



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:09 PM UTC

PDB ID : 1FOH / pdb_00001foh
Title : PHENOL HYDROXYLASE FROM TRICHOSPORON CUTANEUM
Authors : Enroth, C.; Neujahr, H.; Schneider, G.; Lindqvist, Y.
Deposited on : 1998-03-26
Resolution : 2.40 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

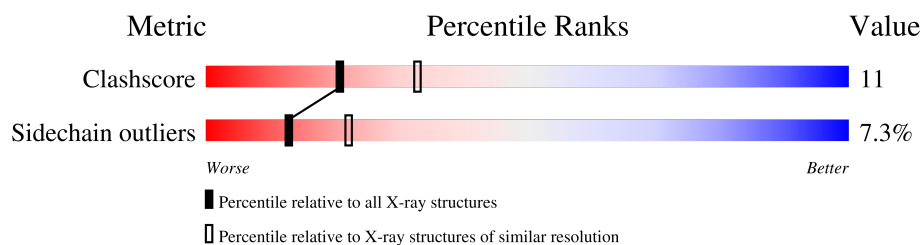
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	664	 73% 20% . . .
1	B	664	 73% 19% 5% . .
1	C	664	 72% 20% 5% . .
1	D	664	 73% 20% 5% . .

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
2	FAD	C	801	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22235 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.

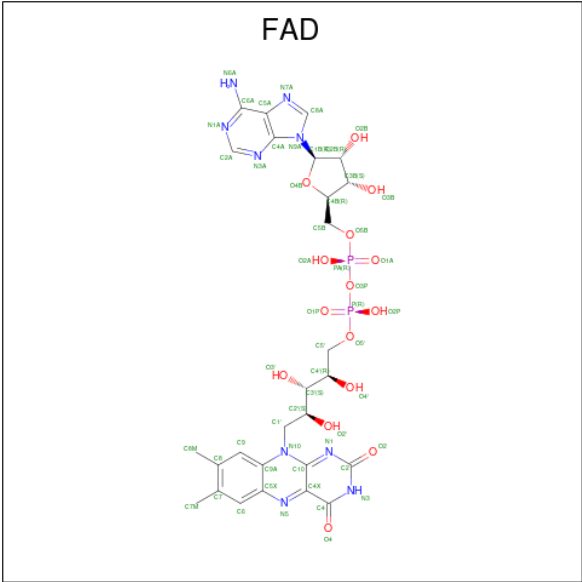
- Molecule 1 is a protein called PHENOL HYDROXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5174	3254	907	989	24			
1	B	651	Total	C	N	O	S	0	0	0
			5186	3261	909	992	24			
1	C	656	Total	C	N	O	S	0	0	0
			5230	3287	920	999	24			
1	D	654	Total	C	N	O	S	0	0	0
			5216	3279	916	997	24			

There are 4 discrepancies between the modelled and reference sequences:

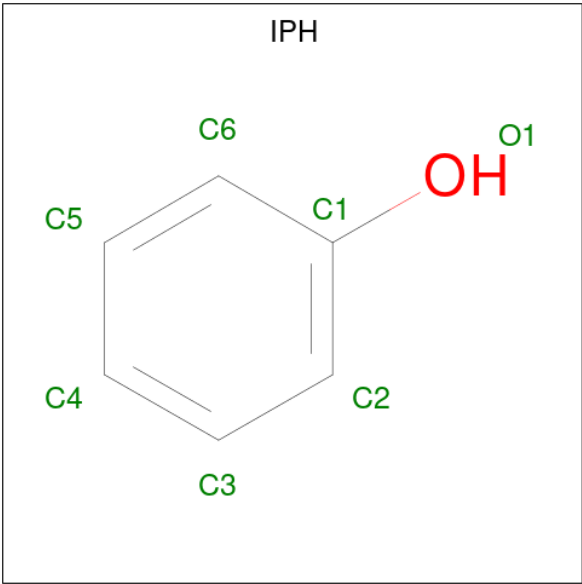
Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ARG	PRO	conflict	UNP P15245
B	265	ARG	PRO	conflict	UNP P15245
C	265	ARG	PRO	conflict	UNP P15245
D	265	ARG	PRO	conflict	UNP P15245

- 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		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 6 1	0	0
3	B	1	Total C O 7 6 1	0	0
3	C	1	Total C O 7 6 1	0	0
3	D	1	Total C O 7 6 1	0	0

- Molecule 4 is water.

