



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 12:30 pm BST

PDB ID : 1VAO
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

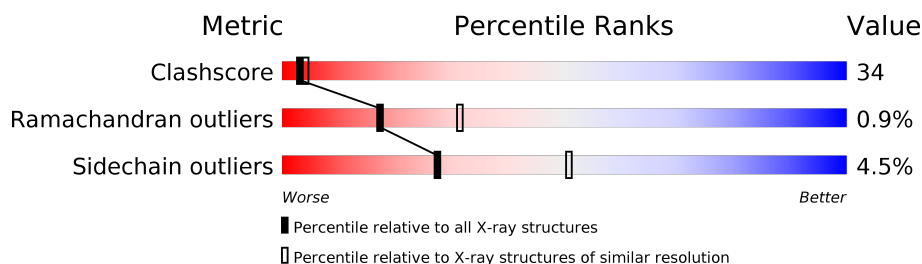
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	

2 Entry composition [i](#)

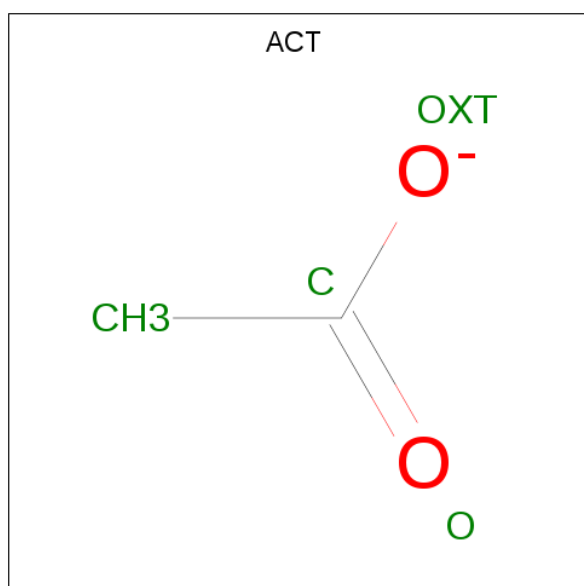
There are 5 unique types of molecules in this entry. The entry contains 9134 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	36	0	0
			4351	2793	744	790	24			
1	B	550	Total	C	N	O	S	36	0	0
			4351	2793	744	790	24			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

