



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:59 PM UTC

PDB ID : 1AHZ / pdb_00001ahz
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-
ALCOHOL OXIDASE IN COMPLEX WITH 4-(1-HEPTENYL)PHENOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 3.30 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

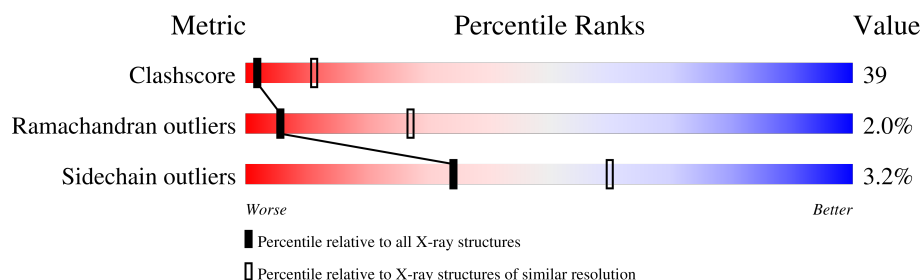
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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	 41% 46% 12% ..
1	B	560	 41% 45% 12% ..

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
4	EPT	A	602	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8904 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.

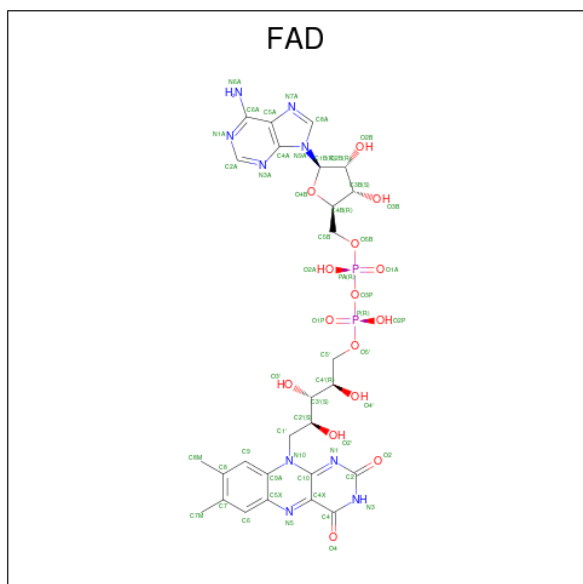
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

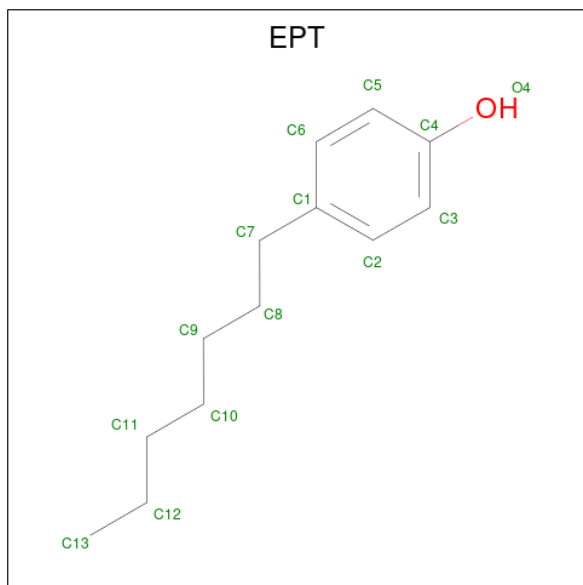
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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		

- Molecule 4 is HEPTANYL-P-PHENOL (CCD ID: EPT) (formula: $C_{13}H_{20}O$).



