



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:14 AM UTC

PDB ID : 1AHU / pdb_00001ahu
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH P-CRESOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 2.70 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

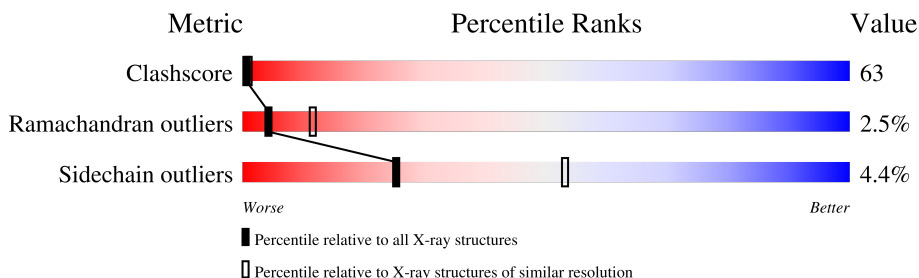
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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](#)

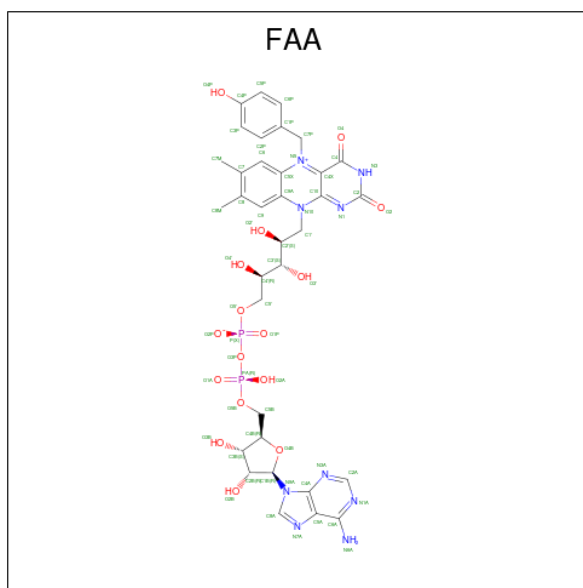
There are 3 unique types of molecules in this entry. The entry contains 9011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	37	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	37	0	0
			4391	2817	751	799	24			

- Molecule 2 is N5-(4-HYDROXYBENZYL)FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAA) (formula: C₃₄H₃₉N₉O₁₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			61	34	9	16	2		
2	B	1	Total	C	N	O	P	0	0
			61	34	9	16	2		

- Molecule 3 is water.

