



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:21 AM UTC

PDB ID : 1AHV / pdb_00001ahv
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH 2-NITRO-P-CRESOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 3.10 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

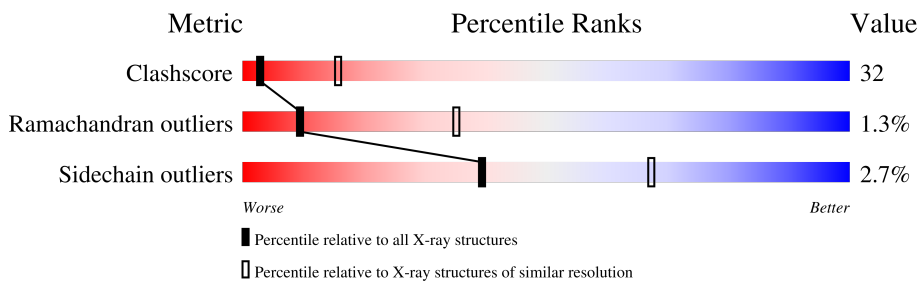
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	

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	NCR	A	601	-	-	X	-
3	NCR	B	601	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8910 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.

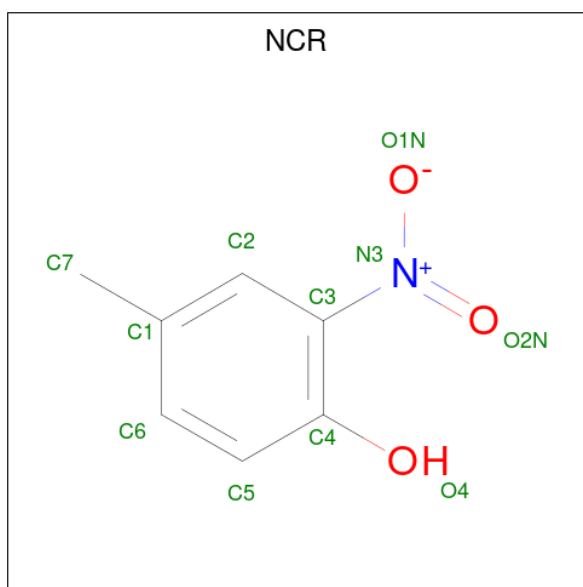
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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-NITRO-P-CRESOL (CCD ID: NCR) (formula: C₇H₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		



I540	I541	K545	S546	W549	P550	S551	Q552	H555	W558	K559	L560	V460	G461	M462	R463	E464	M465	H466	H467	I468	C470	I471	M474	Q480	K481	V484	Q485	M488	R489	I492	C495	A496	A497	N498	G499	W500	G501	E502	Y503	R504	T505	A508	F509	M510	D511	Q512	I513	M518	W519	S522	R526	F527	V530	L531	W535	D536	P537	T389	P390	E391	N392	S393	V394	L395	R396	K400	Q403	G404	I405	E410	L411	K412	W413	D415	W416	L417	P418	N419	R422	F424	F425	S426	P427	I428	A429	K430	V431	S432	G433	E434	M437	M438	Q439	V442	T443	K444	K445	R446	C447	Q448	E449	A450	G451	L452	D453	T457	F458	T459	R161	D162	K163	L164	W165	L166	D167	V168	P169	D170	L171	G172	G173	G174	S175	V176	L177	G178	R183	G184	V185	G186	Y187	T188	P189	Y190	G191	D192	H193	W194	M195	M196	H197	S198	E201	V202	N206	R211	M214	G215	A216	L217	P218	K221	R222	P223	E224	T225	L228	K229	P230	E231	D232	Q233	P234	W235	S236	K237	L238	A239	H240	L241	F242	P243	Y244	G247	P248	I250	D251	S257	N258	M259	V262	T263	K264	L265	W268	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	I296	R297	P298	L301	A304	L305	Q306	N307	W308	P309	T310	I311	R312	H313	I314	I315	L316	D317	A318	A319	V320	L321	G322	D323	K324	R325	R330	T331	E332	P333	E337	A343	L348	G349	R350	W351	N352	F353	G359	P360	E361	P362	I363	R364	R365	V366	L367	I371	V381	K382	F383	Y384	F385	P386	E387	D388
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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	140.62Å 140.62Å 132.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10	Depositor
% Data completeness (in resolution range)	94.3 (30.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.62	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.205 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8910	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: FAD, NCR

