wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2024 – 07:43 PM EST

PDB ID	:	1AHZ
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 (i) 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 (1)) were used in the production of this report:

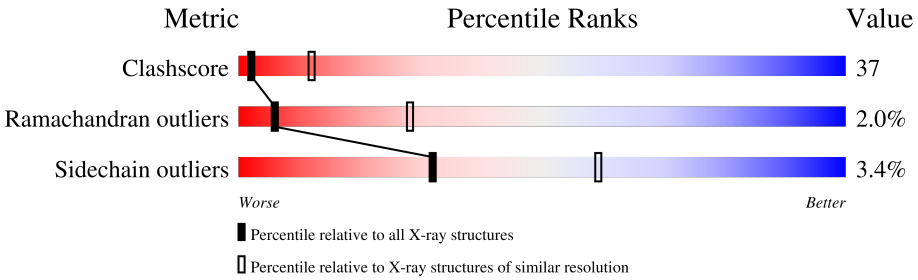
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	48% 45% 5%
1	B	560	48% 45% 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
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.

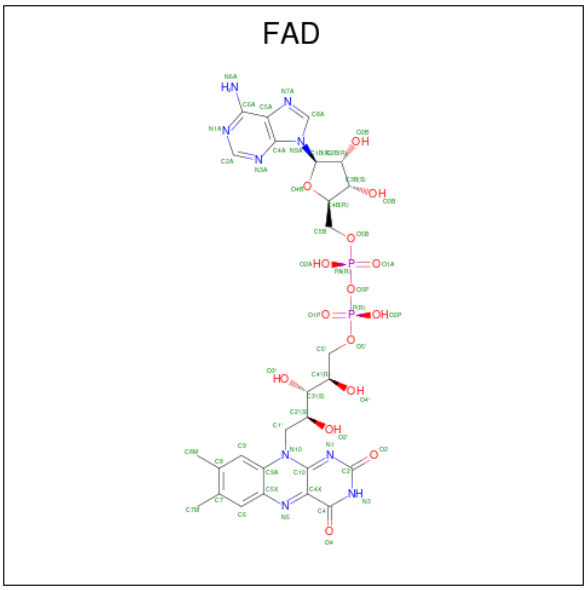
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

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 (three-letter code: CL) (formula: Cl).

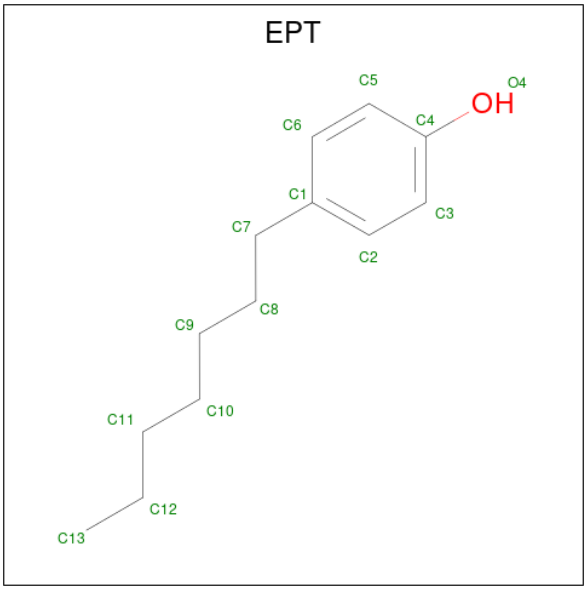
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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 (three-letter code: EPT) (formula: $C_{13}H_{20}O$).



