



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 2VAO / pdb_00002vao
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH ISOEUGENOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 2.80 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

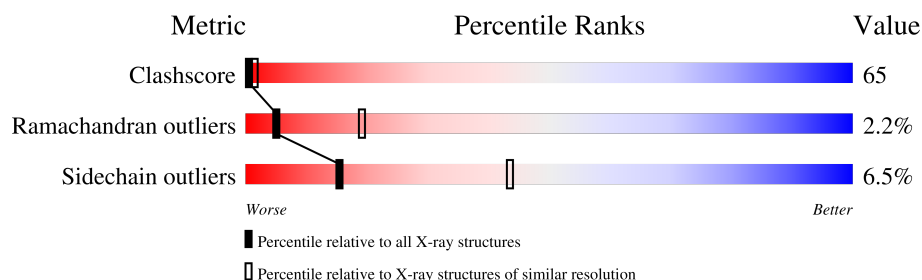
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

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

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8948 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.

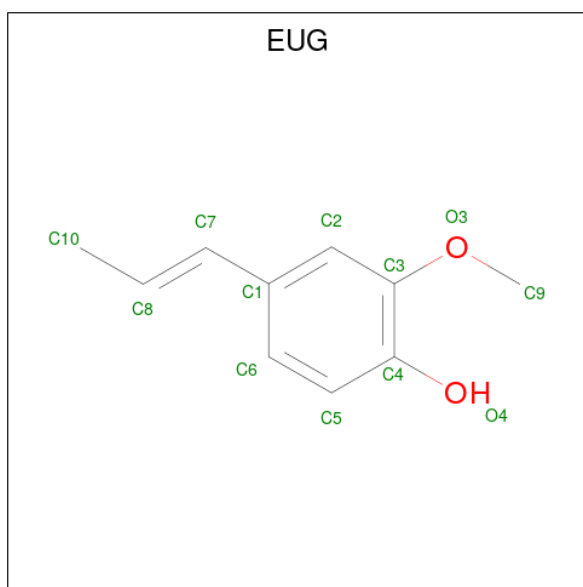
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	51	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	51	0	0
			4391	2817	751	799	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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 2-methoxy-4-[(1E)-prop-1-en-1-yl]phenol (CCD ID: EUG) (formula: $C_{10}H_{12}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	9	2		
3	B	1	Total	C	O	0	0
			11	9	2		

- Molecule 4 is water.

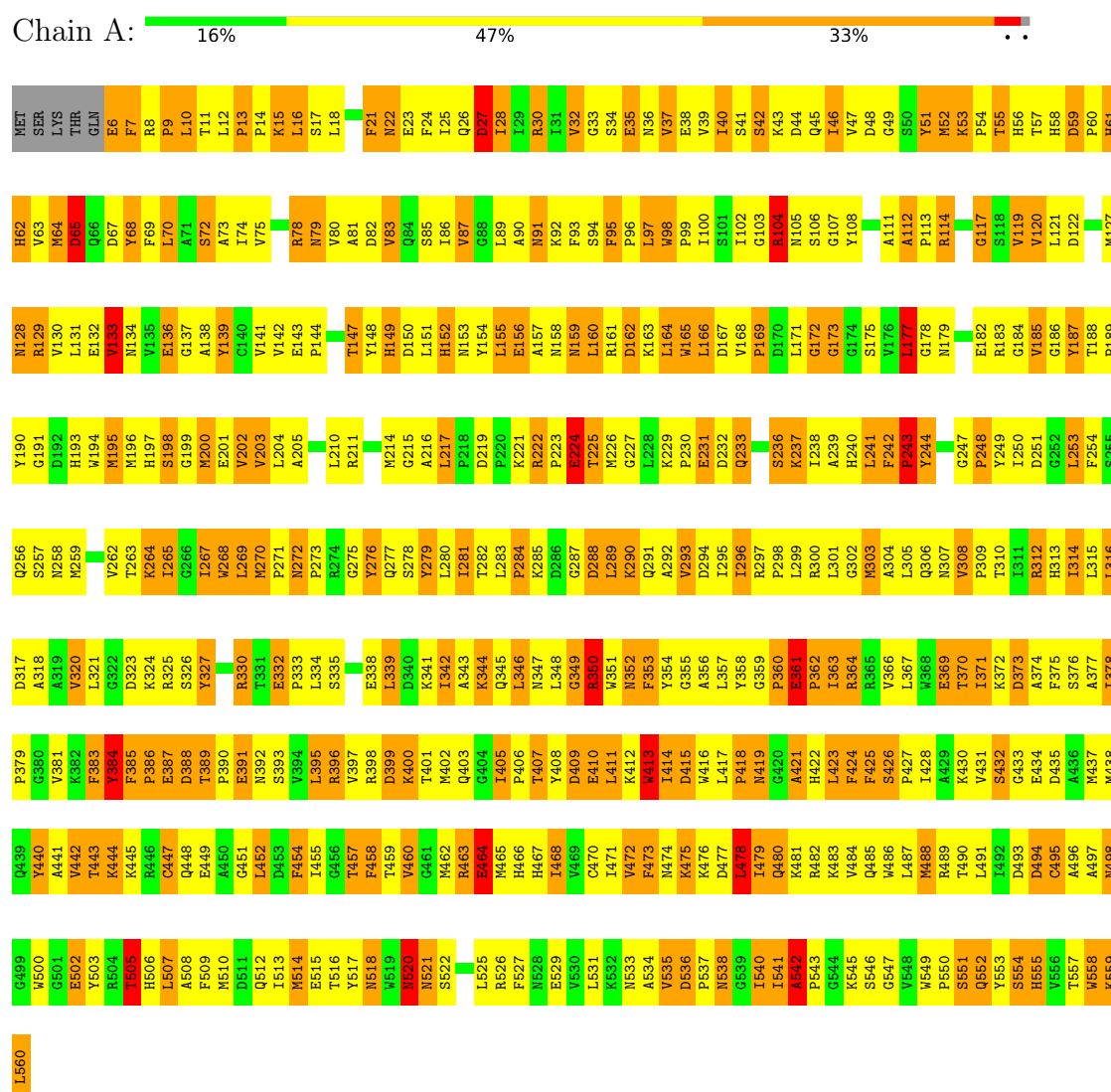
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	24	Total	O	0	0
			24	24		

