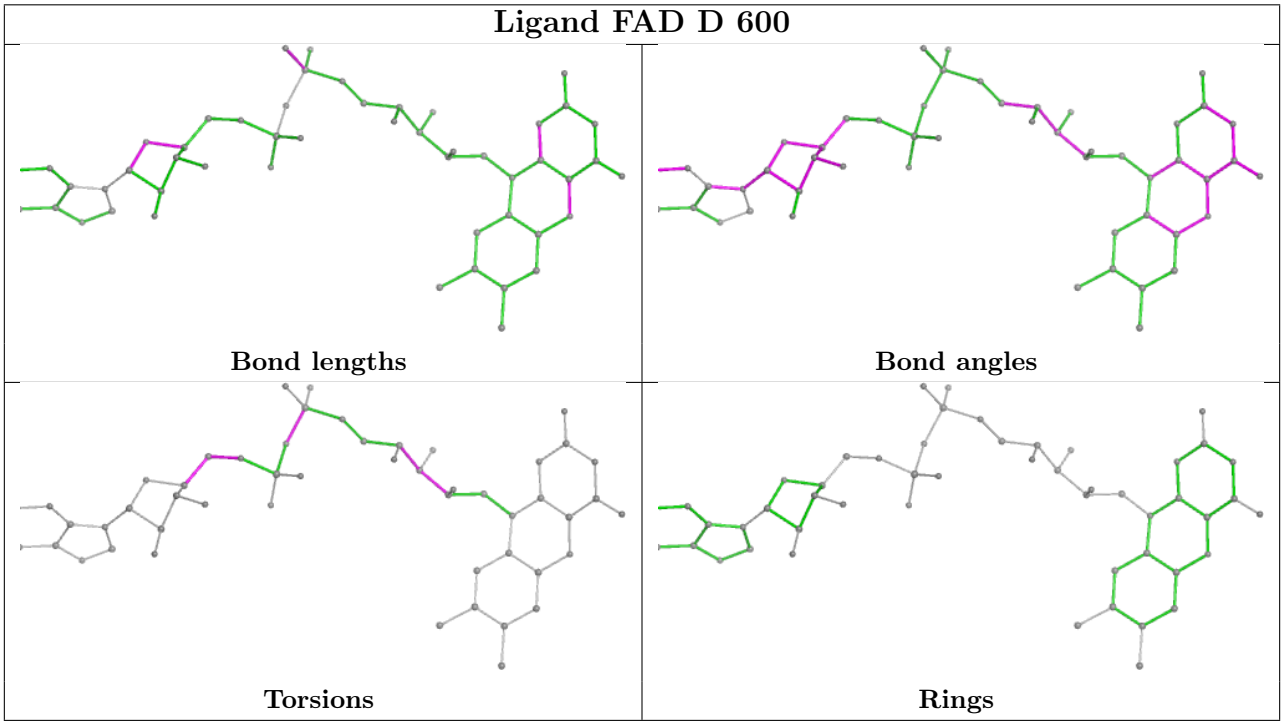


Rings

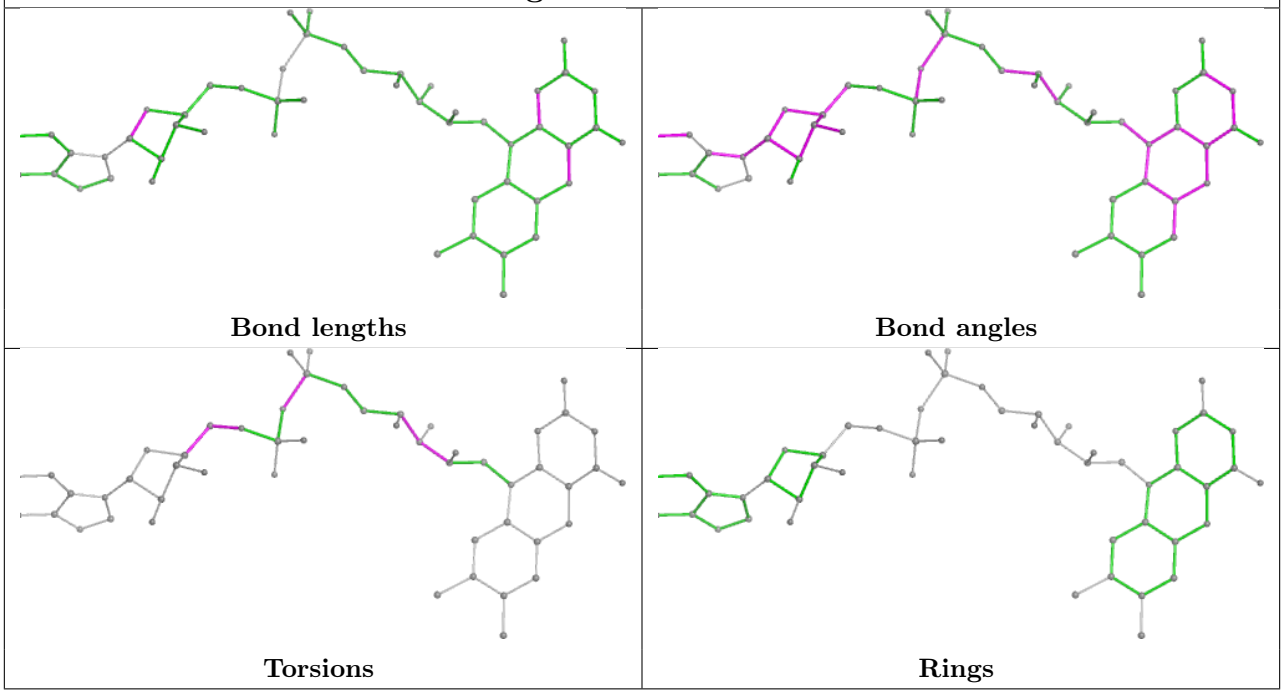
Ligand FAD H 600



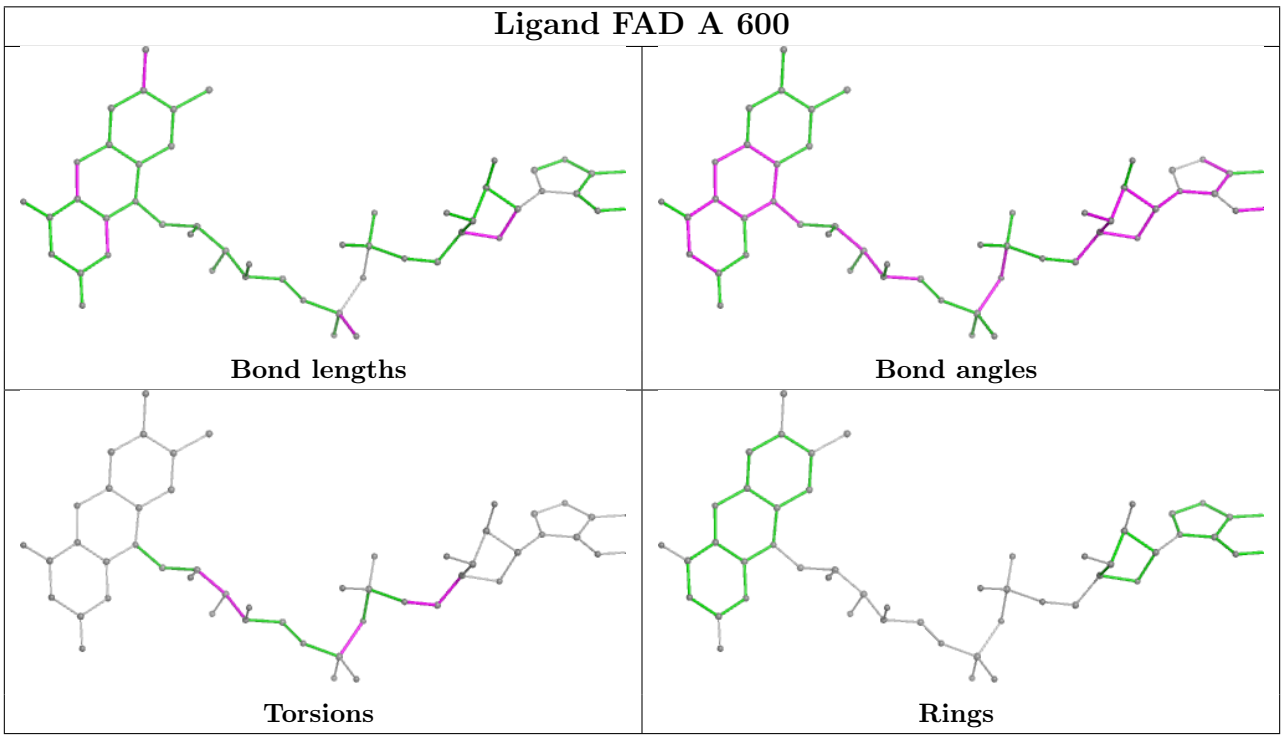
Ligand FAD D 600



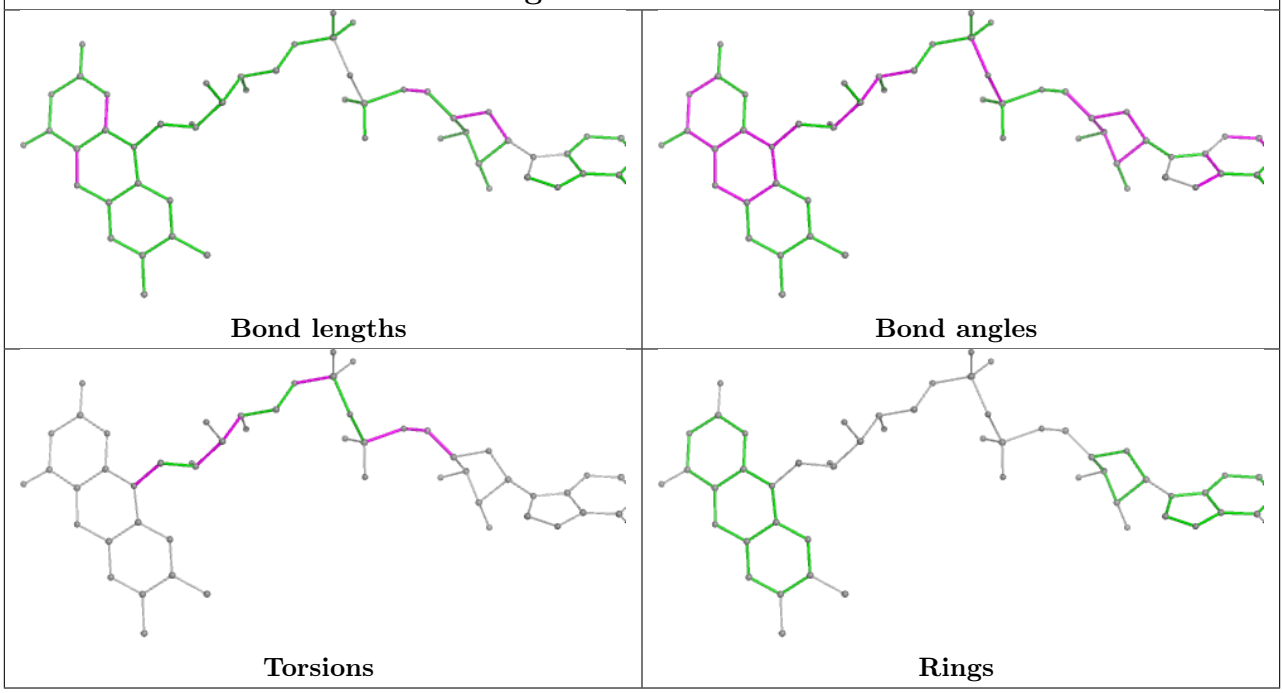
Ligand FAD C 600



Ligand FAD A 600



Ligand FAD G 600



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	4
1	H	4
1	B	3
2	G	3
1	E	2
1	A	2
1	F	1
1	D	1

The worst 5 of 20 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	7:TYR	C	8:GLN	N	1.20