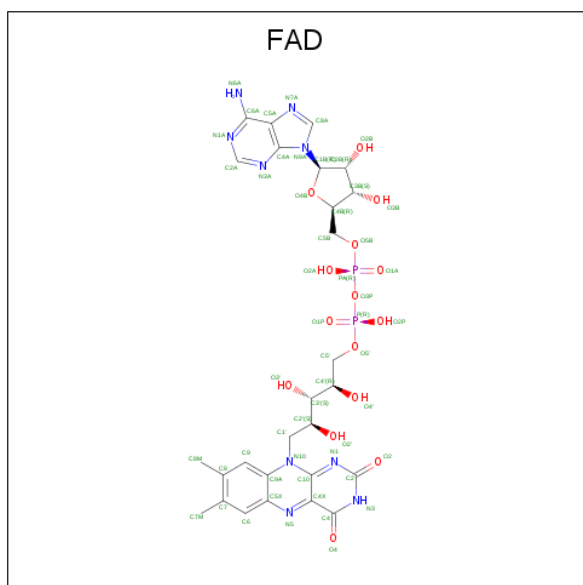


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

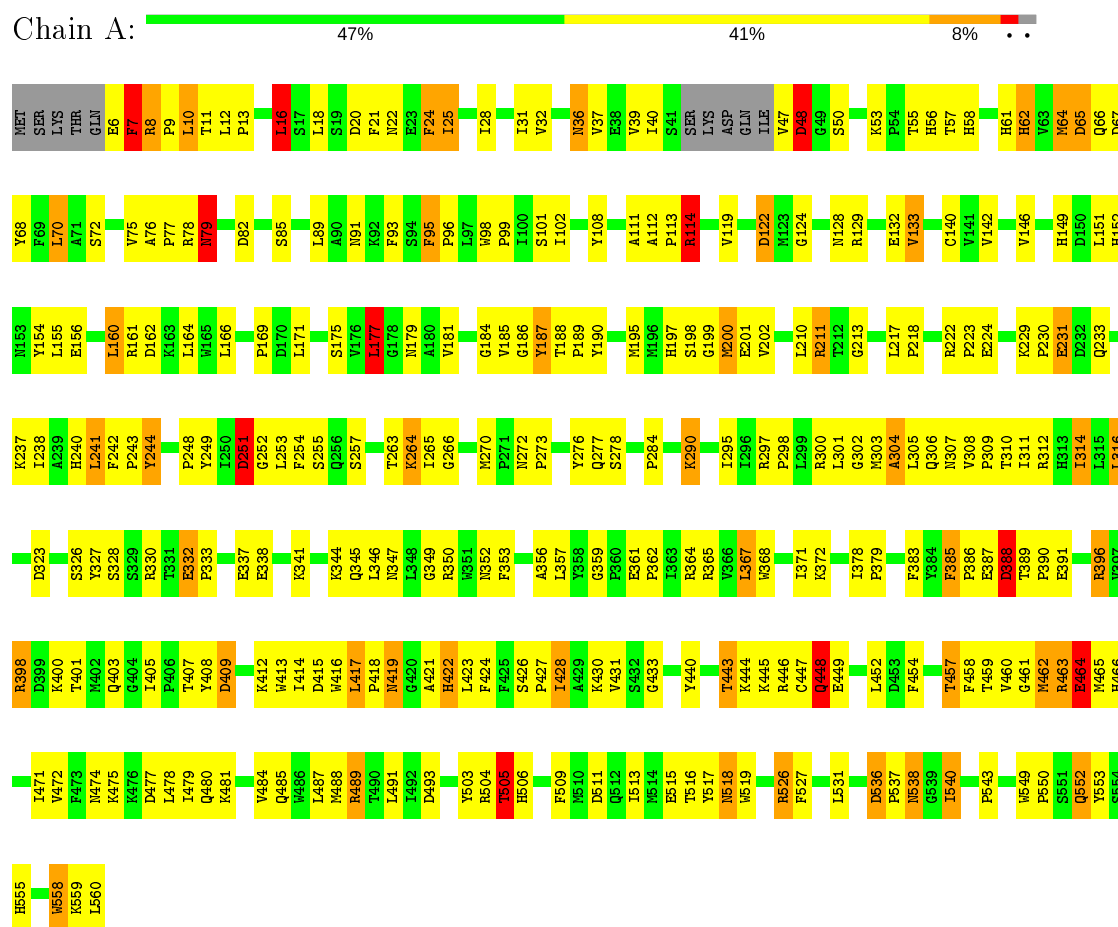


3 Residue-property plots

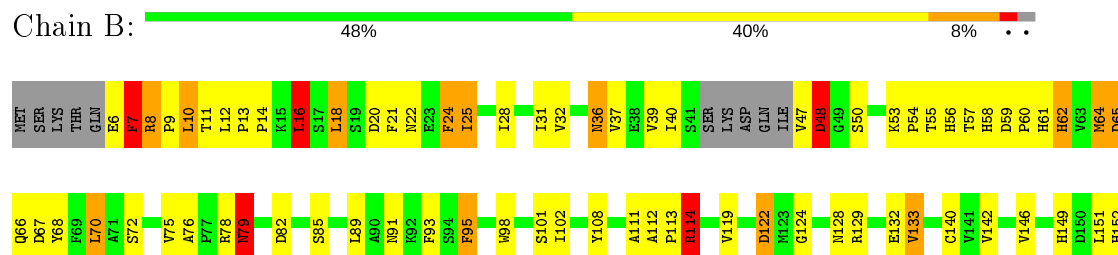
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