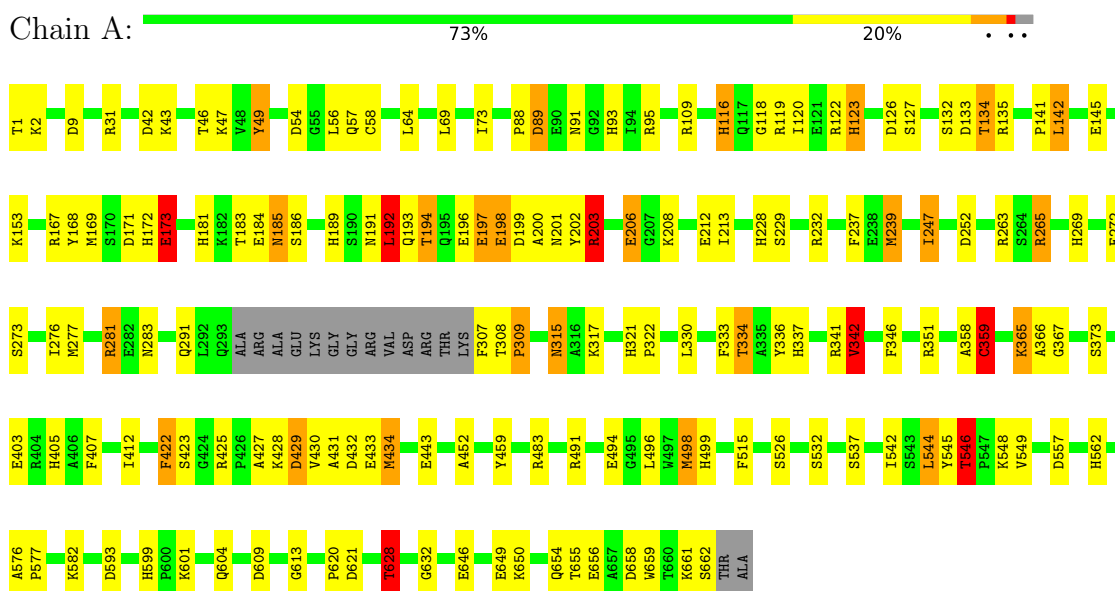
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	341	Total O 341 341	0	0
4	B	296	Total O 296 296	0	0
4	C	302	Total O 302 302	0	0
4	D	250	Total O 250 250	0	0

3 Residue-property plots

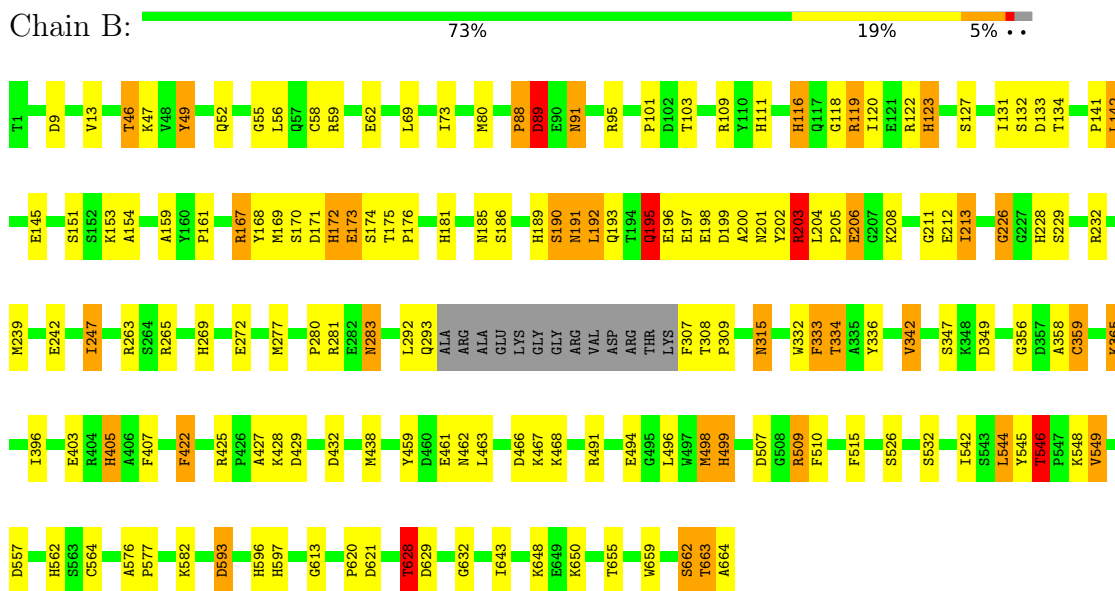
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

