wwPDB X-ray Structure Validation Summary Report (i)

Jan 28, 2024 – 02:35 PM EST

PDB ID	:	1EGE
Title	:	STRUCTURE OF T255E, E376G MUTANT OF HUMAN MEDIUM CHAIN ACYL-COA DEHYDROGENASE
Authors	:	Lee, H.J.; Wang, M.; Paschke, R.; Nandy, A.; Ghisla, S.; Kim, J.P.
Deposited on	:	1996-04-11
Resolution	:	2.75 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:

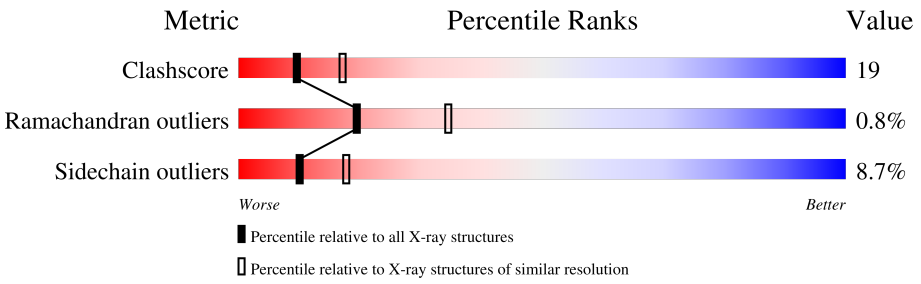
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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	396	53% 39% 5% • •
1	B	396	62% 31% • • •
1	C	396	56% 37% 5% •
1	D	396	49% 41% 8% •

2 Entry composition (i)

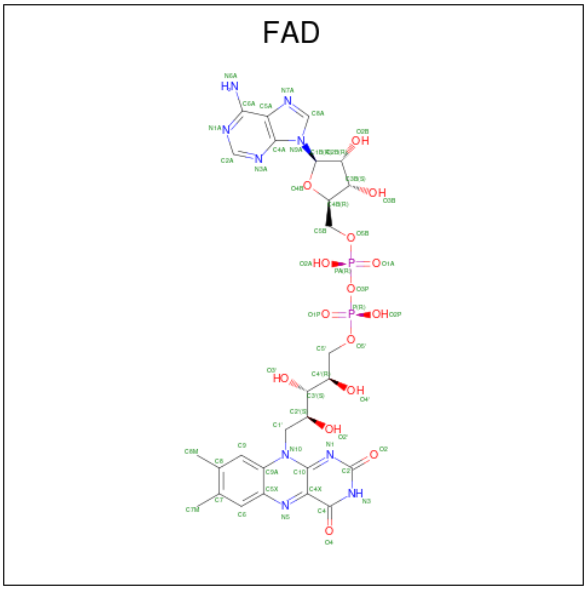
There are 2 unique types of molecules in this entry. The entry contains 12184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MEDIUM CHAIN ACYL-COA DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	2993	1894	515	566	18	0	0	0
1	B	387	2993	1894	515	566	18	0	0	0
1	C	387	2993	1894	515	566	18	0	0	0
1	D	387	2993	1894	515	566	18	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
2	D	1	53	27	9	15	2	0	0

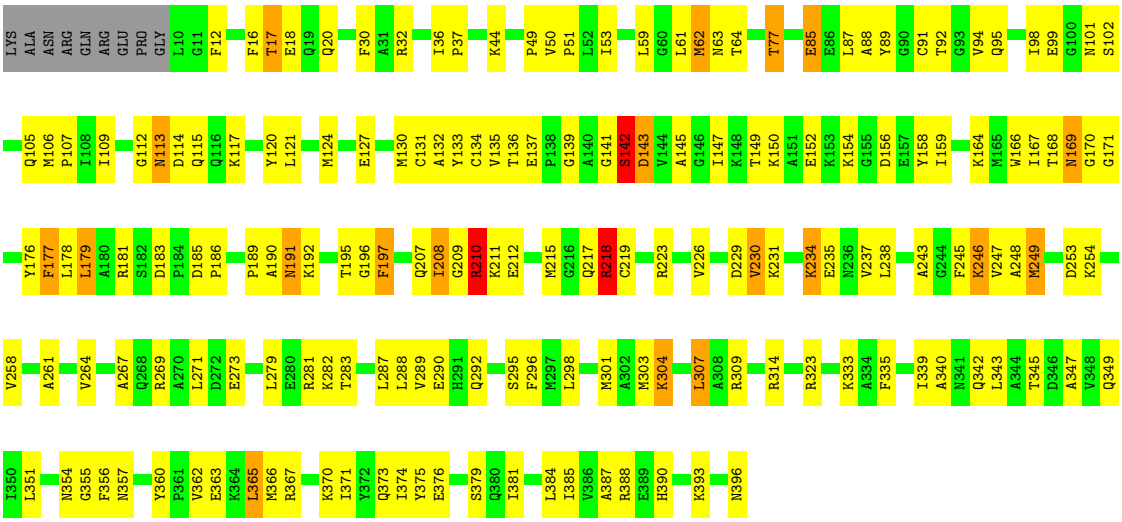
3 Residue-property plots (i)

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.