3 Residue-property plots

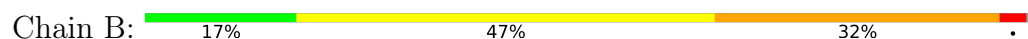
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



G499	W500	G501	E502	Y503	R504	T505	H506	L507	A508	F509	E510	N511	Q512	I513	N514	E515	T516	Y517	N518	W519	N520	N521	S522	L525	R526	F527	N528	E529	E530	L531	R532	A533	A534	V535	D536	P537	N538	G539	I540	I541	A542	K545	S546	G547	V548	W549	P550	S551	Q552	Y553	S554	H555	T557	W558	K559	L560			
Q439	Y440	A441	V442	T443	K444	K445	K446	C447	Q448	E449	A450	G451	L452	D453	F454	I455	G456	T457	F458	T459	V460	G461	M462	R463	E464	M465	H466	H467	I468	V469	C470	L471	F472	F473	N474	K475	K476	D477	L478	I479	Q480	K481	R482	K483	V484	Q485	V486	L487	M488	R489	T490	L491	I492	D493	D494	C495	A496	M497	M498
P379	G380	V381	K382	F383	Y384	F385	F386	E387	D388	T389	P390	E391	N392	S393	V394	L395	R396	V397	R398	D399	K400	T401	M402	Q403	G404	I405	H406	T407	Y408	D409	E410	L411	K412	N413	I414	D415	W416	L417	P418	N419	G420	A421	H422	L423	F424	P425	S426	P427	L428	A429	K430	V431	S432	G433	A434	D435	A436	M437	M438
D317	A318	A319	V320	L321	G322	D323	K324	R325	S326	Y327	R330	T331	E332	P333	L334	S335	E338	L339	D340	K341	I342	A343	K344	Q345	L346	N347	L348	D349	G350	W351	N352	F353	Y354	G355	A356	L357	Y358	G359	P360	E361	P362	I363	R364	R365	V366	L367	V368	E369	T370	I371	K372	D373	A374	F375	S376	A377	I378		
Q256	S257	N258	M259	V262	T263	K264	L265	G266	I267	W268	L269	M270	P271	N272	P273	R274	G275	Y276	Q277	S278	Y279	L280	I281	T282	L283	P284	K285	D286	G287	D288	L289	K290	Q291	A292	V293	D294	L295	R296	R297	P298	L299	R300	L301	G302	N303	A304	L305	Q306	N307	V308	P309	T310	R311	G312	H313	I314	L315	L316	
Y190	G191	D192	H193	W194	M195	L196	H197	S198	G199	M200	E201	V202	V203	L204	A205	L210	R211	M214	G215	A216	L217	P218	D219	P220	K221	R222	P223	R224	T225	M226	G227	L228	K229	P230	E231	D232	Q233	S236	K237	L238	A239	H240	L241	N242	P243	Y244	G247	P248	Y249	L250	D251	G252	L253	F254	S255				
N128	R129	V130	L131	W132	Y133	M134	V135	E136	G137	A138	Y139	C140	V141	E142	N143	P144	T147	Y148	H149	D150	L151	H152	N153	Y154	L155	K156	A157	N158	N159	S160	R161	D162	K163	L164	W165	P166	D167	V168	P169	D170	L171	G172	G173	S174	Y175	V176	L177	G178	N179	E182	R183	Y184	V185	G186	Y187	T188	P189		
H62	V63	M64	D65	Q66	D67	Y68	F69	L70	A71	S72	A73	I74	V75	R78	N79	V80	A81	D82	V83	Q84	S85	I86	V87	G88	L89	A90	N91	K92	F93	S94	P95	P96	L97	W98	P99	I100	S101	I102	G103	N105	S106	G107	Y108	A111	A112	P113	R114	G117	S118	V119	V120	T57	L121	D122	M127				