1	C	99:GLN	C	100:SER	N	1.20
1	E	393:GLU	C	394:ASP	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	394:ASP	C	395:VAL	N	1.19
1	G	303:ARG	C	304:VAL	N	1.19

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	A	478/495 (96%)	-0.60	1 (0%)	95	95	9, 19, 30, 47	10 (2%)
1	B	476/495 (96%)	-0.54	1 (0%)	95	95	9, 19, 35, 48	14 (2%)
1	C	477/495 (96%)	-0.44	3 (0%)	89	89	10, 23, 38, 50	16 (3%)
1	D	478/495 (96%)	-0.38	6 (1%)	77	76	11, 22, 41, 56	18 (3%)
1	E	477/495 (96%)	-0.41	2 (0%)	92	93	9, 23, 41, 50	16 (3%)
1	F	478/495 (96%)	-0.37	5 (1%)	82	83	10, 23, 38, 46	16 (3%)
1	H	478/495 (96%)	-0.23	8 (1%)	70	67	12, 26, 44, 52	18 (3%)
2	G	478/495 (96%)	-0.38	2 (0%)	92	93	11, 23, 39, 51	14 (2%)
All	All	3820/3960 (96%)	-0.42	28 (0%)	87	88	9, 22, 39, 56	122 (3%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	39	PRO	4.0
1	D	288	ALA	3.7
1	F	288	ALA	3.5
1	H	321	ALA	3.2
1	F	38	GLY	3.1

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 (i)

