



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:03 PM UTC

PDB ID : 1W1M / pdb_00001w1m
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE: Glu502Gly Mutant
Authors : Van Den Heuvel, R.H.
Deposited on : 2004-06-22
Resolution : 3.00 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

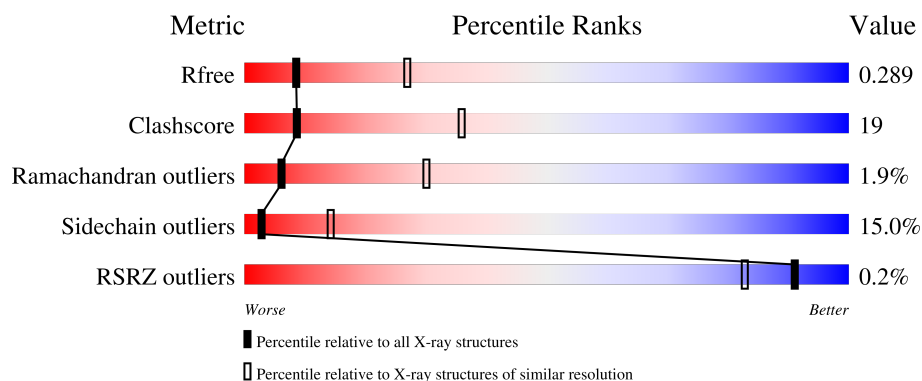
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8820 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	0	0	0
			4346	2790	744	788	24			
1	B	550	Total	C	N	O	S	0	0	0
			4346	2790	744	788	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	GLY	GLU	engineered mutation	UNP P56216
B	502	GLY	GLU	engineered mutation	UNP P56216

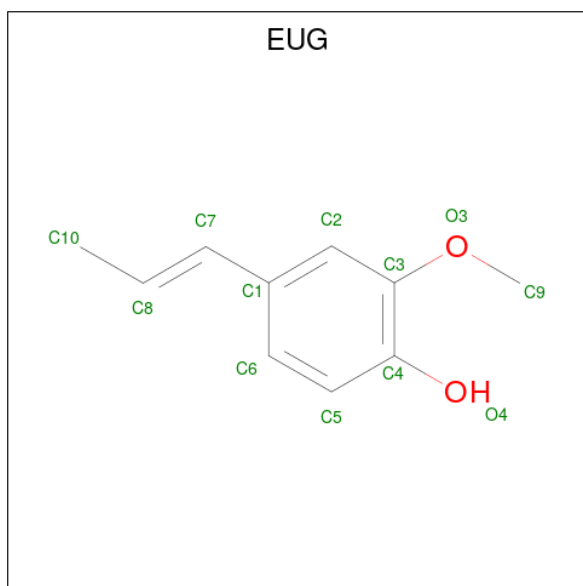
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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: C₁₀H₁₂O₂).