• Molecule 1: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE



Q480	K481	R482	K483	V484	Q485	W486	L487	M488	R489	T490	L491	T492	D493	W500	Y503	R504	T505	H506	F509	M510	D511	Q512	M514	E515	T516	Y517	M518	W519	R526	F527	L531	D536	F537	M538	G539	I540	P543	W549	P550	S551	Q552	Y553	H555	W558	K559	L560							
G404	I405	P406	T407	Y408	D409		K412	W413	I414	D415	W416	L417	P418	N419	G420	A421	H422	L423	F424	I428	A429	K430	V431	S432	G433	Y440	T443	K444	K445	R446	C447	Q448	E449	F454	T457	F458	T459	V460	G461	M462	R463	E464	M465	H466	I471	V472	F473	N474	K475	K476	D477	L478	I479
S328	S329	R330	T331	E332	P333		E337	E338	K341		K344	Q345	L346	N347	L348	G349	R350	K351	N352	F353		A356	L357	K358	P360	E361	P362	I363	R364	R365	V366	W368	I371	K372	I378	P379	F383	Y384	P386	E387	I388	T389	P390	R396	V397	R398	D399	K400	T401	M402	Q403		
P243	Y244	G245	F246	G247	P248	Y249	I250	D251	G252	L253	P254	S255	I261	V262	T263	K264	L265	G266	M270	N271	N272	P273		Y276	Q277	S278	P284	K290	I295	I296	R297	P298	L299	R300	L301	G302	M303	A304	L305	Q306	N307	V308	P309	T310	I311	R312	H313	I314	L315	I316	K324	Y327	
W153	Y154	L155	E156	L160	R161	D162	K163	L164	W165	L166	P169	D170	L171	S175	W176	L177	G178	N179	A180	V181	G184	V185	G186	Y187	T188	P189	Y190	M195	H196	S197	S198	G199	M200	E201	V202	L210	R211	R222	P223	E224	K229	P230	E231	D232	Q233	L238	A239	H240	L241	F242			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	130.24Å 130.24Å 133.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.9 (30.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.88	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9134	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, FAD, ACT

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	0.76	3/4470 (0.1%)	1.68	89/6075 (1.5%)
1	B	0.76	3/4470 (0.1%)	1.68	89/6075 (1.5%)
All	All	0.76	6/8940 (0.1%)	1.68	178/12150 (1.5%)

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	2	0
1	B	2	0
All	All	4	0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	PHE	CE1-CZ	7.54	1.51	1.37
1	B	7	PHE	CE1-CZ	7.50	1.51	1.37
1	A	7	PHE	CD1-CE1	7.35	1.53	1.39
1	B	7	PHE	CD1-CE1	7.35	1.53	1.39
1	A	7	PHE	CD2-CE2	6.36	1.51	1.39

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	ARG	NE-CZ-NH2	-19.95	110.33	120.30
1	A	526	ARG	NE-CZ-NH2	-19.88	110.36	120.30
1	B	526	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	A	526	ARG	NE-CZ-NH1	13.87	127.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	ARG	NE-CZ-NH1	12.01	126.31	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	7	PHE	CA
1	A	332	GLU	CA
1	B	7	PHE	CA
1	B	332	GLU	CA

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	4351	0	4288	307	1
1	B	4351	0	4288	286	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	29	6	0
4	B	53	0	29	5	0
5	A	166	0	0	19	0
5	B	150	0	0	11	0
All	All	9134	0	8640	580	1

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 34.

The worst 5 of 580 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)
4:B:600:FAD:H51A	4:B:600:FAD:H8A	1.22	1.16
4:A:600:FAD:H8A	4:A:600:FAD:H51A	1.23	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.11	1.07
1:A:211:ARG:HG3	1:B:519:TRP:CZ3	1.99	0.98
1:B:555:HIS:HB3	1:B:559:LYS:HE3	1.46	0.97

All (1) 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)
1:A:330:ARG:NH2	1:A:330:ARG:NH2[2_765]	2.15	0.05

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	546/560 (98%)	503 (92%)	38 (7%)	5 (1%)	17	31
1	B	546/560 (98%)	503 (92%)	38 (7%)	5 (1%)	17	31
All	All	1092/1120 (98%)	1006 (92%)	76 (7%)	10 (1%)	17	31

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	B	48	ASP
1	A	199	GLY
1	A	388	ASP
1	B	199	GLY

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	470/482 (98%)	449 (96%)	21 (4%)	27	51
1	B	470/482 (98%)	449 (96%)	21 (4%)	27	51
All	All	940/964 (98%)	898 (96%)	42 (4%)	27	51

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	TYR
1	B	64	MET
1	B	464	GLU
1	A	505	THR
1	B	7	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	GLN
1	B	66	GLN
1	B	520	ASN
1	B	56	HIS
1	B	79	ASN

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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	ACT	B	601	-	1,3,3	4.27	1 (100%)	0,3,3	0.00	-
4	FAD	A	600	1	51,58,58	1.24	4 (7%)	60,89,89	1.59	6 (10%)
4	FAD	B	600	1	51,58,58	1.23	4 (7%)	60,89,89	1.59	7 (11%)
2	ACT	A	601	-	1,3,3	4.20	1 (100%)	0,3,3	0.00	-

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	FAD	A	600	1	-	6/30/50/50	0/6/6/6
4	FAD	B	600	1	-	6/30/50/50	0/6/6/6