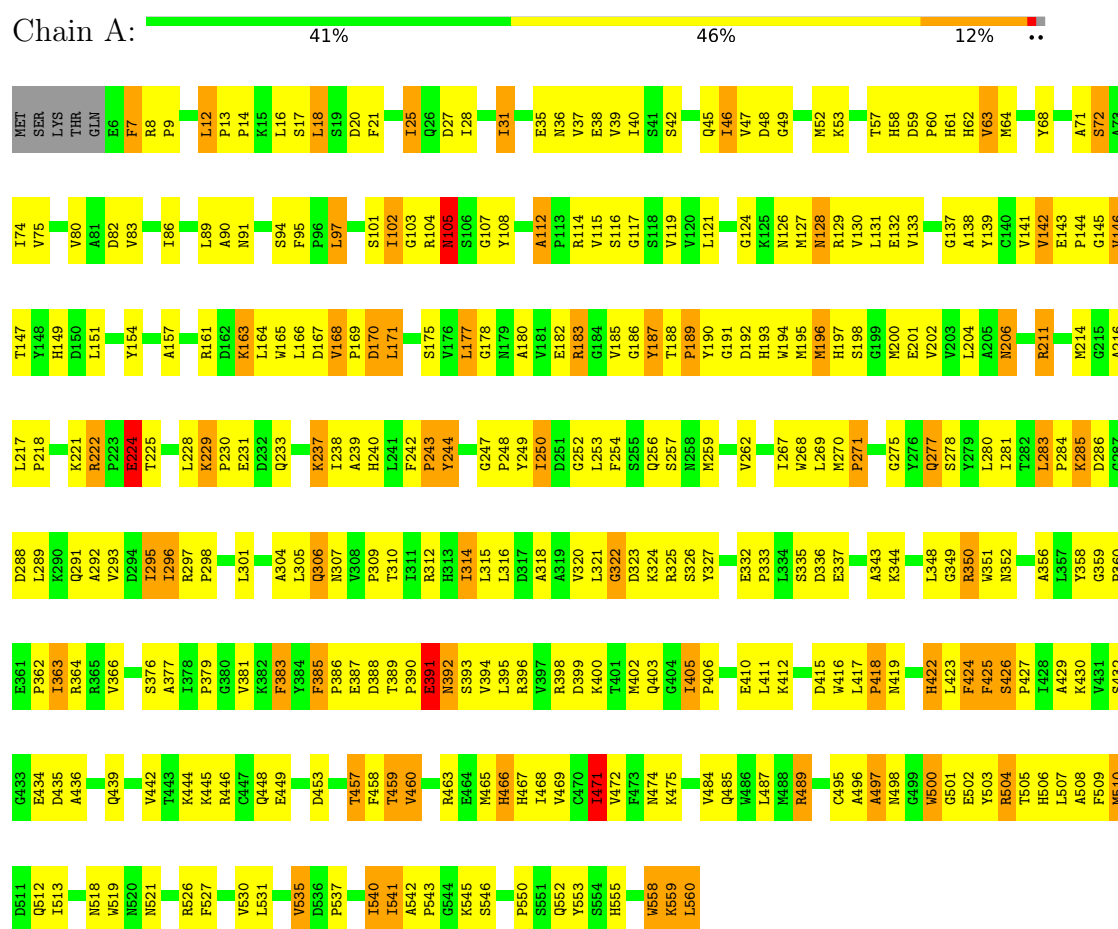
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	13	1		

3 Residue-property plots

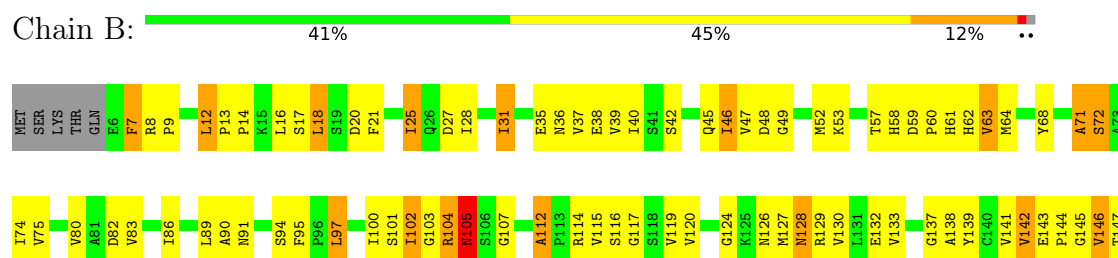
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