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	0.43	0/4511	1.47	77/6131 (1.3%)
1	B	0.43	0/4511	1.47	77/6131 (1.3%)
All	All	0.43	0/9022	1.47	154/12262 (1.3%)

There are no bond length outliers.

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	TYR	N-CA-C	15.44	131.68	112.23
1	B	187	TYR	N-CA-C	15.42	131.66	112.23
1	B	7	PHE	N-CA-C	15.23	130.89	111.24
1	A	7	PHE	N-CA-C	15.21	130.87	111.24
1	B	129	ARG	N-CA-C	13.22	129.79	110.10

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	293	0
1	B	4391	0	4330	292	0
2	A	53	0	29	6	0
2	B	53	0	29	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	11	0	6	6	0
3	B	11	0	6	7	0
All	All	8910	0	8730	566	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 32.

The worst 5 of 566 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:314:ILE:HD11	1:A:350:ARG:HG3	1.32	1.08
1:B:314:ILE:HD11	1:B:350:ARG:HG3	1.32	1.08
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.38	1.02
2:B:600:FAD:H51A	2:B:600:FAD:H8A	1.38	1.02
1:A:202:VAL:HG12	1:A:262:VAL:HA	1.52	0.92

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%)	510 (92%)	36 (6%)	7 (1%)	9	35
1	B	553/560 (99%)	509 (92%)	37 (7%)	7 (1%)	9	35
All	All	1106/1120 (99%)	1019 (92%)	73 (7%)	14 (1%)	9	35

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	GLY

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Mol	Chain	Res	Type
1	A	170	ASP
1	A	418	PRO
1	B	49	GLY

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%)	462 (97%)	13 (3%)	39	67
1	B	475/482 (98%)	462 (97%)	13 (3%)	39	67
All	All	950/964 (98%)	924 (97%)	26 (3%)	39	67

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	128	ASN
1	B	177	LEU
1	B	503	TYR
1	B	163	LYS
1	B	206	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	352	ASN
1	B	485	GLN
1	A	352	ASN
1	A	306	GLN
1	B	498	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](#)

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$
3	NCR	A	601	-	11,11,11	0.77	0	11,15,15	1.22	0
2	FAD	A	600	1	58,58,58	0.92	4 (6%)	85,89,89	0.77	1 (1%)
2	FAD	B	600	1	58,58,58	0.92	4 (6%)	85,89,89	0.78	1 (1%)
3	NCR	B	601	-	11,11,11	0.76	0	11,15,15	1.23	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	NCR	A	601	-	-	0/2/4/4	0/1/1/1
2	FAD	A	600	1	-	6/34/50/50	0/6/6/6
2	FAD	B	600	1	-	6/34/50/50	0/6/6/6
3	NCR	B	601	-	-	0/2/4/4	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	P-O3P	3.23	1.63	1.59
2	A	600	FAD	P-O3P	3.19	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	PA-O3P	3.00	1.62	1.59
2	B	600	FAD	PA-O3P	2.98	1.62	1.59
2	B	600	FAD	C5X-N5	-2.34	1.35	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	C4-N3-C2	-2.32	121.52	125.64
2	A	600	FAD	C4-N3-C2	-2.31	121.54	125.64