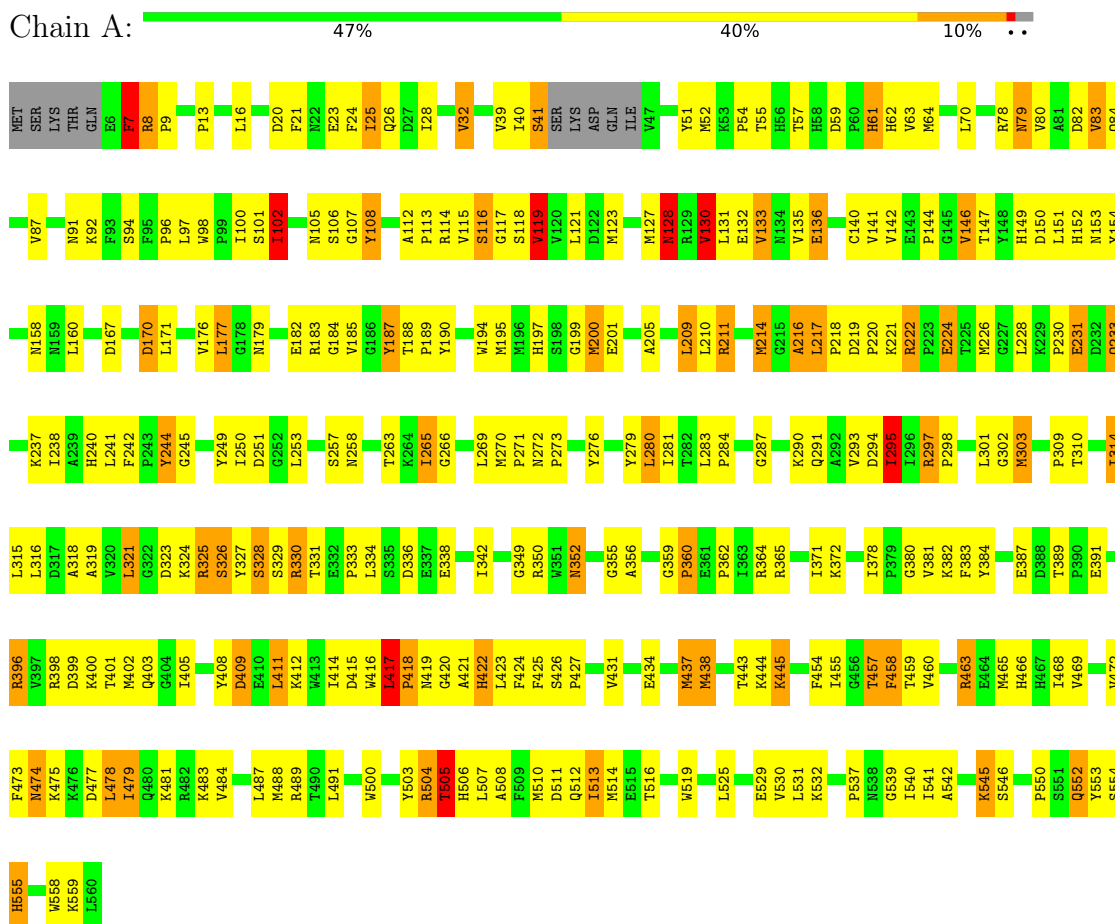


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	9	2		
3	B	1	Total	C	O	0	0
			11	9	2		

3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: VANILLYL-ALCOHOL OXIDASE



E201	V202	L210	R211	M214	L217	K229	P230	E231	I238	L241	Y244	G245	F246	G247	P248	D251	F254	S255	N258	I261	V262	T263	K264	I265	G266	I267	W268	L269	M270	P271	N272	F273	R274	S278	T282	K285	D288	L289	K290	V293	I296			
R297	P298	L301	G302	M303	N307	V308	P309	T310	I311	R312	A319	V320	L321	G322	D323	K324	S329	R330	T331	F332	P333	D336	K341	K344	G349	N352	F353	Y354	L357	Y358	E361	P362	W368	E369	K372	P390	E391	N392	S393	R396	V397	R398	D399	
Q403	G404	I405	P406	T407	L411	K412	W413	I414	D415	W416	L417	P418	A421	H422	S426	K430	V431	S432	G433	W438	T443	K444	K445	R446	C447	Q448	G451	T457	F458	T459	V460	R463	H466	H467	I468	V472	F473	N474	D477	Q480	K483	V484	L487	M488
R489	A496	A497	N498	G499	W500	Y503	R504	T505	H506	L507	D511	Q512	I513	T516	Y517	N518	W519	N520	L525	R526	F527	N528	E529	V530	L531	K532	V535	D536	I540	I541	P550	S551	Q552	Y553	L560									

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	129.91Å 129.91Å 134.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (40.00-3.00) 97.4 (40.00-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1.27	Depositor
R, R_{free}	0.217 , 0.307 0.199 , 0.289	Depositor DCC
R_{free} test set	1114 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h 0.013 for -l,-k,-h 0.022 for -h,-l,-k 0.008 for -h,l,k 0.042 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8820	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.95	5/4465 (0.1%)	1.25	25/6068 (0.4%)
1	B	0.70	1/4465 (0.0%)	1.05	6/6068 (0.1%)
All	All	0.83	6/8930 (0.1%)	1.16	31/12136 (0.3%)

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	0	2
1	B	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	MET	SD-CE	6.62	1.96	1.79
1	B	303	MET	SD-CE	5.89	1.94	1.79
1	A	119	VAL	CA-CB	5.88	1.60	1.53
1	A	389	THR	CA-C	5.54	1.57	1.52
1	A	530	VAL	CA-CB	5.31	1.60	1.54

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	THR	N-CA-C	10.35	121.89	108.34
1	B	48	ASP	N-CA-C	7.66	120.70	111.82
1	B	505	THR	N-CA-C	7.53	120.18	108.96
1	A	244	TYR	N-CA-C	6.89	120.92	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	VAL	N-CA-C	-6.84	97.59	107.78

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	MET	Peptide
1	A	457	THR	Peptide
1	B	127	MET	Peptide

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	4346	0	4285	215	0
1	B	4346	0	4285	125	0
2	A	53	0	29	1	0
2	B	53	0	29	9	0
3	A	11	0	7	1	0
3	B	11	0	7	1	0
All	All	8820	0	8642	329	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 19.