D511	G433	P360	G287	A216	Y148
Q512	E434	E361	D288	L217	H149
I513	D435	P362	L289	P218	D150
	A436	I363	K290		L151
T516		R364	Q291	K221	
Y517	Q439	R365	A292	R222	Y154
N518	V442	V366	V293	P223	
W519			D294	E224	A157
N521	T443	S376	I295	T225	
	K444	A377	I296		R161
R526	K445	T378	R297	L228	D162
F527	K446	P379	P298	K229	K163
	G447	G380		P230	L164
V530	Q448	V381	L301	E231	W165
L531	E449	K382		D232	L166
		F383	A304	Q233	D167
	D453	Y384	L305		V168
V535		F385	Q306	K237	P169
D536	T457	P386	N307	I238	D170
F537	F458	E387	V308	A239	L171
	T459	D388	P309	H240	
I540	V460	T389	T310	L241	
I541		P390	I311	F242	S175
A542	R463	E391	R312	P243	V176
P543	E464	N392	H313	Y244	L177
G544	M465	S393	I314		G178
K545	H466	V394	L315	G247	A180
S546	L467	L395	L316	P248	V181
	T468	R396	D317	Y249	E182
	V469		A318	L250	R183
P550	G470	D399	A319	D251	G184
S551	L471	K400	V320	G252	V185
Y553	F472	T401	L321	L253	G186
	V473	M402	G322	F254	Y187
H555	N474	Q403	D323	S255	T188
	K475	G404	K324	Q256	P189
		I405	R325	S257	Y190
W558	V484	P406	Y327	P258	G191
K559	L485	E485		M259	D192
L560		R489	E332		H193
			P333	V262	W194
		D415	L334		M195
	C495	W416	S335	L267	M196
	A496	L417	D336	W268	H197
	A497	P418	E337	L269	S198
	N498	N419		M270	G199
	G499		A343	P271	M200
		H422	K344		E201
		L423		G275	V202
	F501	F424	L348	Y276	V203
	Y502	F425	G349	Q277	L204
	R504	S426	R350	S278	A205
	T505	P427	W351	Y279	N206
	H506	T428	N352	L280	
	L507	L429	A356	L281	L209
	A508	K430	L357	T282	I210
	F509	V431	G358	L283	R211
		S432	T359	P284	
				K285	M214
				D286	G215

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	140.97 Å 140.97 Å 133.45 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30	Depositor
% Data completeness (in resolution range)	90.7 (30.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.224 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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: EPT, FAD, CL

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	0.64	0/4511	1.67	97/6131 (1.6%)
1	B	0.64	0/4511	1.67	95/6131 (1.5%)
All	All	0.64	0/9022	1.67	192/12262 (1.6%)

There are no bond length outliers.

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ARG	N-CA-C	14.24	130.88	110.23
1	A	129	ARG	N-CA-C	14.21	130.83	110.23
1	B	102	ILE	N-CA-C	13.37	123.31	111.81
1	A	102	ILE	N-CA-C	13.33	123.27	111.81
1	A	7	PHE	N-CA-C	11.92	129.80	111.56

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	4391	0	4330	357	0
1	B	4391	0	4330	352	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	29	9	0
3	B	53	0	29	8	0
4	A	14	0	20	14	0
All	All	8904	0	8738	678	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 39.

The worst 5 of 678 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)
3:A:600:FAD:H8A	3:A:600:FAD:H51A	1.31	1.10
1:A:510:MET:HE2	1:A:546:SER:H	1.15	1.10
1:A:314:ILE:HD11	1:A:350:ARG:HG3	1.37	1.06
3:B:600:FAD:H51A	3:B:600:FAD:H8A	1.31	1.06
1:B:314:ILE:HD11	1:B:350:ARG:HG3	1.37	1.03

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%)	503 (91%)	39 (7%)	11 (2%)	6	27
1	B	553/560 (99%)	504 (91%)	38 (7%)	11 (2%)	6	27
All	All	1106/1120 (99%)	1007 (91%)	77 (7%)	22 (2%)	6	27

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE

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Mol	Chain	Res	Type
1	A	388	ASP
1	A	418	PRO
1	A	475	LYS
1	B	46	ILE

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	475/482 (98%)	460 (97%)	15 (3%)	34	60
1	B	475/482 (98%)	460 (97%)	15 (3%)	34	60
All	All	950/964 (98%)	920 (97%)	30 (3%)	34	60

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	560	LEU
1	B	391	GLU
1	B	115	VAL
1	B	560	LEU
1	B	224	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	485	GLN
1	B	498	ASN
1	B	555	HIS
1	A	485	GLN
1	A	352	ASN

5.3.3 RNA ⓘ

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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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$
4	EPT	A	602	-	14,14,14	1.29	1 (7%)	16,16,16	1.75	5 (31%)
3	FAD	A	600	1	58,58,58	0.95	5 (8%)	85,89,89	0.77	1 (1%)
3	FAD	B	600	1	58,58,58	0.94	5 (8%)	85,89,89	0.76	1 (1%)

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	EPT	A	602	-	-	5/7/7/7	0/1/1/1
3	FAD	A	600	1	-	4/34/50/50	0/6/6/6
3	FAD	B	600	1	-	4/34/50/50	0/6/6/6