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

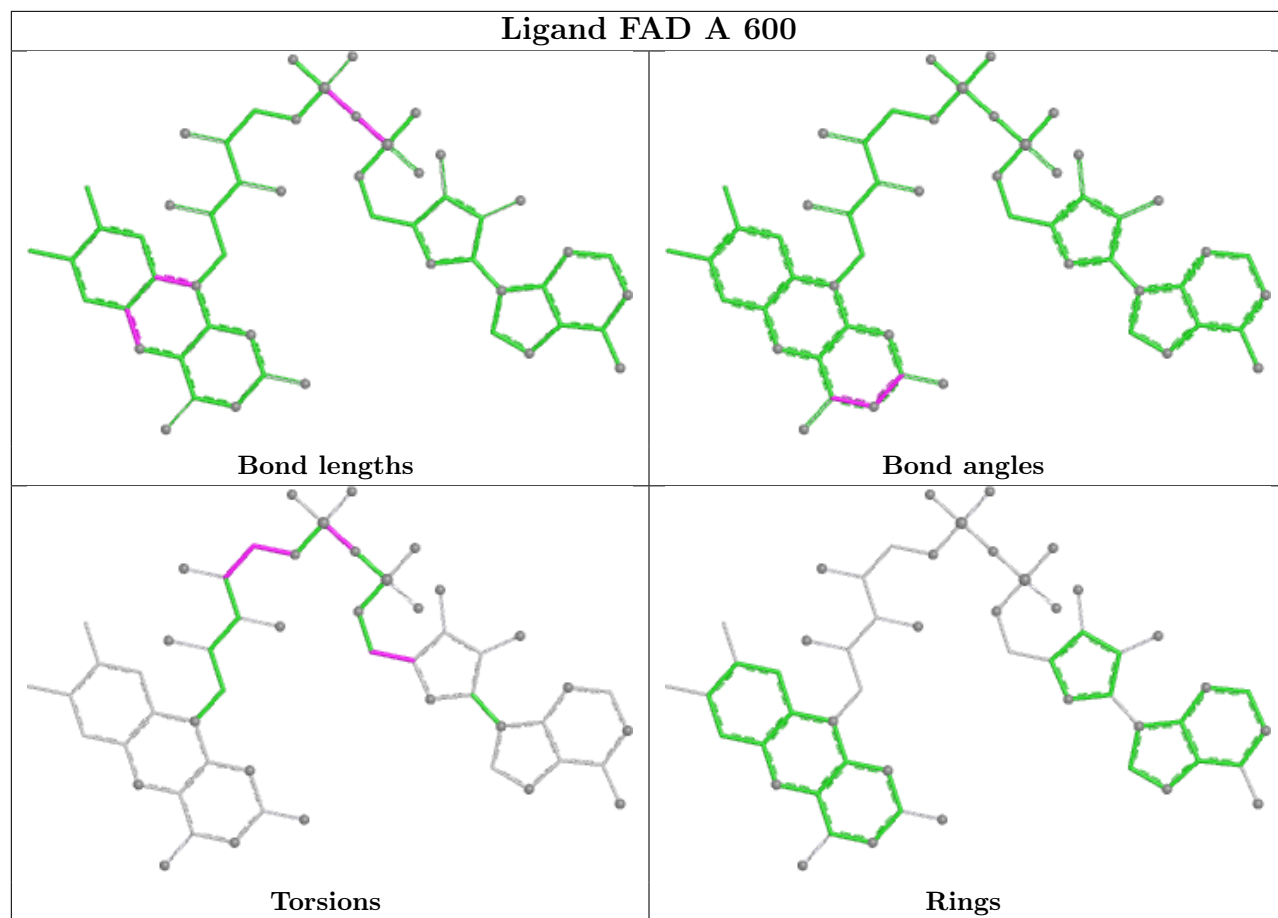
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C3'-C4'-C5'-O5'
2	B	600	FAD	C3'-C4'-C5'-O5'
2	A	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	O4'-C4'-C5'-O5'