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

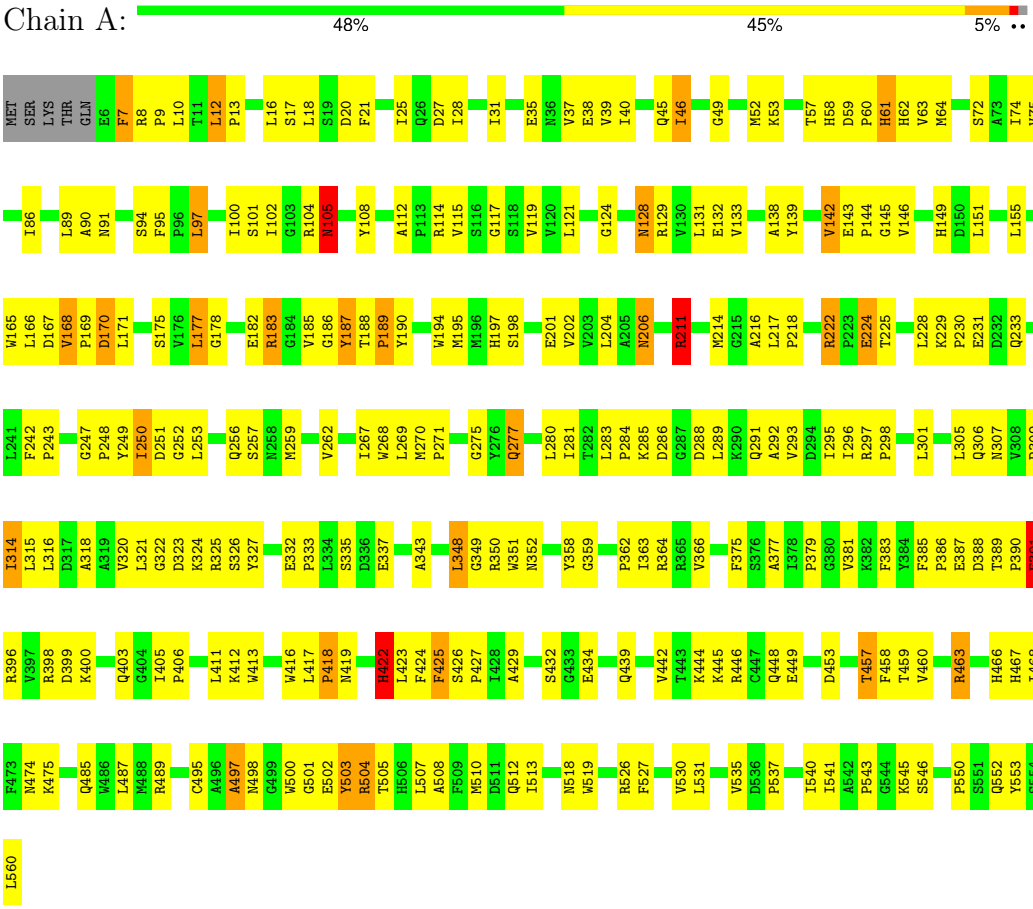
3 Residue-property plots (i)

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. 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.