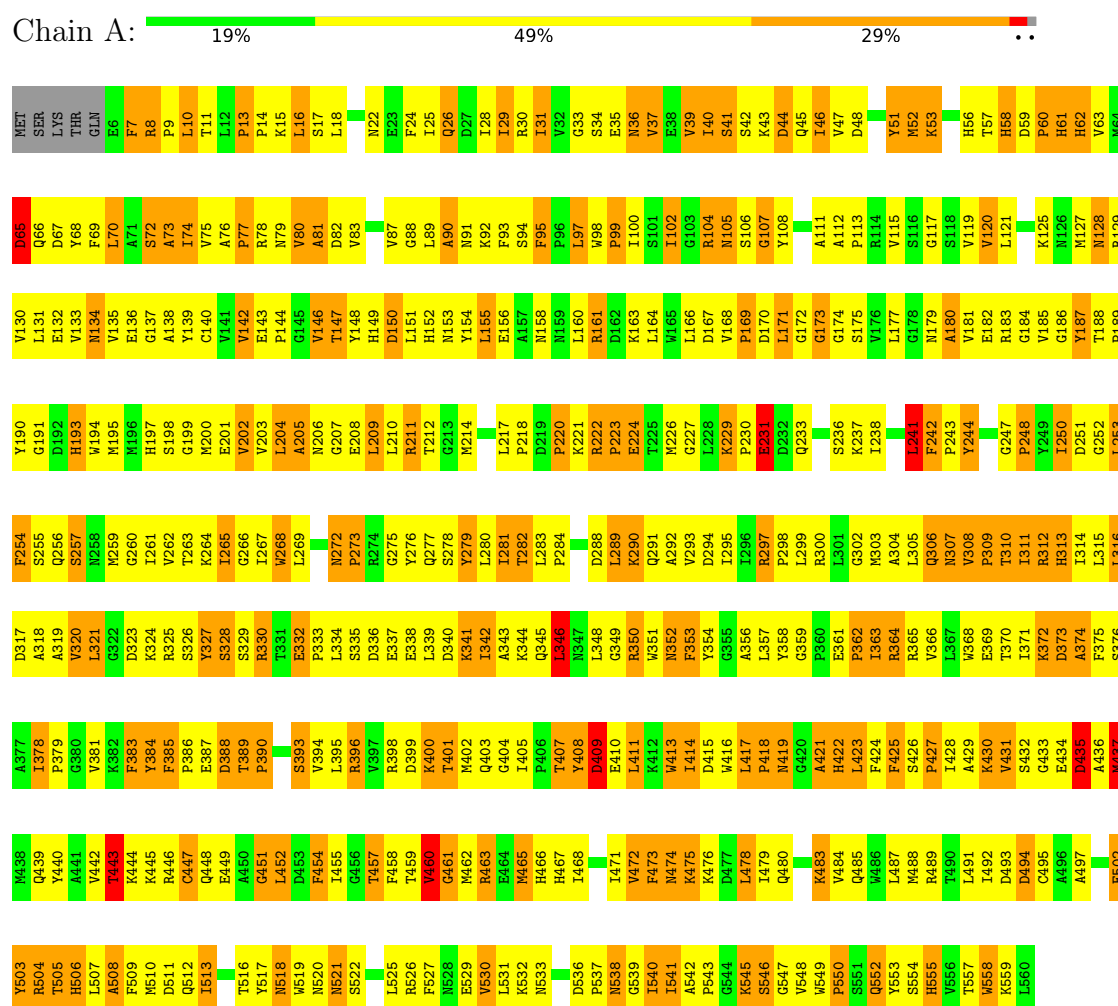
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	52	Total 52	O 52	1	0

3 Residue-property plots

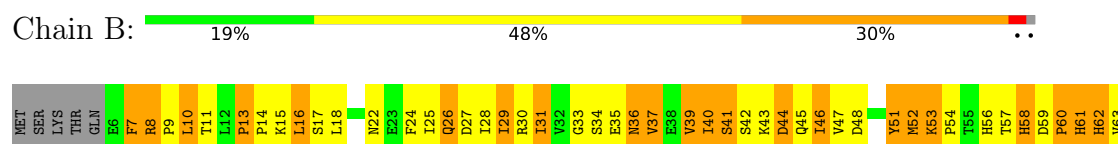
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



A436	F375	L315	L253	P189	R129	W64
R437	S376	L316	F254	Y190	V130	D65
M438	A377	D317	S255	G191	E131	Q66
Q439	I378	A318	S256	D192	E132	D67
Y440	P379	A319	S257	H193	V133	Y68
A441	G380	V320	M258	W194	M134	F69
V442	V381	L321	M259	M195	V135	L70
T443	K382	G322	G260	M196	E136	A71
K444	F383	D323	L261	H197	G137	S72
K445	Y384	K324	V262	S198	A138	A73
R446	F385	K325	T263	G199	Y139	I74
C447	P386	S326	K264	M200	C140	V75
Q448	E387	Y327	L265	E201	V141	A76
E449	D388	S328	G266	V202	V142	P77
A450	T389	S329	L267	V203	E143	R78
L452	P390	R330	W268	L204	P144	N79
D453	S393	T331	L269	A205	G145	V80
F454	V394	E332	M270	N206	V146	A81
I455	L395	P333	P271	G207	T147	D82
G456	R396	L334	M272	E208	Y148	V83
T457	V397	S335	P273	L209	H149	
F458	R398	D336	R274	L210	D150	V87
T459	D399	E337	G275	R211	L151	G88
Y460	K400	E338	Y276	T212	H152	L89
G461	T401	L339	Q277	G213	N153	A90
M462	M402	D340	S278	M214	Y154	N91
R463	Q403	K341	Y279	L217	L155	R92
E464	G404	L342	L280	E156	F93	F93
M465	I405	K343	T281	P218	A157	S94
H466	Q406	K344	T282	D219	N158	F95
H467	T407	Q345	L283	P220	M159	P96
I468	Y408	R346	P284	K221	L160	L97
	D409	M347		R222	R161	W98
I471	E410	L348	D288	P223	K162	P99
V472	L411	R350	K290	E224	K163	I100
F473	K412	W351	Q291	T225	L164	S101
M474	W413	N352	A292	M226	W165	I102
K475	I414	F353	G293	G227	L166	G103
K476	D415	Y354	D294	L228	D167	R104
D477	W416	G355	T295	K229	V168	N105
L478	L417	A356	I296	P230	P169	S106
I479	P418	L357	R297	E231	D170	G107
M419	M419	Y358	P298	D232	L171	Y108
G420	G420	G359	L299	Q233	G172	
K483	A421	P360	R300	S236	G173	A111
V484	H422	E361	L301	G174	S175	A112
Q485	L423	P362	G302	S176	P113	P113
W486	F424	I363	M303	I238	V176	R114
L487	F425	R364	A304	L177	G178	V115
M488	S426	R365	L305	L241	S116	G117
R489	P427	V366	Q306	F242	N179	G117
T490	I428	L367	N307	P243	A180	S118
W491	A429	W368	V308	Y244	V181	V119
I492	K430	E369	P309	G247	E182	V120
D493	V431	T370	I310	P248	R183	G184
D494	S432	I371	I311	Y249	V185	K125
C495	E433	K372	R312	D250	G186	M126
A496	E434	D373	H187	T188	Y187	M127
A497	D435	A374	I314			N128