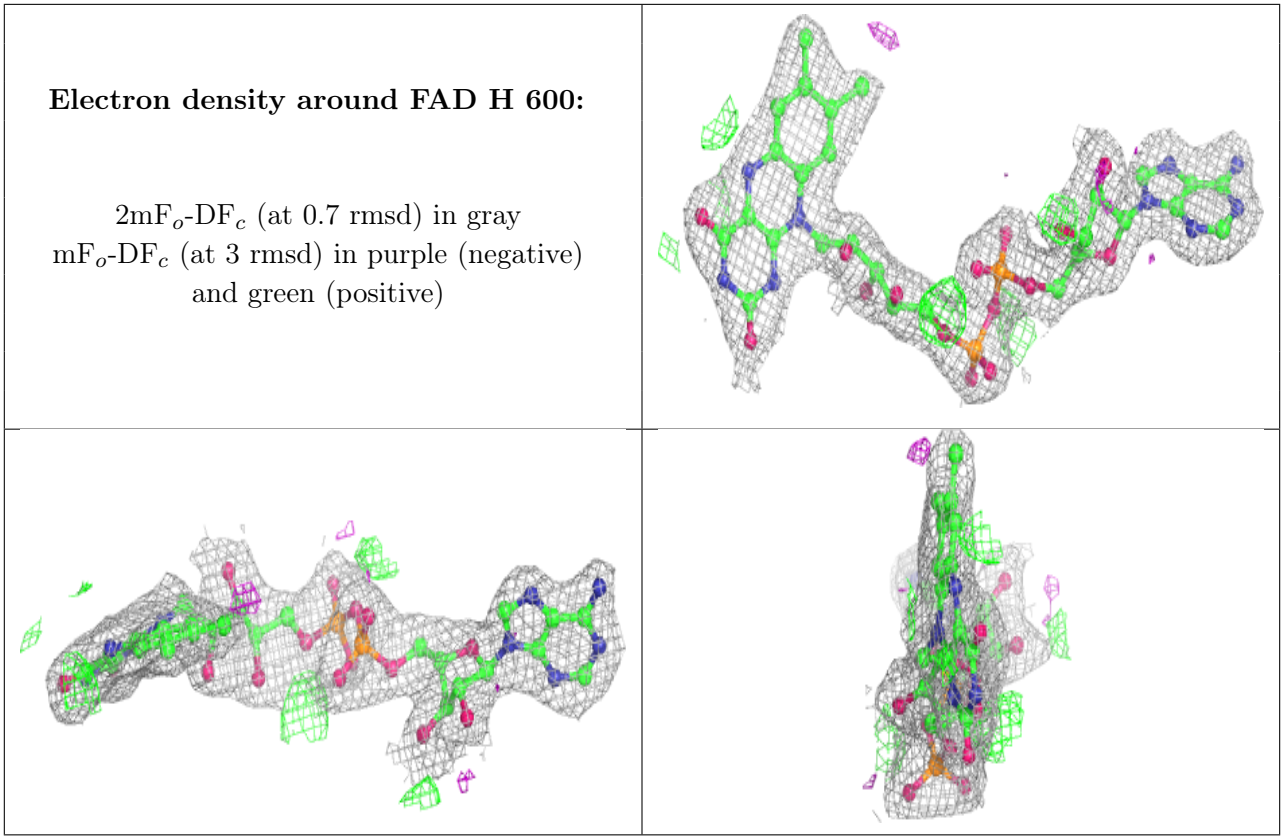
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	EDO	C	601	4/4	0.82	0.18	24,27,31,32	0
4	EDO	G	601	4/4	0.85	0.21	26,28,31,34	0
4	EDO	F	601	4/4	0.95	0.17	21,24,27,31	0
3	FAD	H	600	53/53	0.96	0.13	19,24,29,30	0
3	FAD	D	600	53/53	0.96	0.13	10,19,26,27	0
3	FAD	F	600	53/53	0.96	0.12	15,20,25,25	0
3	FAD	G	600	53/53	0.96	0.13	17,22,32,32	0
4	EDO	D	601	4/4	0.97	0.14	20,23,25,27	0
3	FAD	C	600	53/53	0.97	0.13	13,19,27,28	0
3	FAD	E	600	53/53	0.97	0.12	14,19,29,30	0
4	EDO	G	602	4/4	0.97	0.12	29,31,31,31	0
3	FAD	B	600	53/53	0.98	0.12	10,18,22,23	0
4	EDO	A	601	4/4	0.98	0.13	23,25,26,26	0
3	FAD	A	600	53/53	0.98	0.12	13,18,20,22	0
4	EDO	C	602	4/4	0.98	0.09	29,32,33,33	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.