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	128.38Å 128.38Å 130.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	90.6 (30.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.214 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8948	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: FAD, EUG

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	1.06	7/4511 (0.2%)	2.49	342/6131 (5.6%)
1	B	1.06	7/4511 (0.2%)	2.49	339/6131 (5.5%)
All	All	1.06	14/9022 (0.2%)	2.49	681/12262 (5.6%)

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 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	MET	SD-CE	7.34	1.97	1.79
1	A	303	MET	SD-CE	7.32	1.97	1.79
1	A	64	MET	SD-CE	6.35	1.95	1.79
1	B	64	MET	SD-CE	6.32	1.95	1.79
1	B	120	VAL	CA-CB	-6.22	1.46	1.54

The worst 5 of 681 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	SER	N-CA-C	-17.32	91.73	113.55
1	A	72	SER	N-CA-C	-17.27	91.79	113.55
1	A	129	ARG	N-CA-C	15.71	133.53	110.28
1	B	129	ARG	N-CA-C	15.70	133.51	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ALA	N-CA-C	-15.54	94.43	111.36

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	363	ILE	CA
1	A	410	GLU	CA
1	B	363	ILE	CA
1	B	410	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	4391	0	4330	576	0
1	B	4391	0	4330	574	0
2	A	53	0	31	17	0
2	B	53	0	31	16	0
3	A	11	0	7	5	0
3	B	11	0	7	5	0
4	A	14	0	0	2	0
4	B	24	0	0	0	0
All	All	8948	0	8736	1136	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 65.

The worst 5 of 1136 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:A:422:HIS:NE2	2:A:600:FAD:HM83	1.00	1.30
1:B:422:HIS:NE2	2:B:600:FAD:HM83	1.00	1.30
1:A:422:HIS:CE1	2:A:600:FAD:HM83	1.72	1.24
1:B:422:HIS:CE1	2:B:600:FAD:HM83	1.72	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LEU:HA	1:A:510:MET:HE3	1.28	1.12

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	553/560 (99%)	472 (85%)	69 (12%)	12 (2%)	5	19
1	B	553/560 (99%)	472 (85%)	69 (12%)	12 (2%)	5	19
All	All	1106/1120 (99%)	944 (85%)	138 (12%)	24 (2%)	5	19

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	559	LYS
1	B	46	ILE
1	B	559	LYS
1	A	157	ALA

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	475/482 (98%)	444 (94%)	31 (6%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	475/482 (98%)	444 (94%)	31 (6%)	15	43
All	All	950/964 (98%)	888 (94%)	62 (6%)	15	43

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	520	ASN
1	B	464	GLU
1	B	78	ARG
1	B	413	TRP
1	B	520	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	152	HIS
1	B	240	HIS
1	B	197	HIS
1	B	352	ASN
1	A	352	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	58,58,58	1.00	5 (8%)	85,89,89	0.89	4 (4%)
2	FAD	B	600	1	58,58,58	1.00	5 (8%)	85,89,89	0.89	4 (4%)
3	EUG	A	601	-	11,11,12	0.46	0	14,14,15	1.51	2 (14%)
3	EUG	B	601	-	11,11,12	0.47	0	14,14,15	1.52	2 (14%)