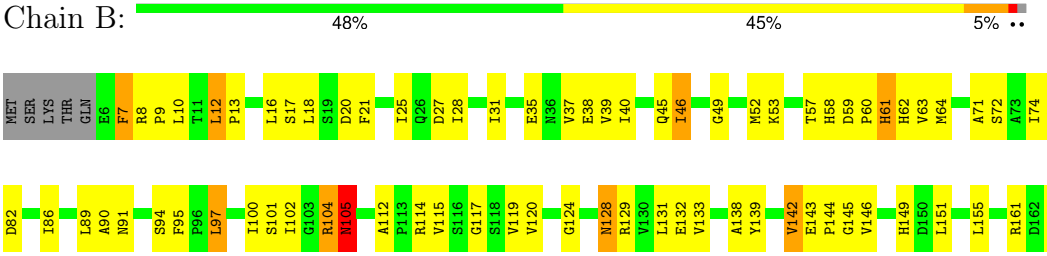
• Molecule 1: VANILLYL-ALCOHOL OXIDASE

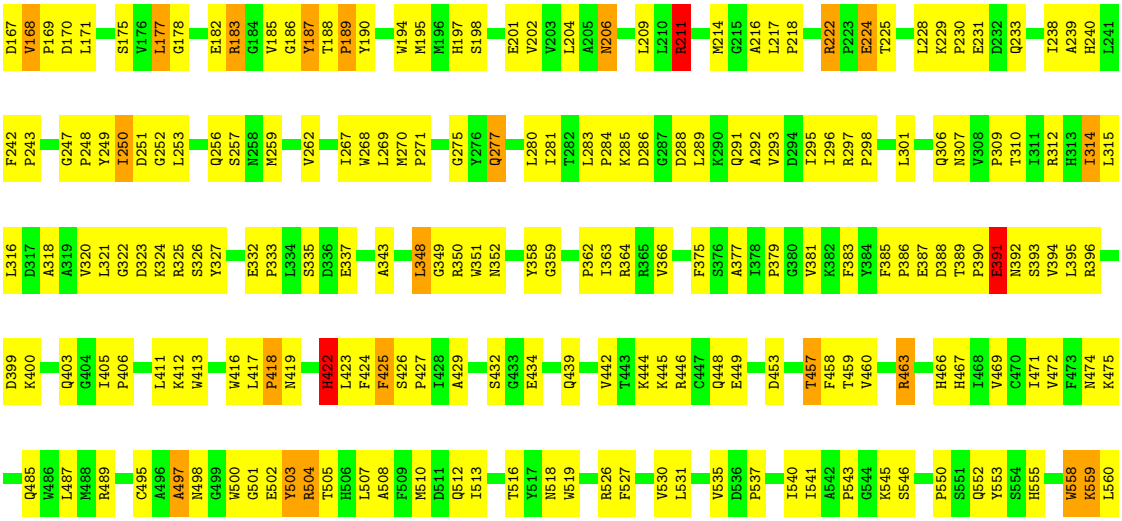
Chain A:



• Molecule 1: VANILLYL-ALCOHOL OXIDASE

Chain B:




D167 V168 P169 D170 L171 S175 V176 L177 G178 E182 R183 G184 V185 G186 Y187 T188 P189 Y190 W194 M195 M196 H197 S198 E201 V202 V203 L204 A205 N206 L209 I210 R211 M214 G215 A216 L217 P218 R222 P223 E224 T225 L228 K229 P230 E231 D232 Q233 I238 A239 H240 L241
F242 P243 G247 P248 Y249 I250 D251 G252 L253 Q256 S257 N258 M259 V262 I267 W268 L269 M270 P271 G275 Y276 Q277 L280 I281 T282 L283 P284 K285 D286 G287 D288 L289 K290 Q291 A292 V293 D294 I295 I296 R297 P298 L301 Q306 N307 V308 P309 T310 I311 R312 H313 I314 L315
L316 D317 A318 A319 V320 L321 G322 D323 K324 R325 S326 Y327 E332 P333 L334 S335 D336 E337 A343 L348 G349 R350 W351 N352 Y358 G359 P362 I363 R364 R365 V366 F375 S376 A377 I378 P379 G380 V381 K382 F383 Y384 F385 P386 E387 D388 T389 P390 E391 N392 S393 V394 L395 R396
D399 K400 Q403 G404 I405 P406 L411 K412 W413 W416 L417 P418 N419 H422 L423 F424 F425 S426 P427 I428 A429 S432 G433 E434 Q439 V442 T443 K444 K445 R446 C447 Q448 E449 D453 T457 F458 T459 V460 R463 H466 H467 I468 V469 C470 I471 V472 F473 N474 K475
Q485 W486 L487 M488 R489 C495 A496 A497 N498 G499 W500 G501 E502 Y503 R504 T505 H506 L507 A508 F509 M510 D511 Q512 I513 T516 Y517 N518 W519 R526 F527 V530 L531 V535 D536 P537 I540 I541 A542 P543 G544 K545 S546 P550 S551 Q552 Y553 S554 H555 W558 K559 L560

4 Data and refinement statistics (i)

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	140.97Å 140.97Å 133.45Å 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, CL, EPT

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	0.50	0/4511	1.23	26/6131 (0.4%)
1	B	0.50	0/4511	1.23	26/6131 (0.4%)
All	All	0.50	0/9022	1.23	52/12262 (0.4%)

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	183	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	183	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	375	PHE	CB-CG-CD1	7.62	126.13	120.80
1	B	375	PHE	CB-CG-CD1	7.61	126.12	120.80
1	A	97	LEU	CA-CB-CG	-7.36	98.36	115.30

There are no chirality outliers.

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	337	0
1	B	4391	0	4330	333	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	642	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 37.