The worst 5 of 329 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)
2:B:1561:FAD:H8A	2:B:1561:FAD:C5B	1.76	1.14
2:B:1561:FAD:H51A	2:B:1561:FAD:C8A	1.80	1.12
1:B:214:MET:HE2	1:B:245:GLY:HA2	1.41	1.01
1:A:552:GLN:H	1:A:552:GLN:HE21	1.10	0.99
1:A:505:THR:HG21	1:A:513:ILE:CD1	1.93	0.98

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	460 (84%)	75 (14%)	11 (2%)	6	28
1	B	546/560 (98%)	495 (91%)	41 (8%)	10 (2%)	6	31
All	All	1092/1120 (98%)	955 (88%)	116 (11%)	21 (2%)	6	30

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	PRO
1	A	83	VAL
1	A	116	SER
1	A	323	ASP
1	B	418	PRO

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	469/481 (98%)	393 (84%)	76 (16%)	2	12
1	B	469/481 (98%)	404 (86%)	65 (14%)	3	17
All	All	938/962 (98%)	797 (85%)	141 (15%)	3	14

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	331	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	357	LEU
1	B	457	THR
1	A	336	ASP
1	A	331	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	HIS
1	B	128	ASN
1	B	520	ASN
1	B	126	ASN
1	B	179	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	B	1561	1	58,58,58	1.24	7 (12%)	85,89,89	1.70	19 (22%)
2	FAD	A	1561	1	58,58,58	1.18	5 (8%)	85,89,89	1.74	22 (25%)
3	EUG	B	1562	-	11,11,12	1.71	1 (9%)	14,14,15	1.49	2 (14%)
3	EUG	A	1562	-	11,11,12	1.70	1 (9%)	14,14,15	1.54	3 (21%)

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	B	1561	1	-	8/34/50/50	0/6/6/6
2	FAD	A	1561	1	-	8/34/50/50	0/6/6/6
3	EUG	B	1562	-	-	4/4/4/5	0/1/1/1
3	EUG	A	1562	-	-	4/4/4/5	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1562	EUG	C4-C3	5.26	1.49	1.40
3	B	1562	EUG	C4-C3	5.25	1.49	1.40
2	B	1561	FAD	C4X-N5	3.53	1.38	1.30
2	A	1561	FAD	C4X-N5	3.48	1.38	1.30
2	A	1561	FAD	C10-N1	3.20	1.39	1.33

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1561	FAD	N3A-C2A-N1A	-6.25	119.13	128.58
2	B	1561	FAD	N3A-C2A-N1A	-6.03	119.46	128.58
2	A	1561	FAD	C5A-C4A-N3A	-5.07	119.74	126.72
2	B	1561	FAD	C5A-C4A-N3A	-4.51	120.50	126.72
3	A	1562	EUG	O3-C3-C4	3.69	120.08	114.55

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1561	FAD	C3'-C4'-C5'-O5'
2	B	1561	FAD	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