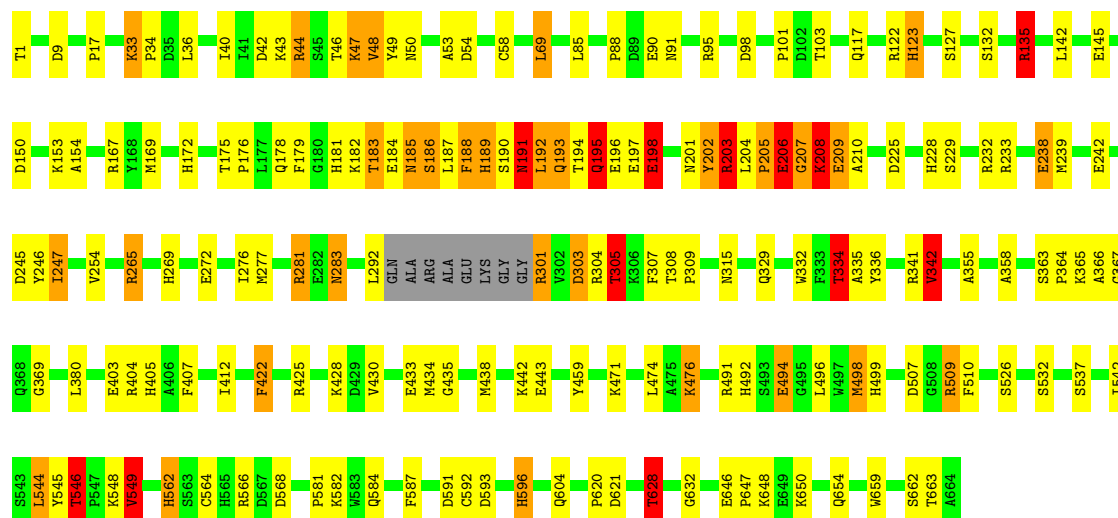


• Molecule 1: PHENOL HYDROXYLASE



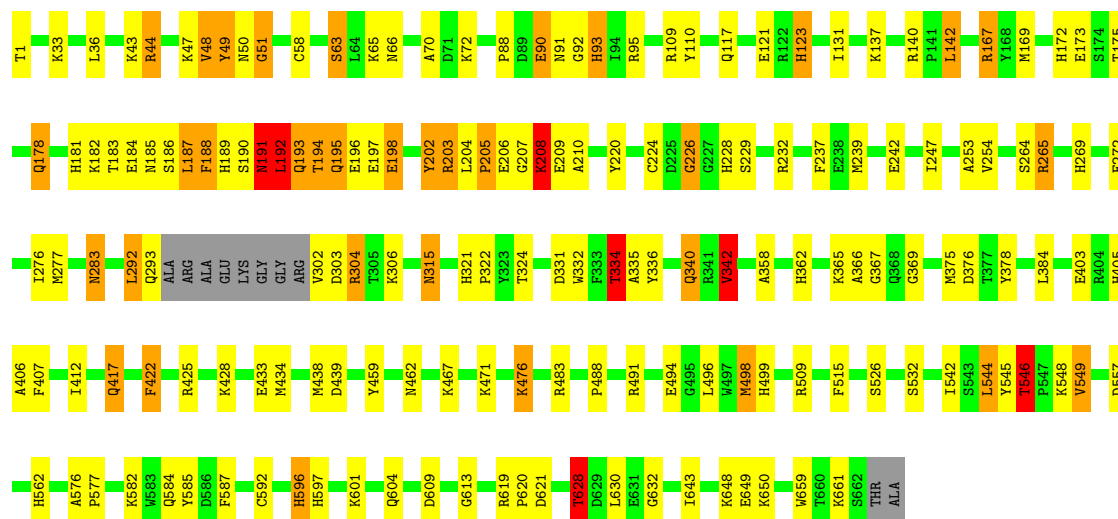
• Molecule 1: PHENOL HYDROXYLASE

Chain C:  72% 20% 5% ..