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	128.82Å 128.82Å 130.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.4 (30.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.97	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.221 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9011	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: FAA

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	6/4511 (0.1%)	2.33	281/6131 (4.6%)
1	B	0.95	6/4511 (0.1%)	2.33	278/6131 (4.5%)
All	All	0.95	12/9022 (0.1%)	2.33	559/12262 (4.6%)

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 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	MET	SD-CE	-6.00	1.64	1.79
1	B	226	MET	SD-CE	-5.99	1.64	1.79
1	B	513	ILE	CA-CB	-5.60	1.47	1.54
1	A	513	ILE	CA-CB	-5.59	1.47	1.54
1	A	264	LYS	CA-C	-5.37	1.46	1.52

The worst 5 of 559 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	TYR	N-CA-C	20.62	133.84	111.36
1	B	187	TYR	N-CA-C	20.58	133.79	111.36
1	B	404	GLY	CA-C-N	-14.25	112.33	122.59
1	B	404	GLY	C-N-CA	-14.25	112.33	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	129	ARG	N-CA-C	14.23	132.68	110.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	187	TYR	CA
1	A	332	GLU	CA
1	B	187	TYR	CA
1	B	332	GLU	CA

There are no planarity outliers.

5.2 Too-close contacts

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	547	0
1	B	4391	0	4330	565	0
2	A	61	0	35	12	0
2	B	61	0	35	13	0
3	A	55	0	0	9	0
3	B	52	0	0	9	0
All	All	9011	0	8730	1090	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 63.

The worst 5 of 1090 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:507:LEU:HA	1:A:510:MET:HE3	1.18	1.18
1:B:507:LEU:HA	1:B:510:MET:HE3	1.18	1.16
2:A:600:FAA:H51A	2:A:600:FAA:H8A	1.21	1.13
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.32	1.11
2:B:600:FAA:H51A	2:B:600:FAA:H8A	1.21	1.10

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%)	470 (85%)	69 (12%)	14 (2%)	4	11
1	B	553/560 (99%)	470 (85%)	69 (12%)	14 (2%)	4	11
All	All	1106/1120 (99%)	940 (85%)	138 (12%)	28 (2%)	4	11

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	B	44	ASP
1	A	30	ARG
1	A	46	ILE
1	A	328	SER

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%)	454 (96%)	21 (4%)	25	53
1	B	475/482 (98%)	454 (96%)	21 (4%)	25	53
All	All	950/964 (98%)	908 (96%)	42 (4%)	25	53

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

Mol	Chain	Res	Type
1	B	231	GLU
1	B	413	TRP
1	B	241	LEU
1	B	363	ILE
1	B	437	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	152	HIS
1	B	403	GLN
1	B	240	HIS
1	B	448	GLN
1	A	448	GLN