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	FAD	P-O3P	3.50	1.63	1.59
3	A	600	FAD	P-O3P	3.37	1.63	1.59
3	A	600	FAD	PA-O3P	3.34	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	FAD	PA-O3P	3.24	1.63	1.59
4	A	602	EPT	C5-C4	-3.16	1.33	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	EPT	C6-C5-C4	3.72	123.81	119.88
4	A	602	EPT	C9-C8-C7	-3.02	101.14	113.74
4	A	602	EPT	C2-C3-C4	-2.85	116.86	119.88
4	A	602	EPT	C5-C6-C1	-2.84	117.27	121.00
4	A	602	EPT	C3-C2-C1	2.48	124.25	121.00

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

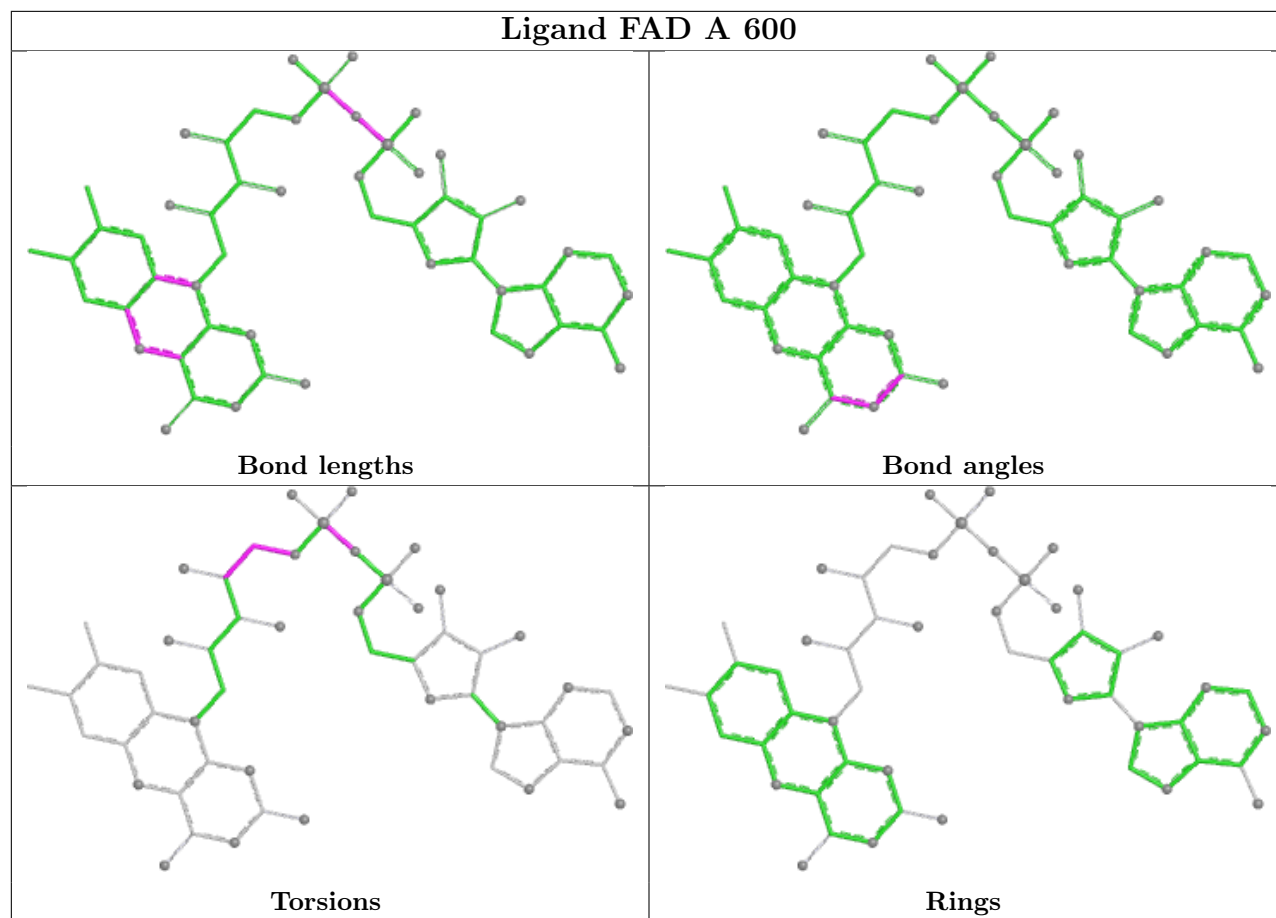
Mol	Chain	Res	Type	Atoms
4	A	602	EPT	C11-C10-C9-C8
3	A	600	FAD	C3'-C4'-C5'-O5'
3	B	600	FAD	C3'-C4'-C5'-O5'
3	A	600	FAD	C4'-C5'-O5'-P
3	B	600	FAD	C4'-C5'-O5'-P