• Molecule 1: PHENOL HYDROXYLASE

Chain D:  73% 20% 5% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.03Å 150.68Å 114.92Å 90.00° 114.68° 90.00°	Depositor
Resolution (Å)	12.00 – 2.40	Depositor
% Data completeness (in resolution range)	98.0 (12.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22235	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: IPH, FAD

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	0.67	0/5292	1.63	62/7160 (0.9%)
1	B	0.67	0/5304	1.63	85/7177 (1.2%)
1	C	0.72	4/5348 (0.1%)	1.73	97/7235 (1.3%)
1	D	0.71	1/5334 (0.0%)	1.70	99/7216 (1.4%)
All	All	0.69	5/21278 (0.0%)	1.67	343/28788 (1.2%)

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	B	0	1
1	C	0	1
1	D	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	562	HIS	CE1-NE2	-10.44	1.22	1.32
1	C	562	HIS	CG-CD2	-6.75	1.28	1.35
1	C	208	LYS	N-CA	-6.65	1.37	1.46
1	C	562	HIS	CG-ND1	-6.15	1.31	1.38
1	D	621	ASP	CA-CB	6.01	1.63	1.53

The worst 5 of 343 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASP	CA-CB-CG	22.85	135.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	562	HIS	ND1-CG-CD2	-20.04	86.06	106.10
1	C	562	HIS	CG-CD2-NE2	18.71	125.91	107.20
1	D	208	LYS	CA-C-O	14.68	137.55	120.66
1	A	620	PRO	CA-C-N	13.99	144.09	120.72

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	89	ASP	Mainchain
1	C	584	GLN	Mainchain
1	D	488	PRO	Mainchain
1	D	584	GLN	Mainchain

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	5174	0	5038	103	0
1	B	5186	0	5050	90	0
1	C	5230	0	5101	143	0
1	D	5216	0	5084	132	0
2	A	53	0	30	1	0
2	B	53	0	30	0	0
2	C	53	0	29	2	0
2	D	53	0	29	6	0
3	A	7	0	6	0	0
3	B	7	0	6	0	0
3	C	7	0	6	0	0
3	D	7	0	6	0	0
4	A	341	0	0	19	0
4	B	296	0	0	17	0
4	C	302	0	0	17	0
4	D	250	0	0	20	0
All	All	22235	0	20415	460	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 11.

The worst 5 of 460 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:C:167:ARG:NE	1:C:203:ARG:HH21	1.52	1.05
1:C:491:ARG:HB2	1:C:498:MET:HE3	1.39	1.05
1:A:491:ARG:HB2	1:A:498:MET:HE3	1.38	1.02
1:D:491:ARG:HB2	1:D:498:MET:HE3	1.40	0.98
1:C:476:LYS:HE2	4:C:1053:HOH:O	1.62	0.98

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	563/573 (98%)	526 (93%)	37 (7%)	15	26
1	B	564/573 (98%)	527 (93%)	37 (7%)	15	26
1	C	569/573 (99%)	520 (91%)	49 (9%)	10	16
1	D	568/573 (99%)	525 (92%)	43 (8%)	12	21
All	All	2264/2292 (99%)	2098 (93%)	166 (7%)	13	22

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	544	LEU
1	D	276	ILE
1	C	628	THR

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Mol	Chain	Res	Type
1	D	142	LEU
1	D	342	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	315	ASN
1	D	191	ASN
1	C	449	ASN
1	C	584	GLN
1	D	243	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](#)

8 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	C	801	-	58,58,58	1.42	8 (13%)	85,89,89	1.52	15 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IPH	D	802	-	7,7,7	1.06	0	8,8,8	0.95	0
2	FAD	B	801	-	58,58,58	1.40	7 (12%)	85,89,89	1.63	23 (27%)
3	IPH	A	802	-	7,7,7	0.59	0	8,8,8	0.61	0
3	IPH	B	802	-	7,7,7	0.78	0	8,8,8	1.15	1 (12%)
3	IPH	C	802	-	7,7,7	0.64	0	8,8,8	0.94	0
2	FAD	D	801	-	58,58,58	1.39	6 (10%)	85,89,89	1.62	20 (23%)
2	FAD	A	801	-	58,58,58	1.47	6 (10%)	85,89,89	1.61	19 (22%)