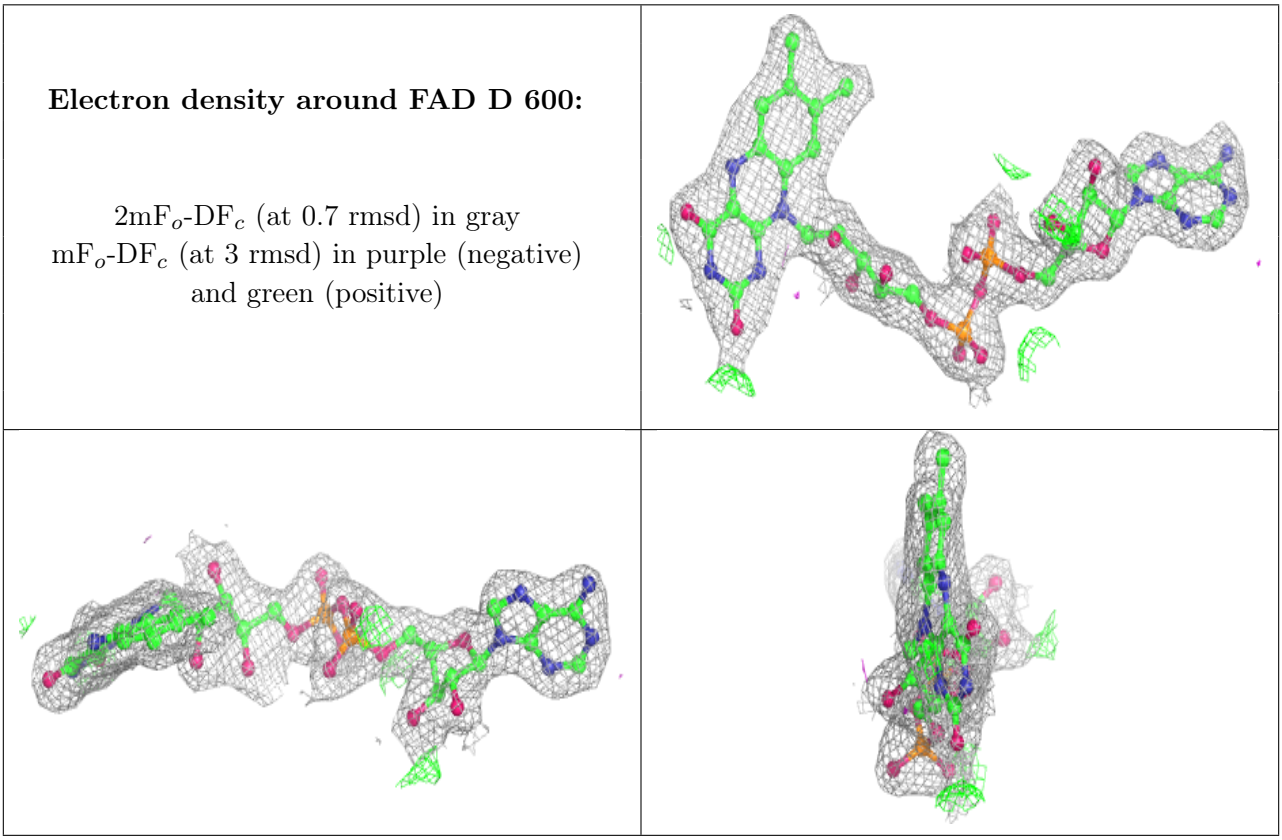
Electron density around FAD H 600:

$2mF_o$-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 D 600:

$2mF_o$-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 F 600:

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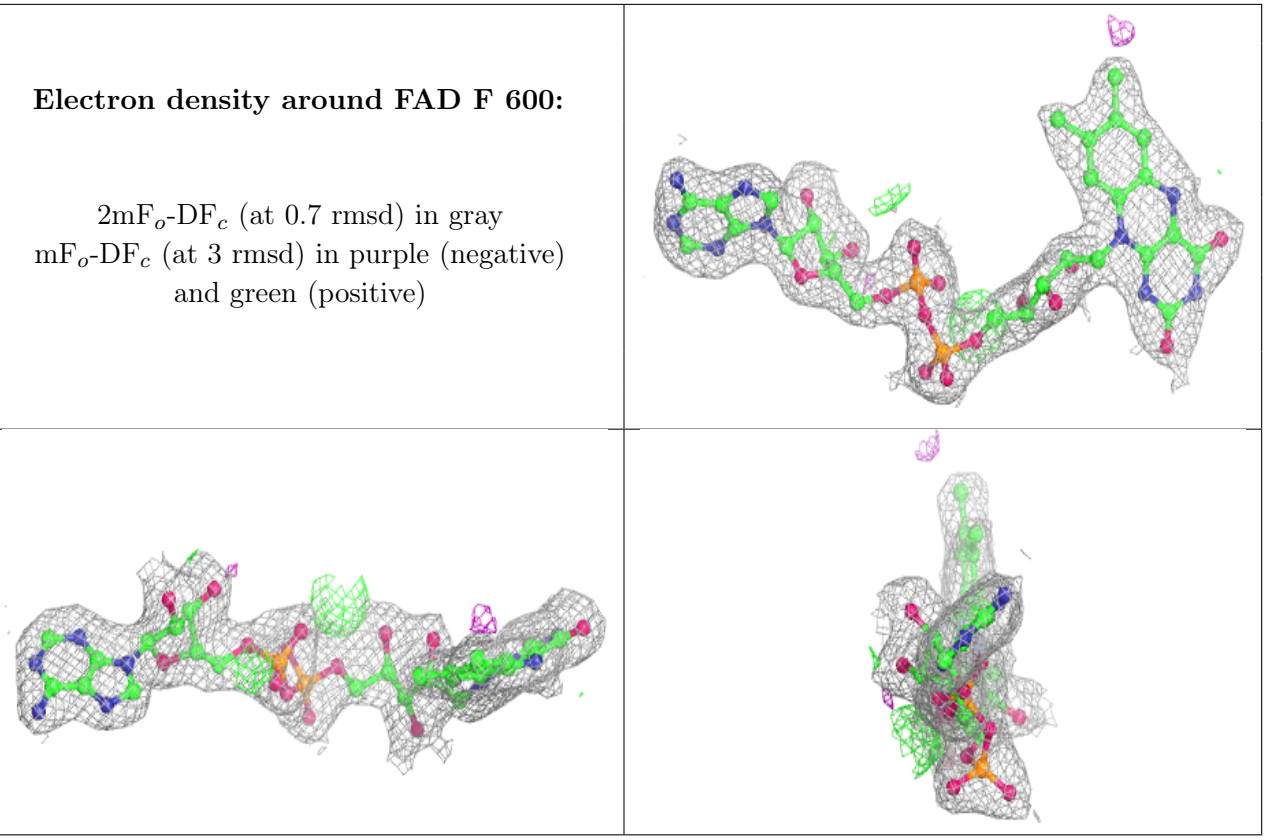
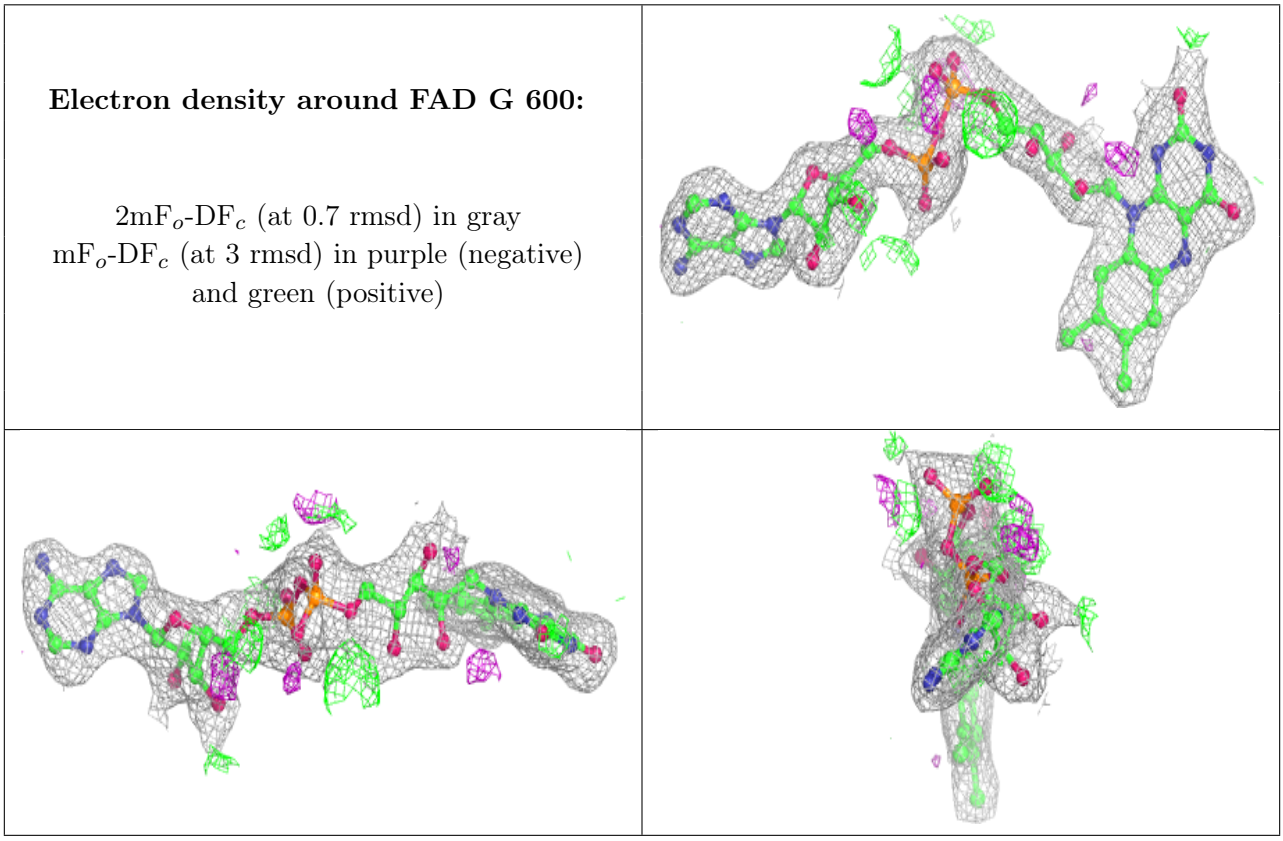
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