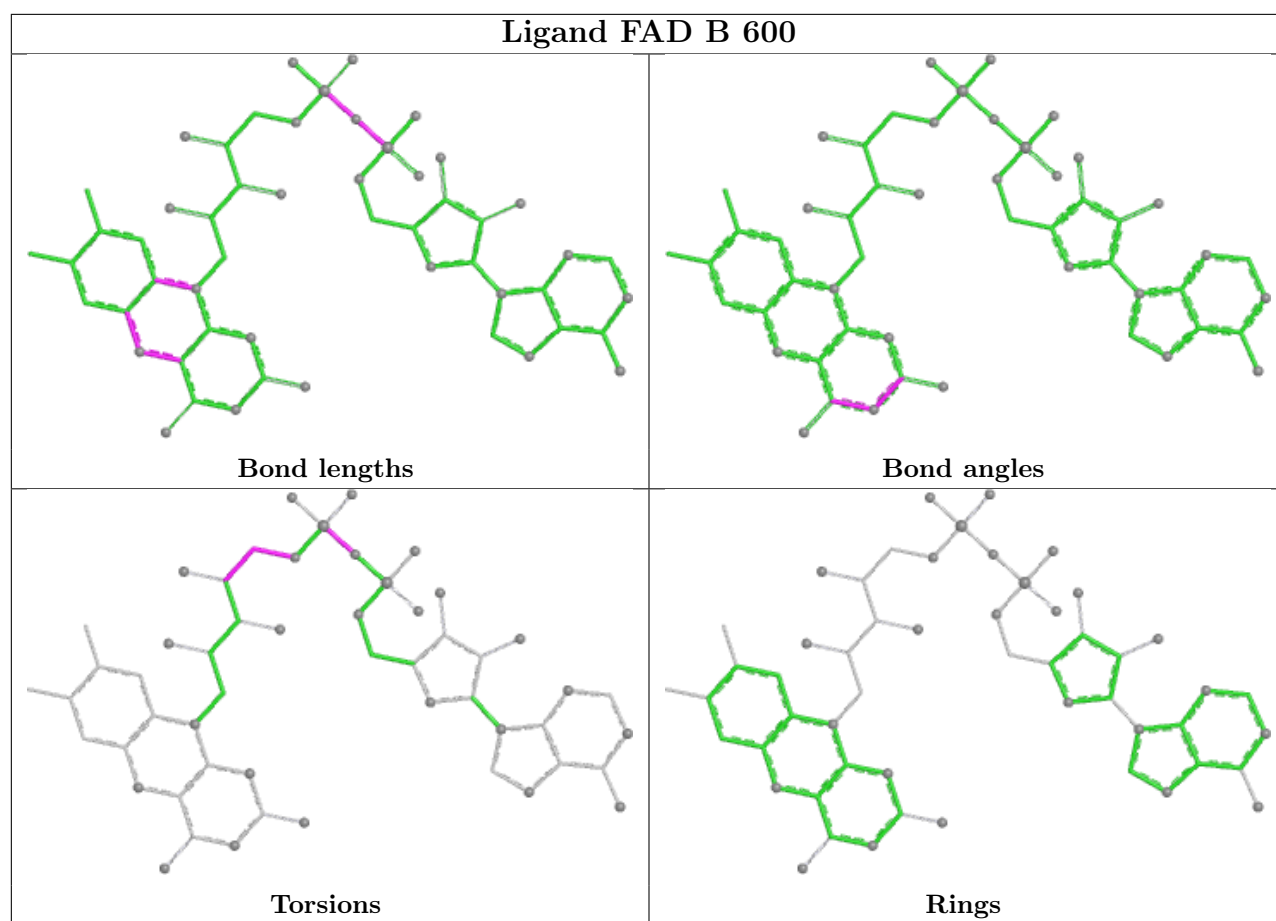
There are no ring outliers.

3 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	EPT	14	0
3	A	600	FAD	9	0
3	B	600	FAD	8	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.