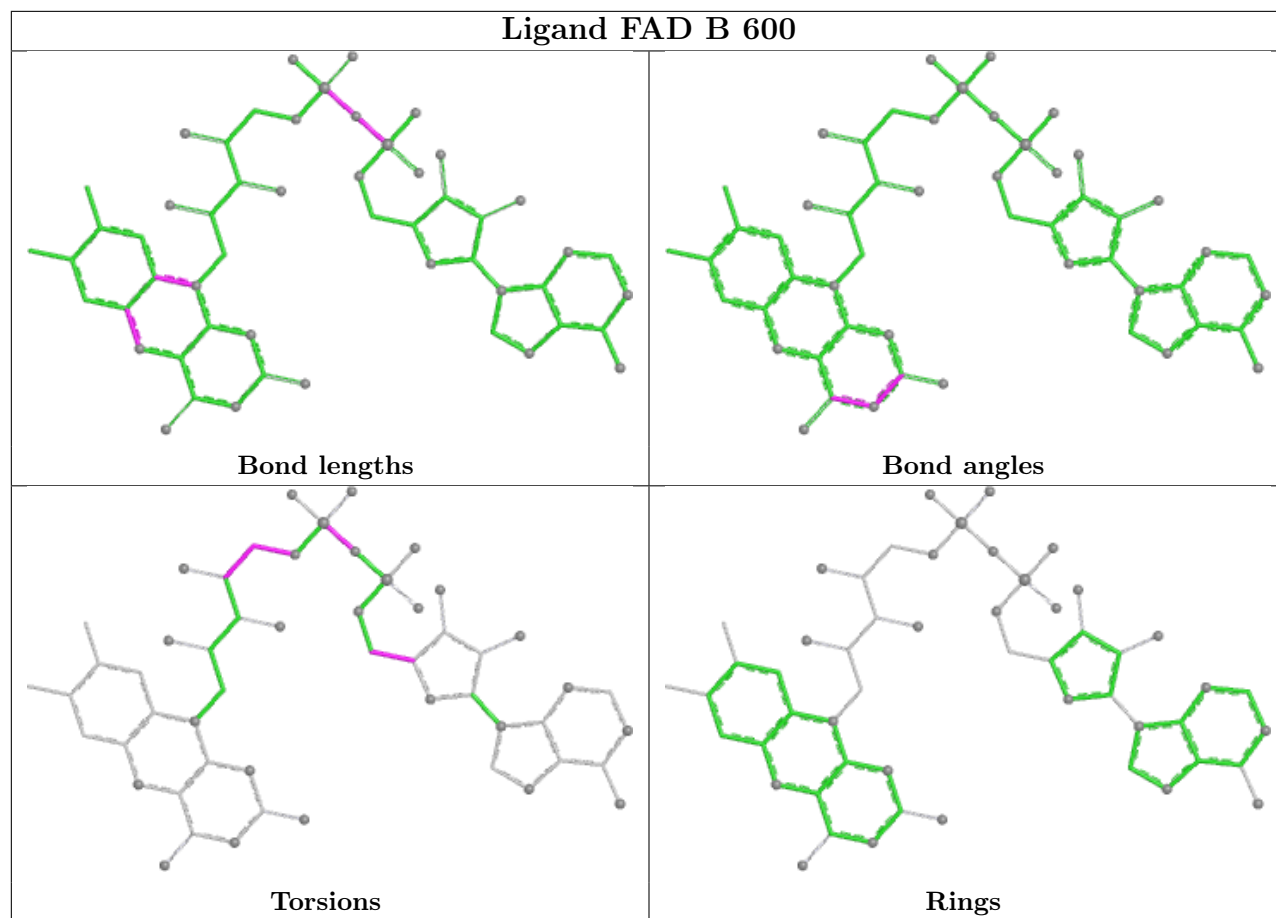
There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NCR	6	0
2	A	600	FAD	6	0
2	B	600	FAD	6	0
3	B	601	NCR	7	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.