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	C	801	-	1/1/9/9	5/34/50/50	0/6/6/6
3	IPH	D	802	-	-	-	0/1/1/1
2	FAD	B	801	-	-	2/34/50/50	0/6/6/6
3	IPH	A	802	-	-	-	0/1/1/1
3	IPH	B	802	-	-	-	0/1/1/1
3	IPH	C	802	-	-	-	0/1/1/1
2	FAD	D	801	-	-	5/34/50/50	0/6/6/6
2	FAD	A	801	-	-	4/34/50/50	0/6/6/6

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C9-C8	-5.18	1.32	1.39
2	B	801	FAD	C9-C8	-5.15	1.32	1.39
2	D	801	FAD	C9-C8	-5.07	1.32	1.39
2	C	801	FAD	C9-C8	-4.89	1.33	1.39
2	A	801	FAD	O2B-C2B	-3.37	1.34	1.43

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O2B-C2B-C1B	4.97	127.22	110.10
2	C	801	FAD	O2B-C2B-C1B	4.84	126.76	110.10
2	C	801	FAD	O2B-C2B-C3B	4.24	125.41	111.82
2	C	801	FAD	C2B-C1B-N9A	4.03	123.33	113.30
2	B	801	FAD	C7M-C7-C6	3.97	126.57	119.57

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	801	FAD	C2B

5 of 16 torsion outliers are listed below:

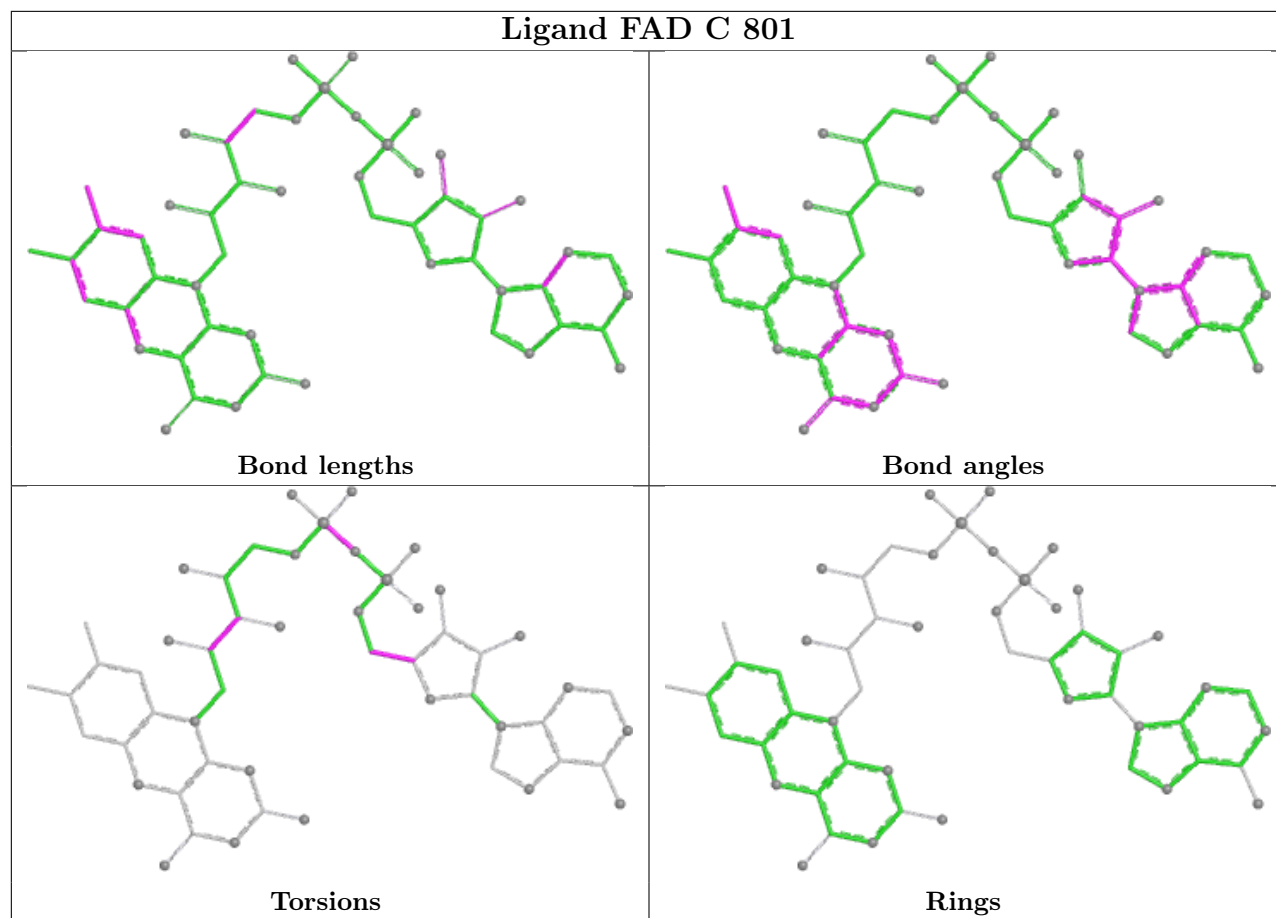
Mol	Chain	Res	Type	Atoms
2	A	801	FAD	N10-C1'-C2'-O2'
2	A	801	FAD	C5'-O5'-P-O1P
2	A	801	FAD	C5'-O5'-P-O3P
2	C	801	FAD	C1'-C2'-C3'-C4'
2	C	801	FAD	PA-O3P-P-O5'