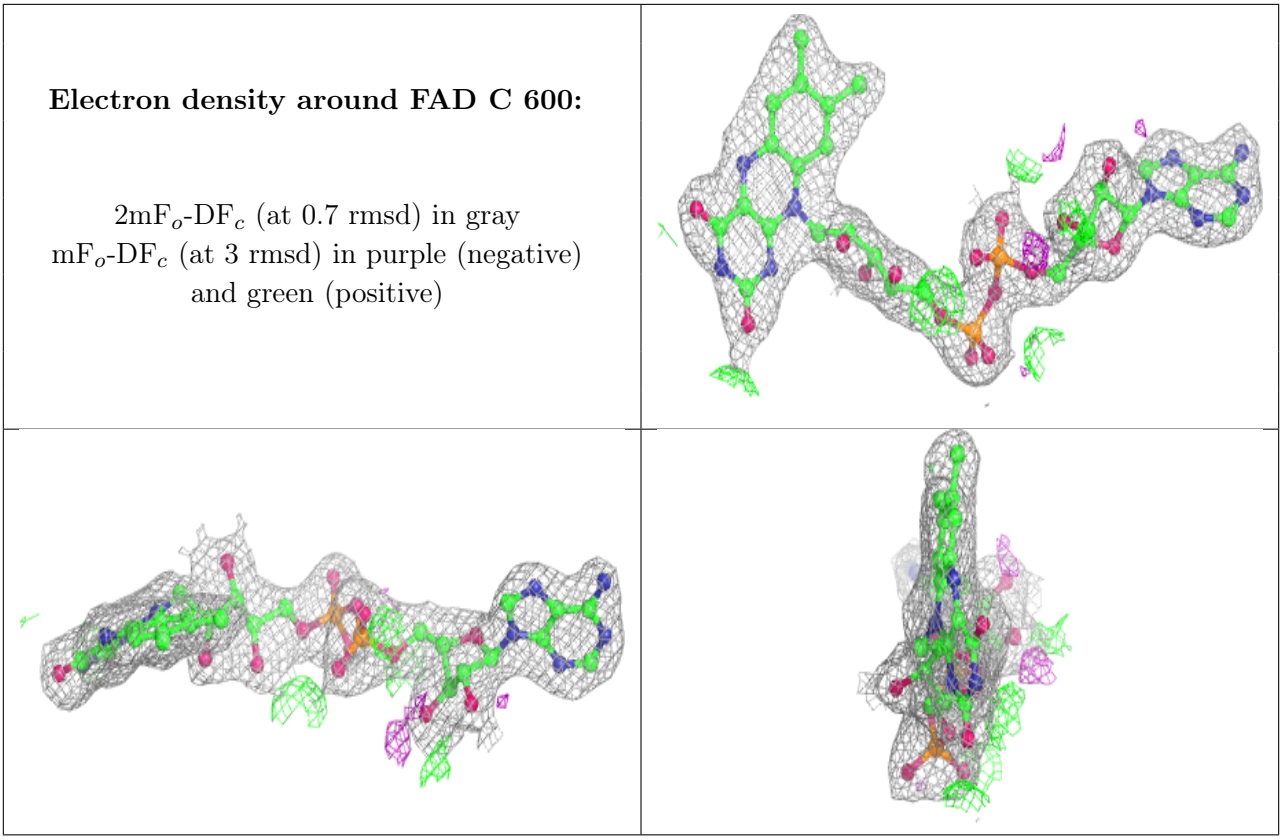
Electron density around FAD G 600:

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



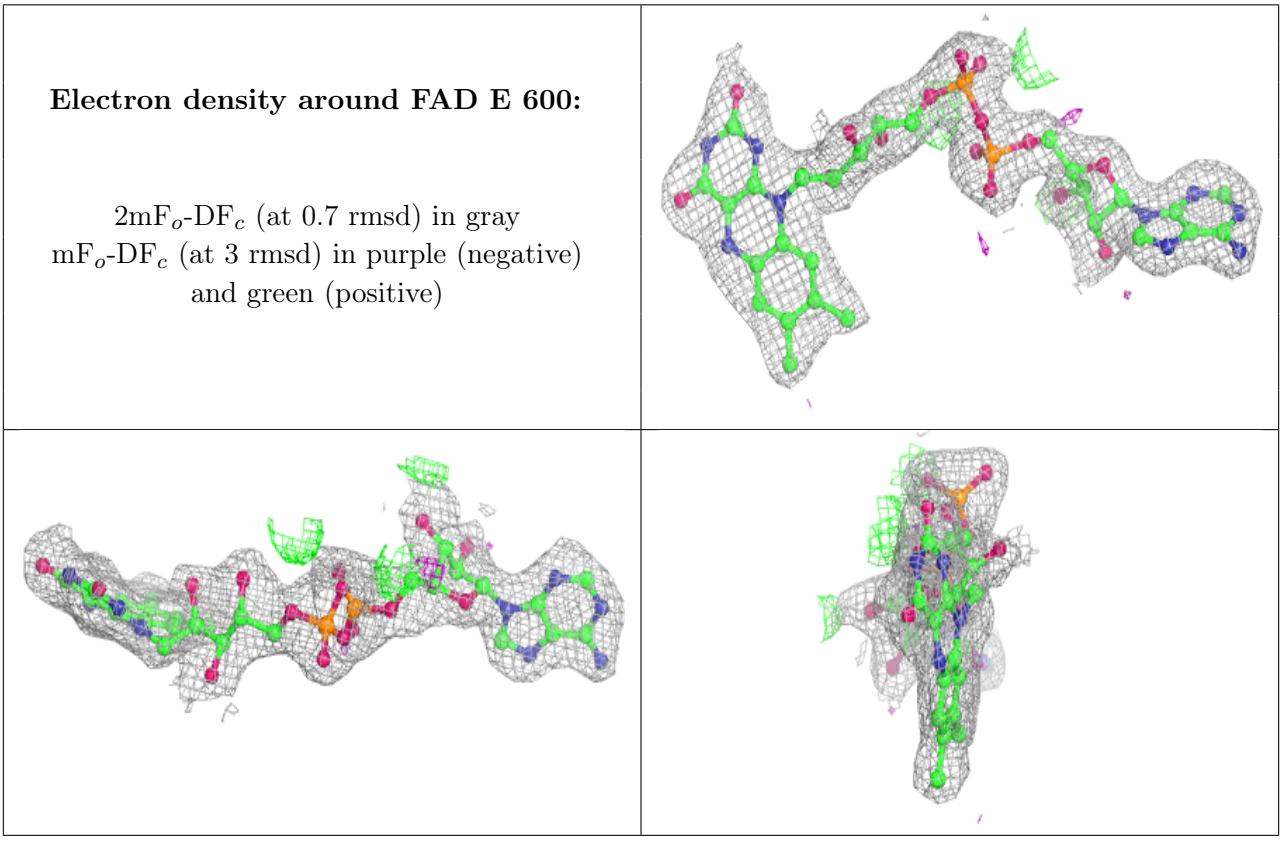
Electron density around FAD C 600:

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



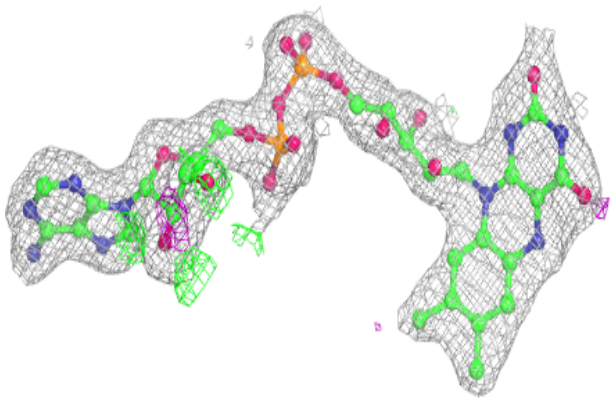
Electron density around FAD E 600:

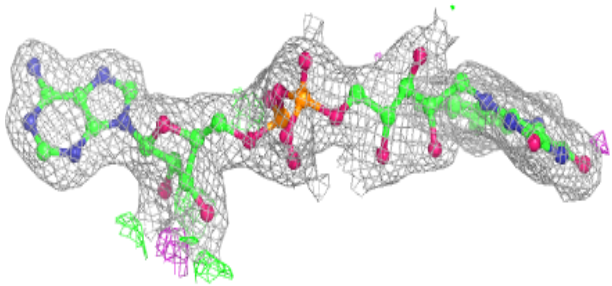
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

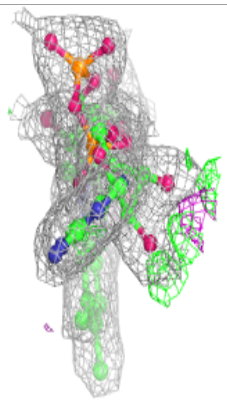


Electron density around FAD B 600:

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

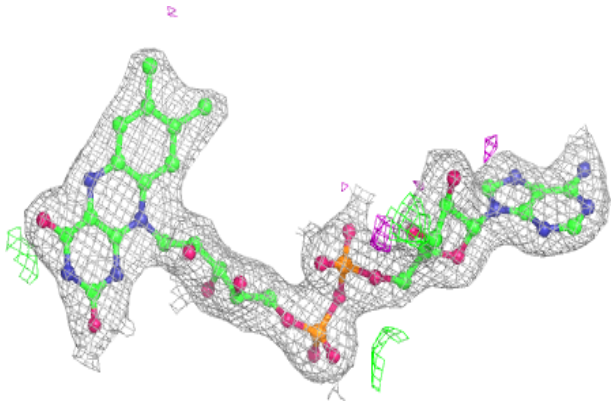


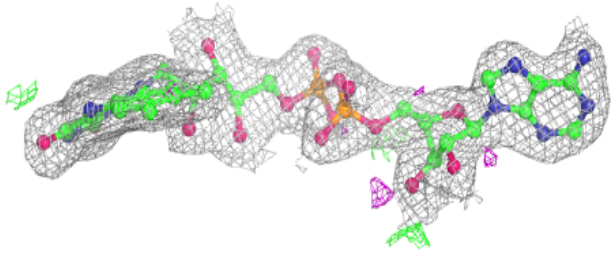


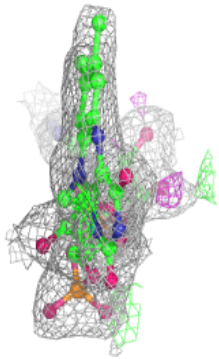


Electron density around FAD A 600:

$2mF_o$-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.