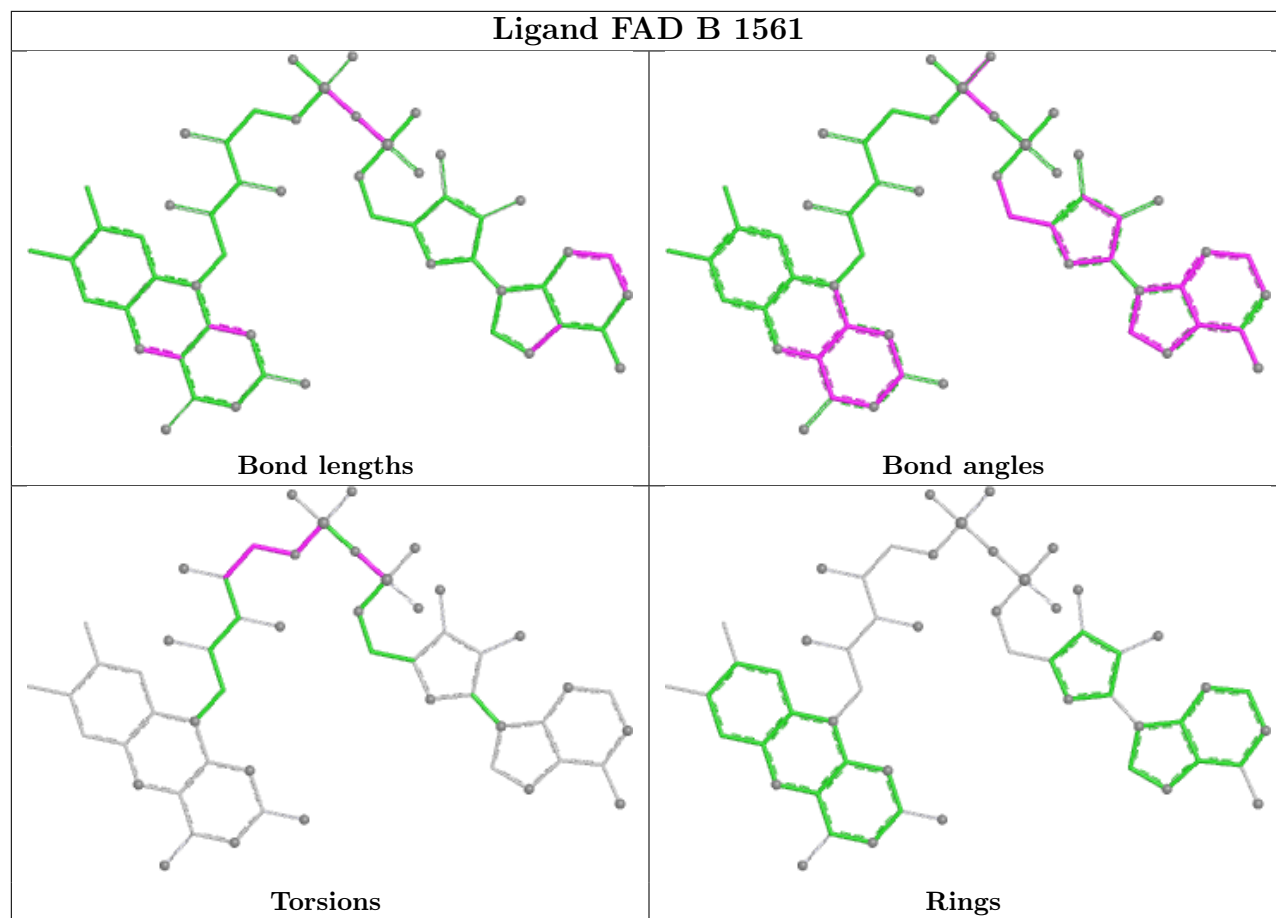
Mol	Chain	Res	Type	Atoms
2	B	1561	FAD	C5'-O5'-P-O1P
3	A	1562	EUG	C2-C1-C7-C8
3	A	1562	EUG	C6-C1-C7-C8