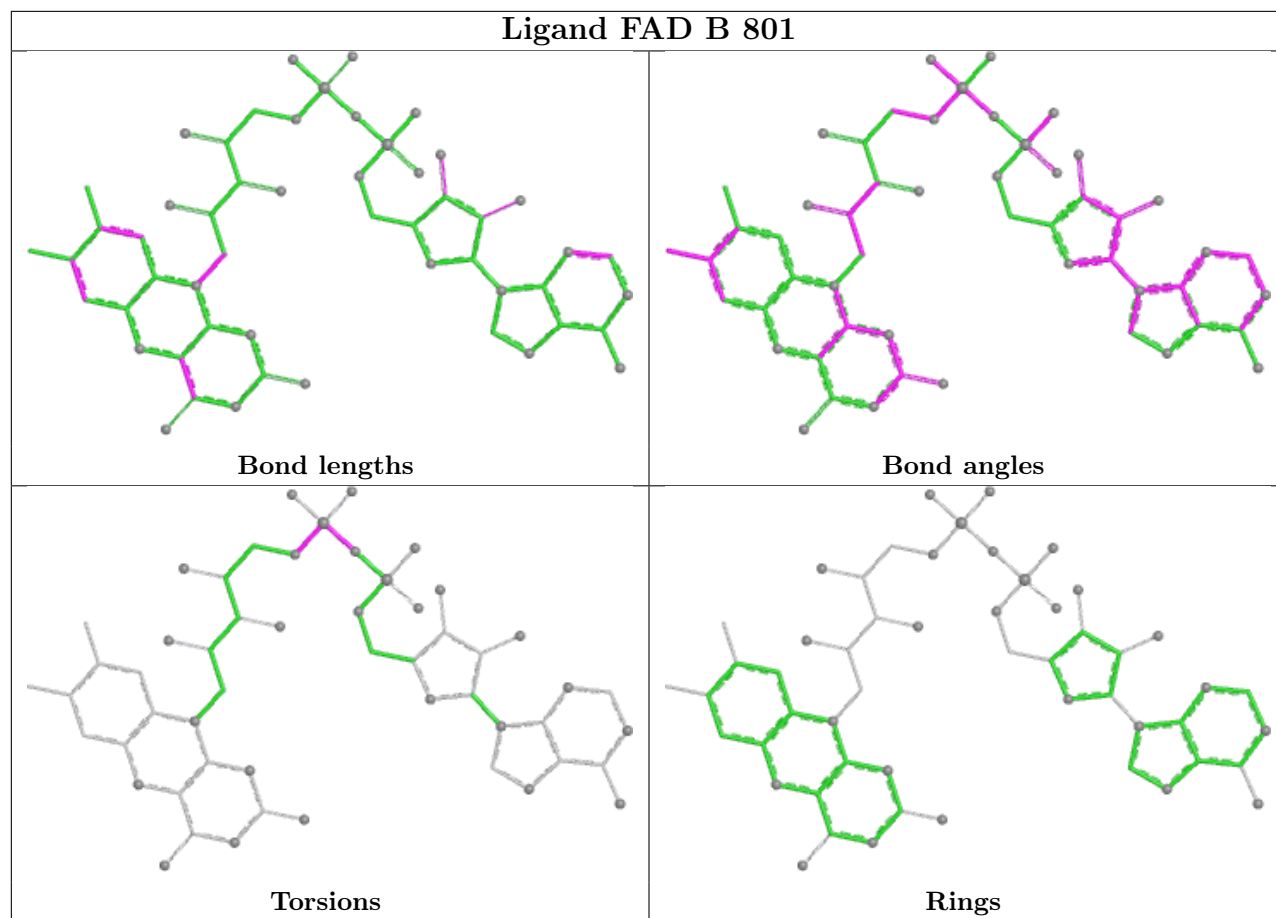
There are no ring outliers.