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ACT	CH3-C	4.27	1.54	1.48
4	A	600	FAD	C4X-C10	4.24	1.43	1.38
2	A	601	ACT	CH3-C	4.20	1.54	1.48
4	B	600	FAD	C4X-C10	4.14	1.43	1.38
4	B	600	FAD	C4-N3	3.64	1.39	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	C4-N3-C2	7.56	121.53	115.14
4	B	600	FAD	C4-N3-C2	7.48	121.46	115.14
4	A	600	FAD	C4X-C4-N3	-5.13	116.42	123.43
4	B	600	FAD	C4X-C4-N3	-5.10	116.46	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	C1'-N10-C9A	2.51	120.27	118.29

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

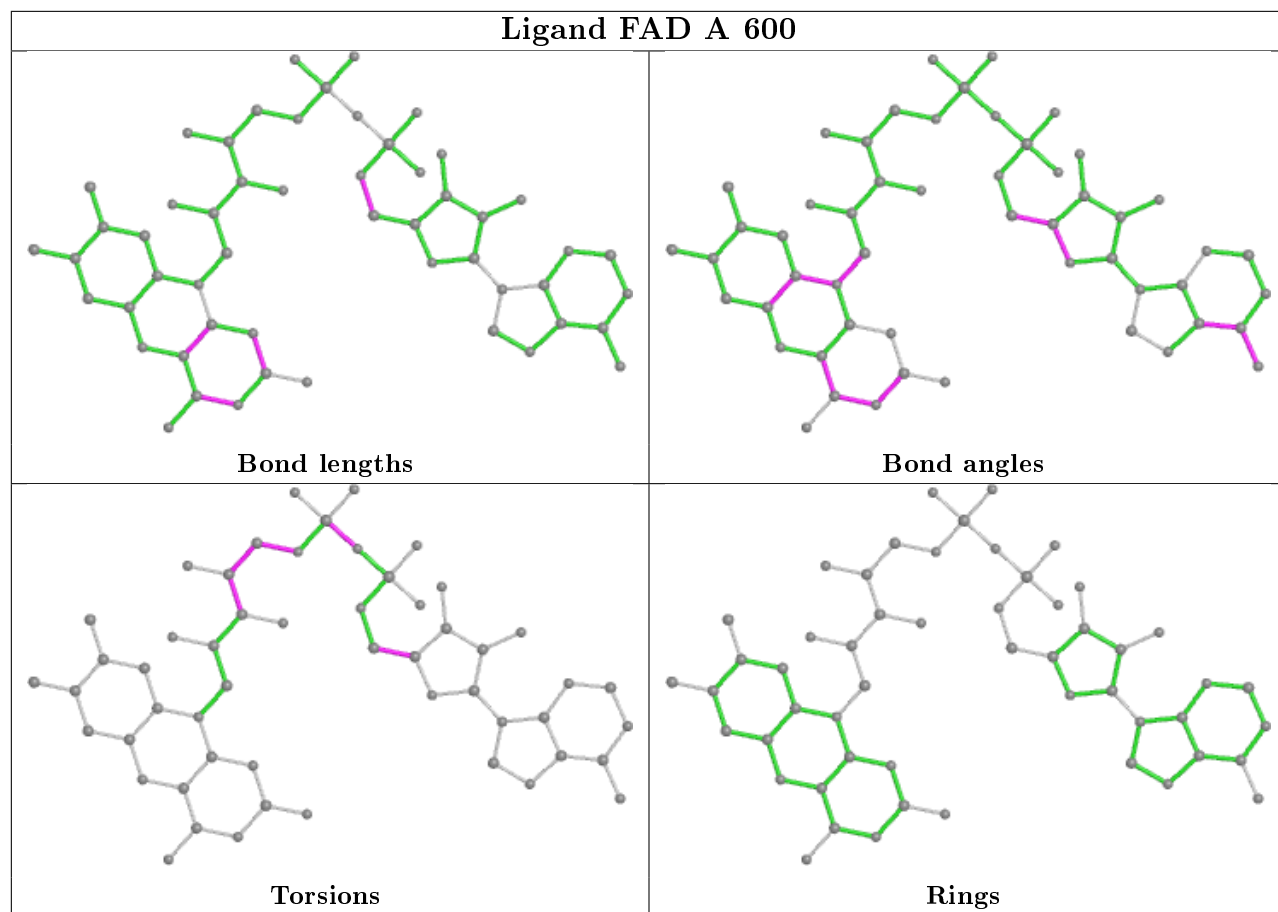
Mol	Chain	Res	Type	Atoms
4	B	600	FAD	C3'-C4'-C5'-O5'
4	B	600	FAD	O4'-C4'-C5'-O5'
4	A	600	FAD	C3'-C4'-C5'-O5'
4	A	600	FAD	O4'-C4'-C5'-O5'
4	B	600	FAD	C4'-C5'-O5'-P