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](#)

2 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	FAA	A	600	1	65,67,67	0.92	4 (6%)	89,102,102	1.52	6 (6%)
2	FAA	B	600	1	65,67,67	0.92	4 (6%)	89,102,102	1.52	6 (6%)

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	FAA	A	600	1	-	11/38/54/54	0/7/7/7
2	FAA	B	600	1	-	11/38/54/54	0/7/7/7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAA	PA-O3P	3.69	1.63	1.59
2	B	600	FAA	PA-O3P	3.57	1.63	1.59
2	B	600	FAA	P-O3P	3.52	1.63	1.59
2	A	600	FAA	P-O3P	3.48	1.63	1.59
2	A	600	FAA	C5X-N5	-2.38	1.36	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAA	C7P-N5-C5X	-11.26	102.71	119.14
2	B	600	FAA	C7P-N5-C5X	-11.26	102.72	119.14
2	B	600	FAA	C1P-C7P-N5	-4.03	106.81	112.85
2	A	600	FAA	C1P-C7P-N5	-4.00	106.85	112.85
2	B	600	FAA	C6-C5X-N5	-2.90	116.92	120.41

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

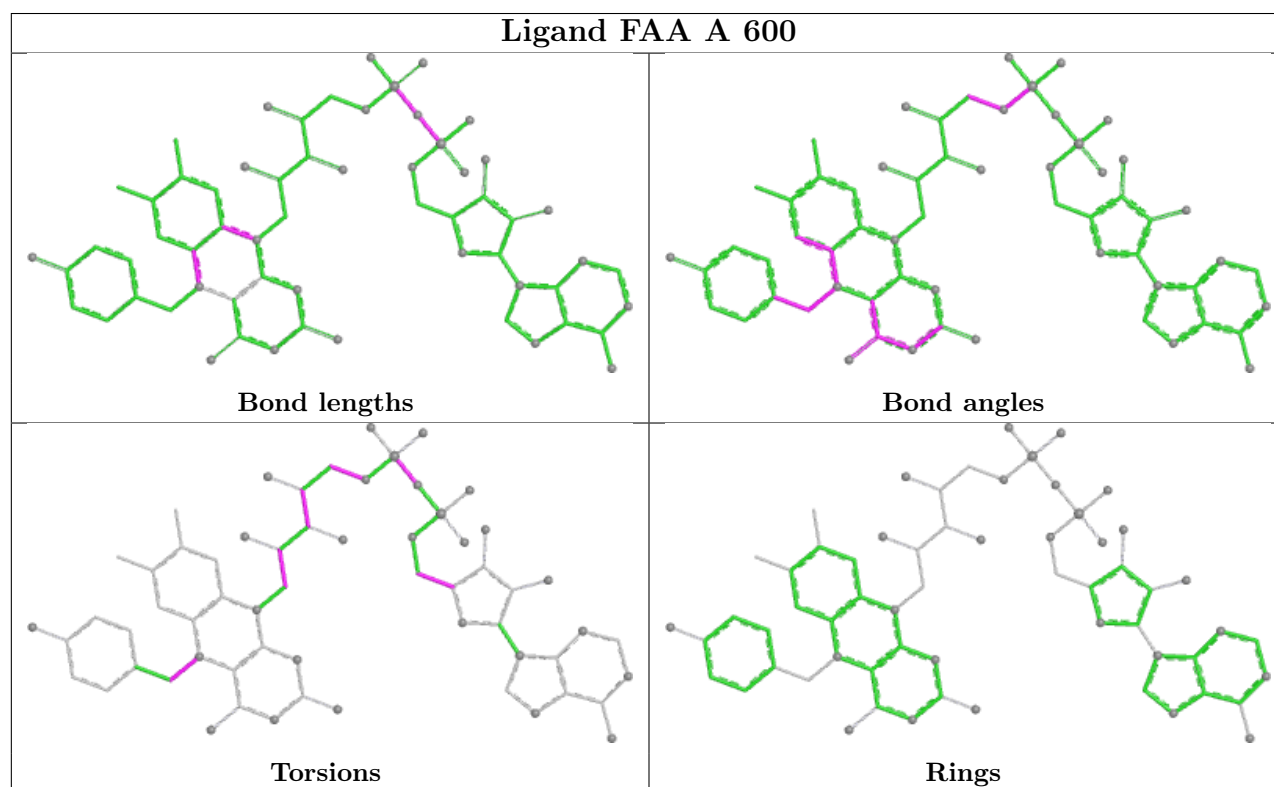
Mol	Chain	Res	Type	Atoms
2	A	600	FAA	C1P-C7P-N5-C4X
2	A	600	FAA	N10-C1'-C2'-O2'
2	A	600	FAA	N10-C1'-C2'-C3'
2	B	600	FAA	C1P-C7P-N5-C4X
2	B	600	FAA	N10-C1'-C2'-O2'