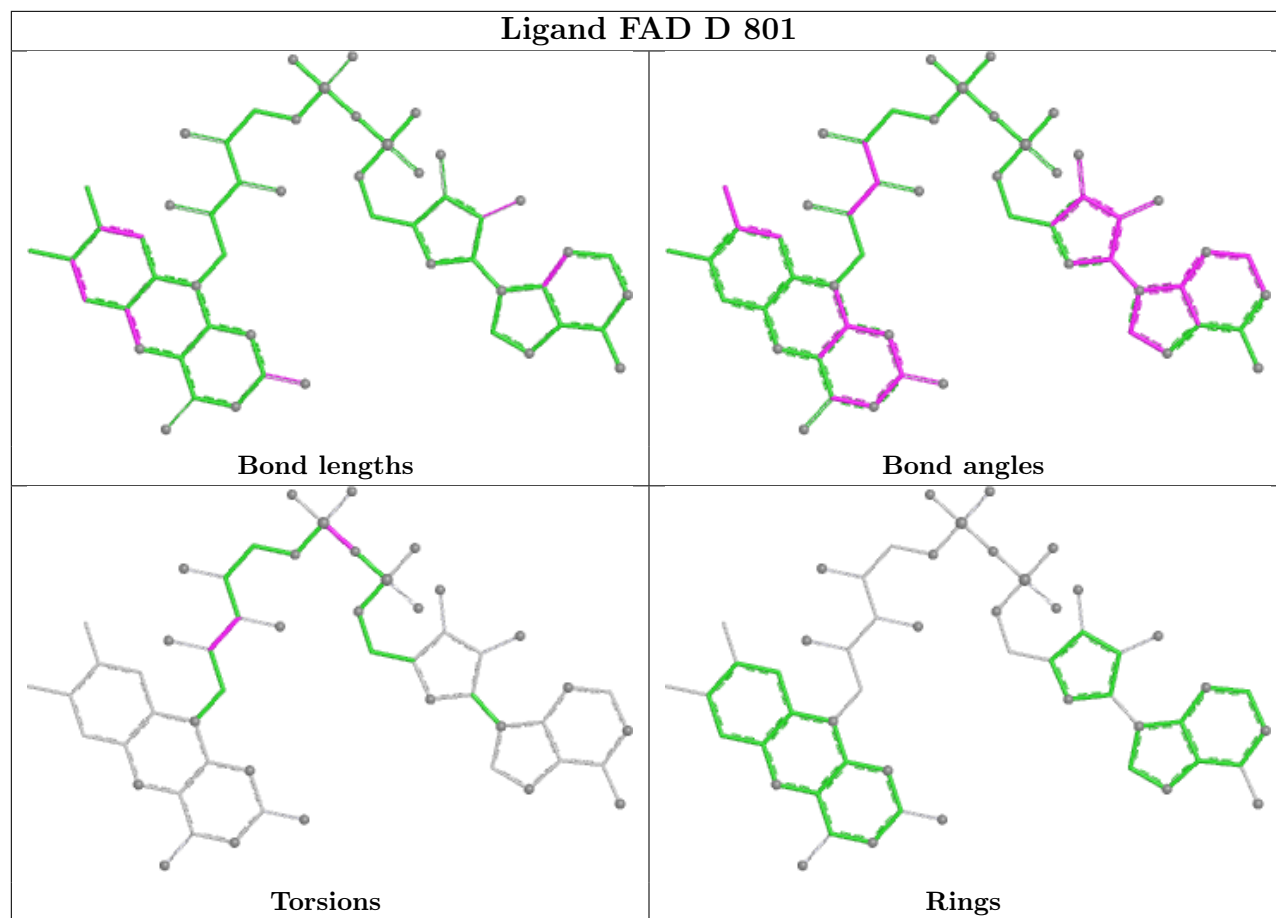
3 monomers are involved in 9 short contacts:

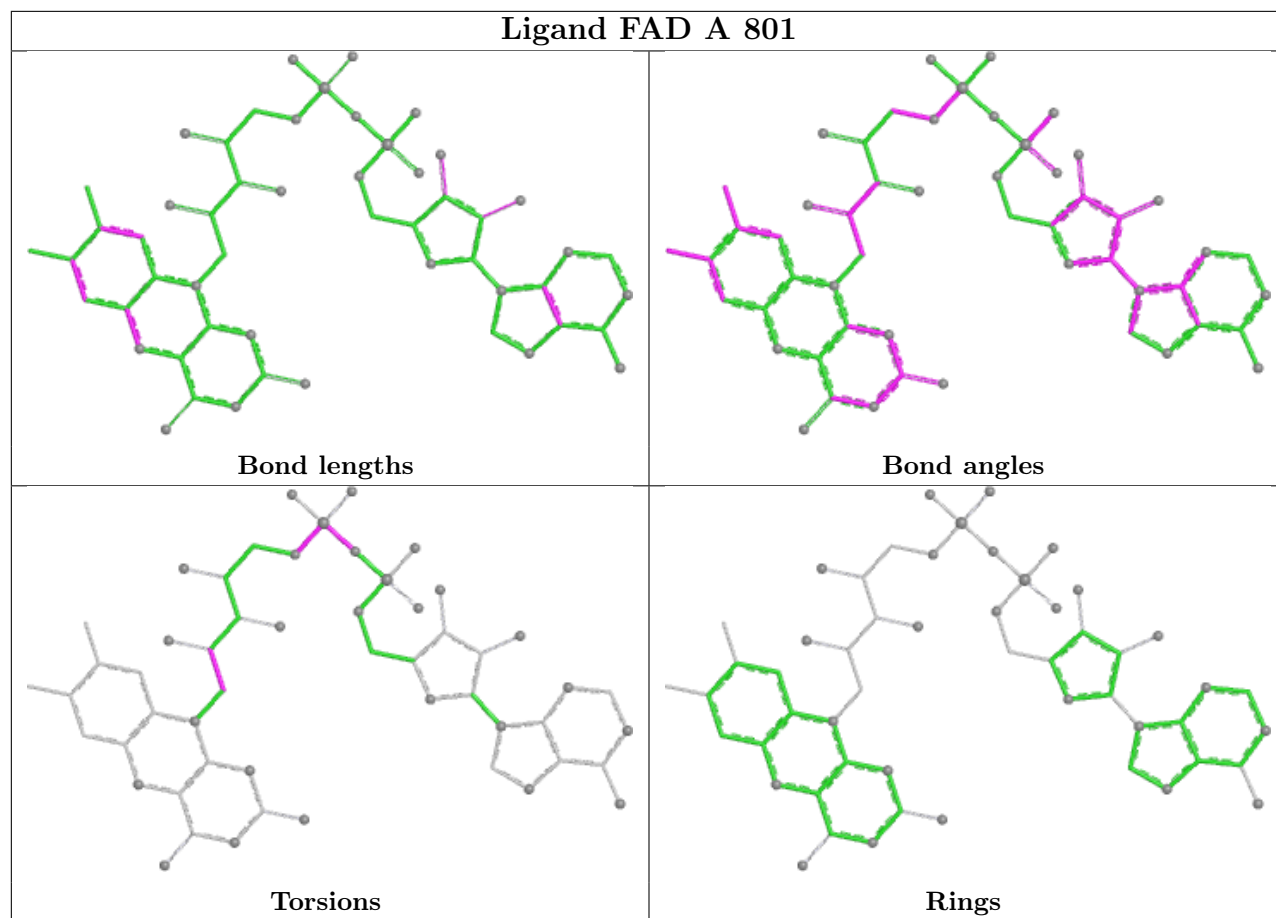
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	FAD	2	0
2	D	801	FAD	6	0
2	A	801	FAD	1	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.