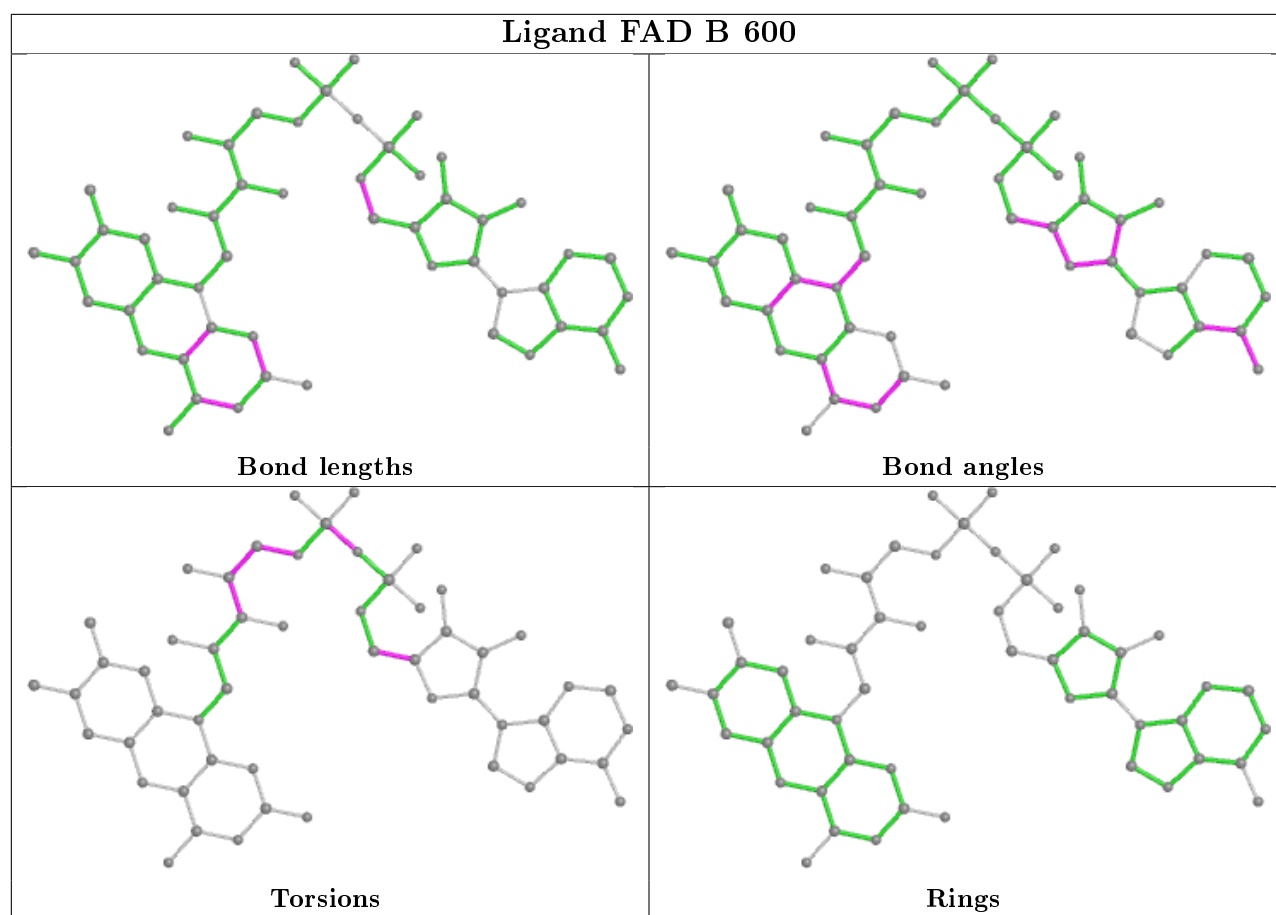
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	FAD	6	0
4	B	600	FAD	5	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.