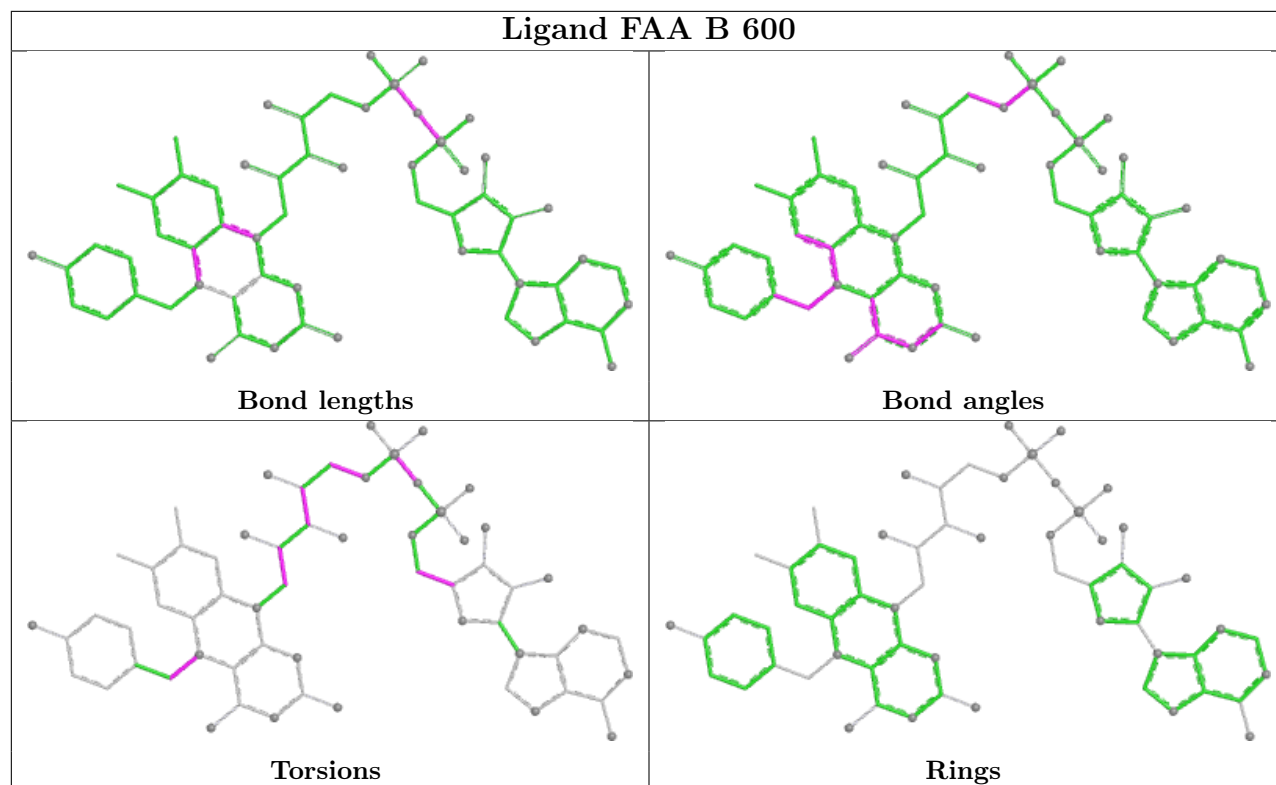
There are no ring outliers.

2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAA	12	0
2	B	600	FAA	13	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.