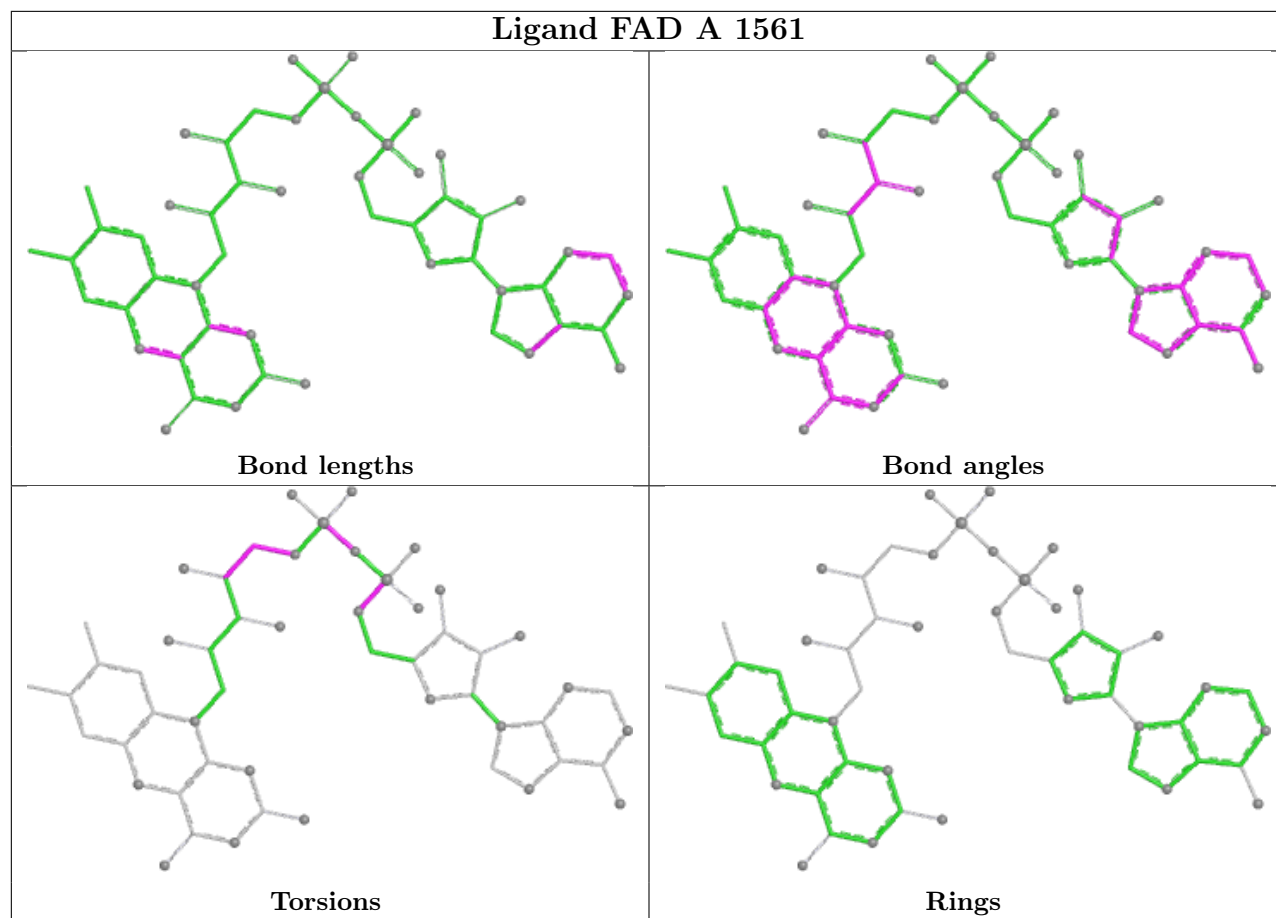
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1561	FAD	9	0
2	A	1561	FAD	1	0
3	B	1562	EUG	1	0
3	A	1562	EUG	1	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](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	550/560 (98%)	-0.72	0	100 100	22, 37, 50, 62	0
1	B	550/560 (98%)	-0.18	2 (0%)	88 76	40, 64, 90, 99	0
All	All	1100/1120 (98%)	-0.45	2 (0%)	91 83	22, 49, 87, 99	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	TYR	2.3
1	B	111	ALA	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