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	-	10/34/50/50	0/6/6/6
2	FAD	B	600	1	-	10/34/50/50	0/6/6/6
3	EUG	A	601	-	-	4/4/4/5	0/1/1/1
3	EUG	B	601	-	-	4/4/4/5	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	PA-O3P	3.42	1.63	1.59
2	B	600	FAD	PA-O3P	3.39	1.63	1.59
2	B	600	FAD	P-O3P	3.27	1.63	1.59
2	A	600	FAD	P-O3P	3.22	1.63	1.59
2	A	600	FAD	C5X-N5	-2.68	1.34	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	EUG	O3-C3-C4	3.89	120.38	114.55
3	A	601	EUG	O3-C3-C4	3.85	120.33	114.55
2	B	600	FAD	PA-O5B-C5B	2.60	136.23	121.35
2	A	600	FAD	PA-O5B-C5B	2.59	136.17	121.35
3	B	601	EUG	C9-O3-C3	2.45	121.11	117.51

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

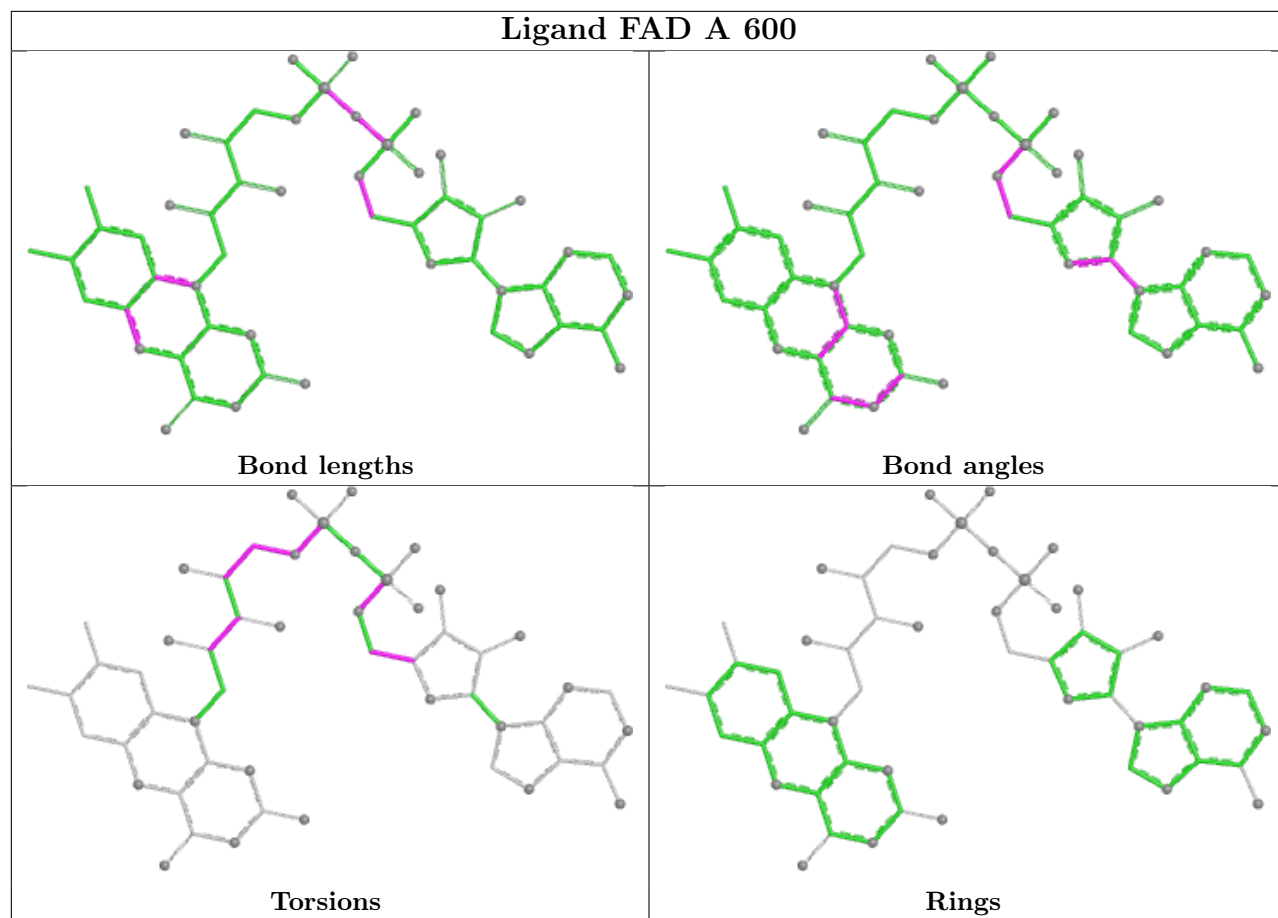
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O3P
2	A	600	FAD	C5'-O5'-P-O1P
2	B	600	FAD	C5B-O5B-PA-O3P
2	B	600	FAD	C5'-O5'-P-O1P
3	A	601	EUG	C6-C1-C7-C8