The worst 5 of 642 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: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
1:A:280:LEU:HD12	1:A:281:ILE:H	1.28	0.99

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 28
1	B	553/560 (99%)	504 (91%)	38 (7%)	11 (2%)	6 28
All	All	1106/1120 (99%)	1007 (91%)	77 (7%)	22 (2%)	6 28

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 (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%)	459 (97%)	16 (3%)	32 59
1	B	475/482 (98%)	459 (97%)	16 (3%)	32 59
All	All	950/964 (98%)	918 (97%)	32 (3%)	32 59

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	277	GLN
1	B	391	GLU
1	A	277	GLN
1	A	251	ASP
1	B	422	HIS

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	91	ASN
1	B	197	HIS
1	B	498	ASN
1	B	128	ASN
1	B	206	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)

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	$\#\|Z\| > 2$
3	FAD	A	600	1	54,58,58	1.03	5 (9%)	71,89,89	0.88	2 (2%)
3	FAD	B	600	1	54,58,58	1.03	5 (9%)	71,89,89	0.87	2 (2%)
4	EPT	A	602	-	14,14,14	1.29	1 (7%)	16,16,16	1.75	5 (31%)

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	FAD	A	600	1	-	4/30/50/50	0/6/6/6
3	FAD	B	600	1	-	4/30/50/50	0/6/6/6
4	EPT	A	602	-	-	5/7/7/7	0/1/1/1

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 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

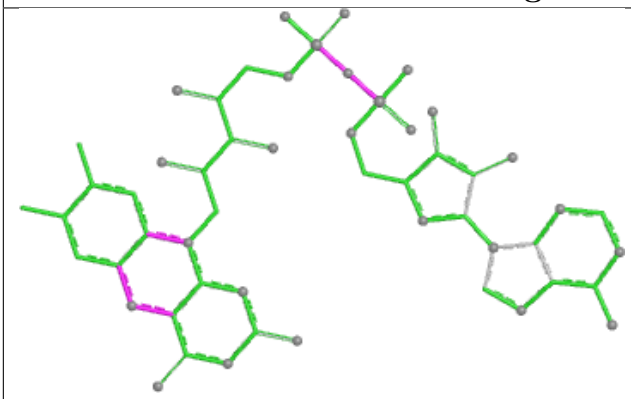
There are no ring outliers.

3 monomers are involved in 31 short contacts:

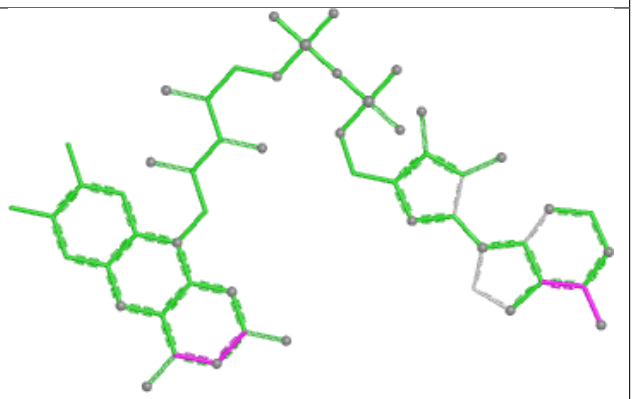
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	FAD	9	0
3	B	600	FAD	8	0
4	A	602	EPT	14	0

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 then 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.