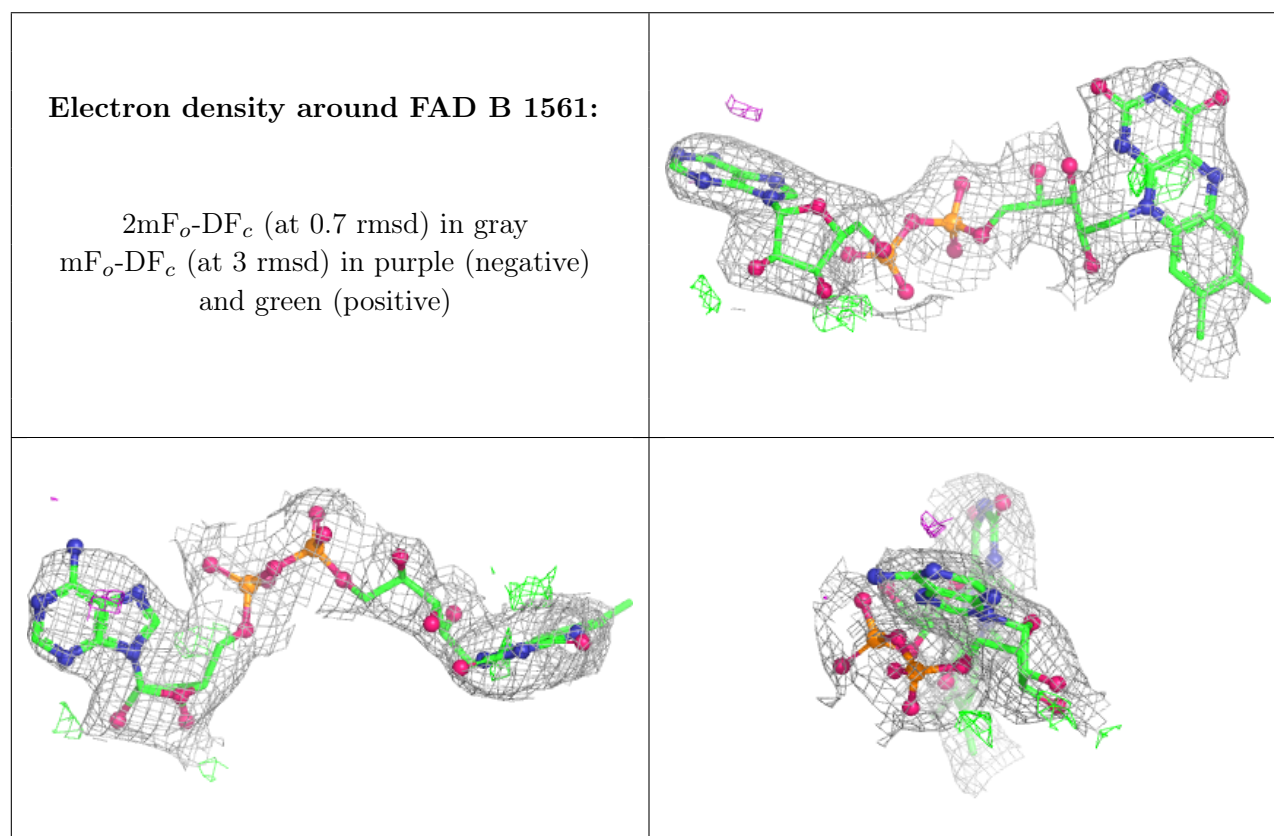
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EUG	A	1562	11/12	0.89	0.13	66,68,70,71	0
2	FAD	B	1561	53/53	0.92	0.10	63,70,83,83	0
3	EUG	B	1562	11/12	0.93	0.09	60,62,63,63	0

Continued on next page...

Continued from previous page...

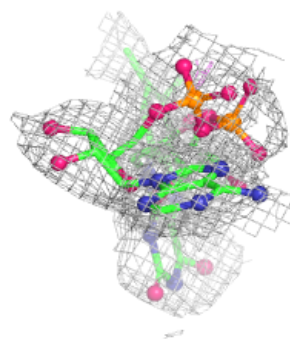
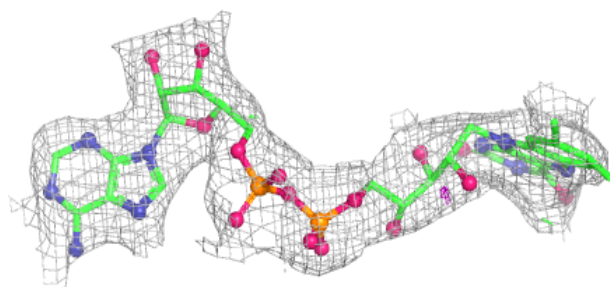
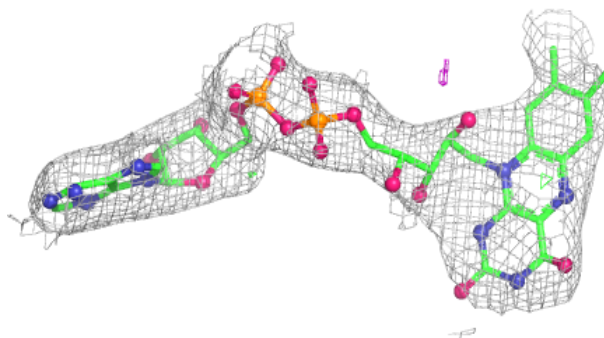
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	1561	53/53	0.95	0.09	54,60,69,71	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around FAD A 1561:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.