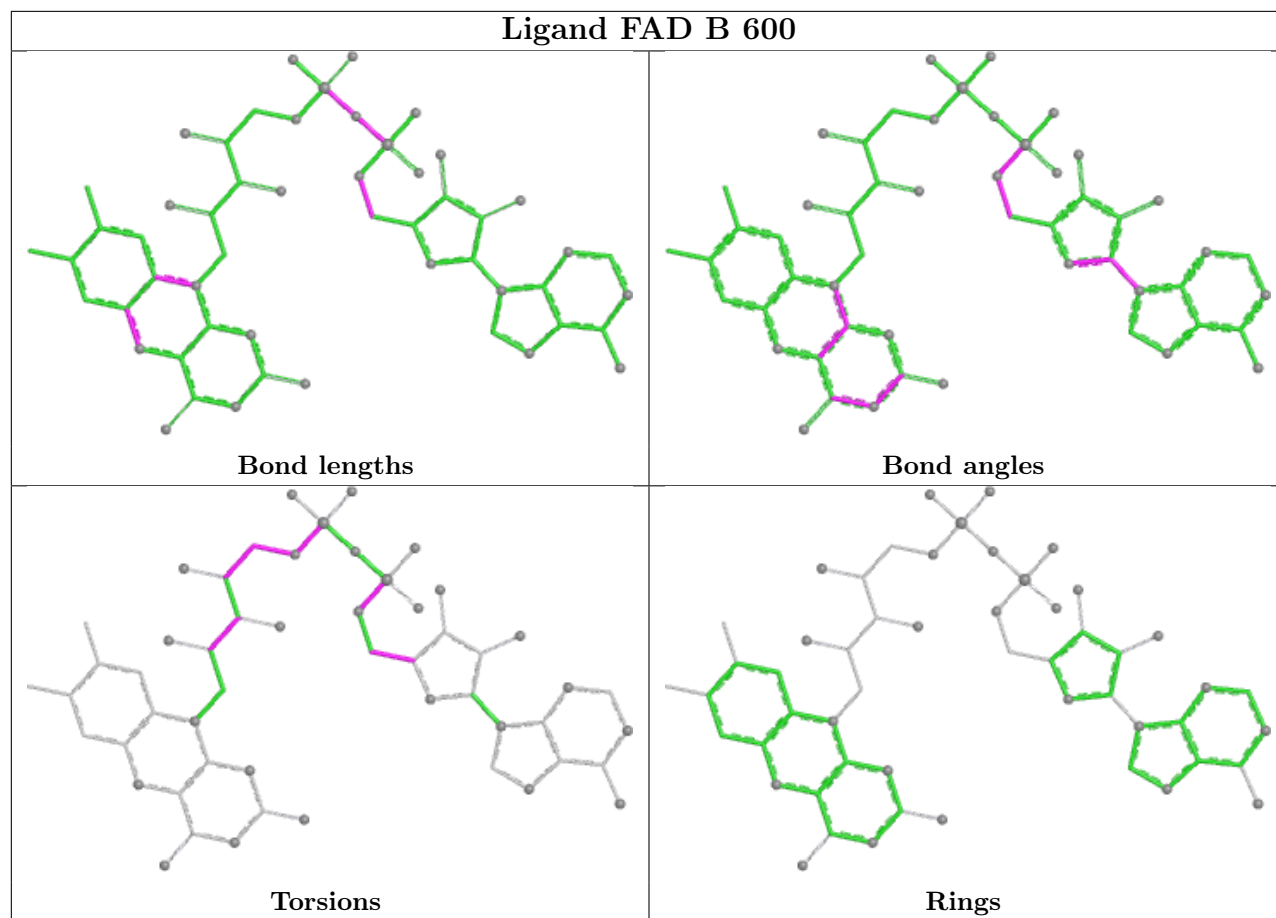
There are no ring outliers.

4 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	17	0
2	B	600	FAD	16	0
3	A	601	EUG	5	0
3	B	601	EUG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.