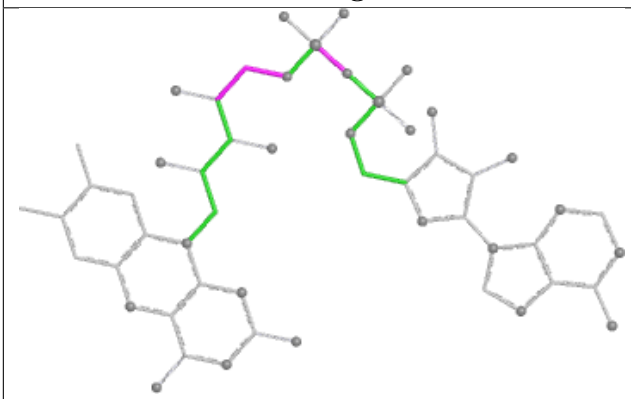
Ligand FAD A 600



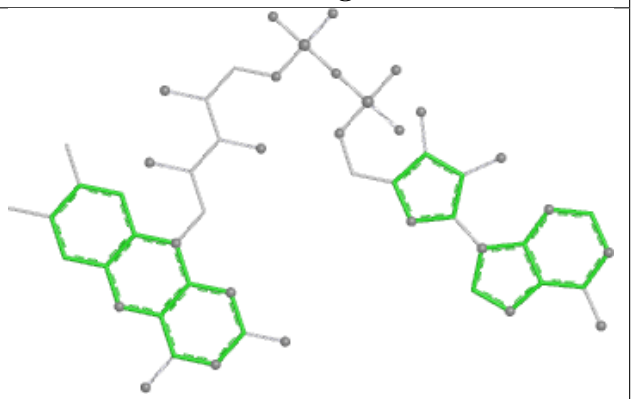
Bond lengths



Bond angles

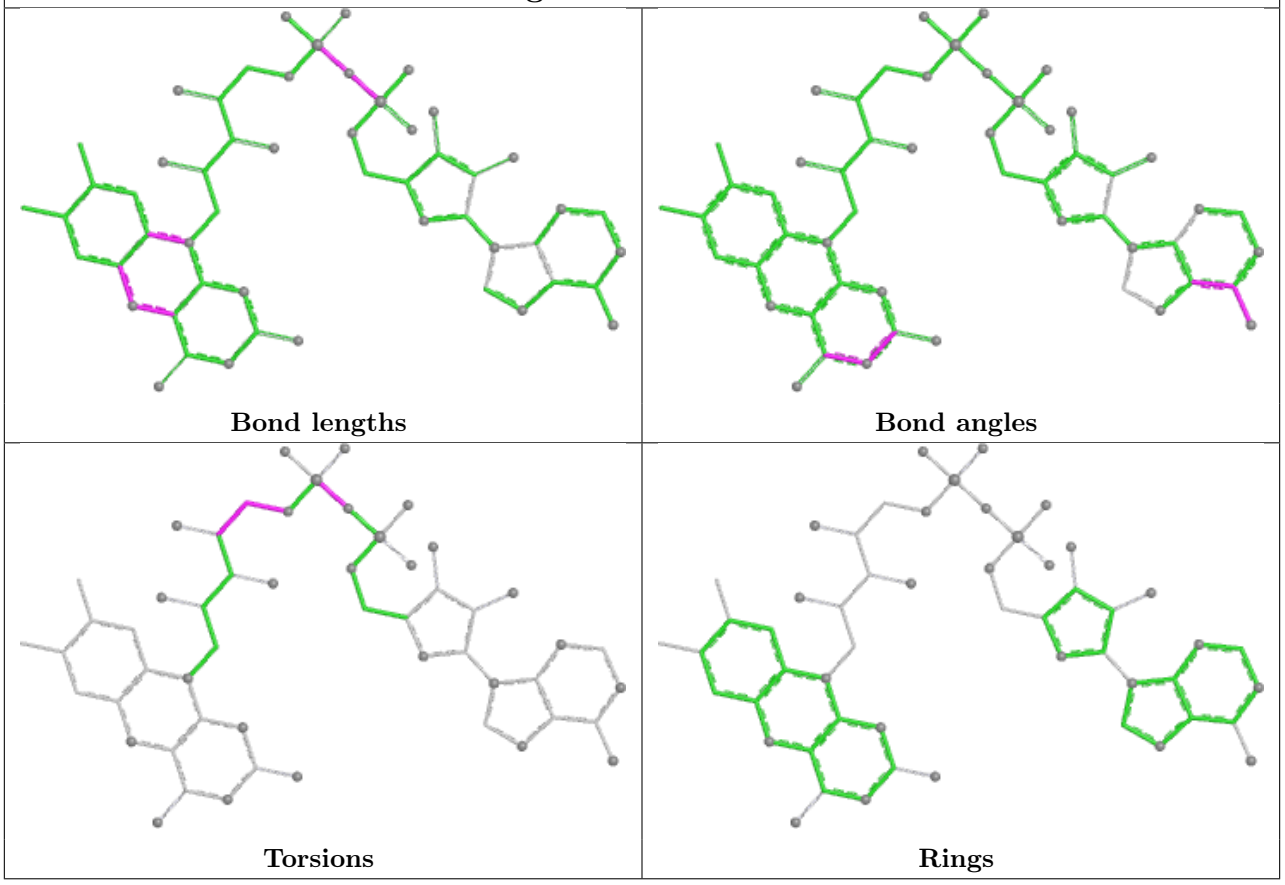


Torsions



Rings

Ligand FAD B 600



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.