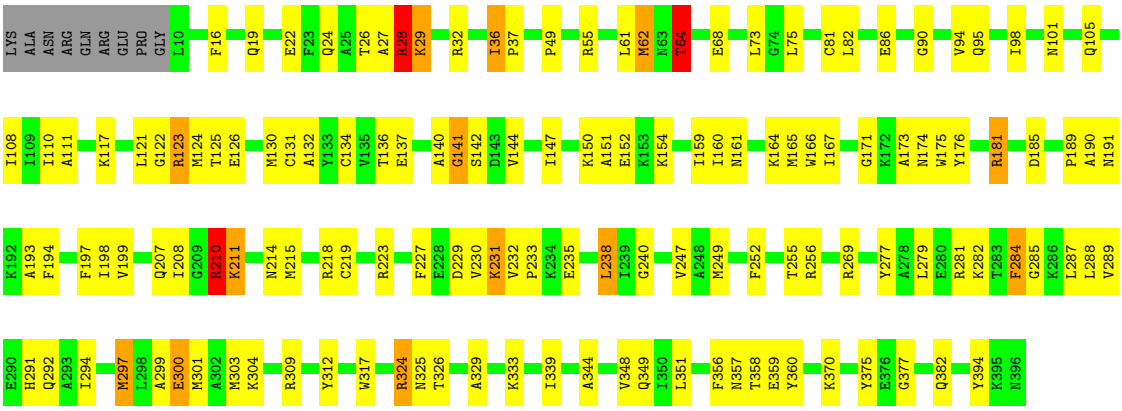
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain A:



• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain B:



• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain C: 56% 37% 5% •

LYS ALA ASN ARG GLN ARG GLU PRO GLY L10 G11 F14 T17 E18 Q19 Q20 K21 R28 A31 R32 E33 E34 I35 V38 A39 A40 E41 Y42 D43 K44 E47 Y48 P49 V50 P51 L52 R55 L59 G60 L61 M62 I66 L75 E85 Y89 G90 C91

V94 I98 N101 S102 L103 G104 Q105 M106 P107 I108 I109 I110 A111 G112 K117 K118 L121 G122 T125 E126 L129 M130 C131 C134 E137 D143 I147 E152 K153 D156 E157 Y158 I159 I160 K164 M165 W166 I167 T168 N169 Y176 F177 L178 L179 A180 R181

D185 P186 K187 A188 N191 F194 F197 A201 D202 T203 P204 Q207 I208 G209 R210 K211 E212 M215 G216 Q217 R218 D221 T222 R223 V226 F227 V230 K234 E235 N236 V237 L238 I239 A243 G244 F245 M249 F252 R256 P257 V258 V259 A260 V264

G265 L266 A267 Q268 R269 E273 A274 V277 A278 L279 E280 R281 K282 T283 F284 G285 K286 L287 E290 H291 Q292 A293 I294 M297 M301 V305 A308 R309 M310 S311 V319 N325 T326 Y327 Y328 I331 A332 K333 A334 Q342 L343 A344 T345 Q349 I350 T358

K364 L365 M366 A369 K370 I371 Y372 Q373 I374 Y375 E376 G377 T378 S379 Q380 I381 Q382 R383 L384 I385 V386 A387 R388 I391 K395 N396

• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain D: 49% 41% 8% •

LYS ALA ASN ARG GLN ARG GLU PRO GLY L10 F14 E15 F16 T17 Q20 K21 E22 F23 Q24 R28 K29 F30 A31 R32 E33 E34 I35 I36 P37 A40 E41 Y42 D43 K44 T45 G46 E47 Y48 P49 V50 P51 L52 I53 R54 R55 A56 W57 M62 H65 I66 P67 E68 G72

L73 G74 L75 G76 T77 F78 L82 I83 L87 V94 Q95 I98 N101 S102 Q105 I108 I109 I110 A111 G112 N113 D114 Q115 Q116 K117 K118 K119 Y120 L121 G122 R123 M124 T125 P128 C131 A132 Y133 C134 V135 T136 E137 P138 S142 A145 G146 I147 K148 T149 K150

A151 E152 E157 Y158 I159 I160 N161 G162 Q163 K164 I167 T168 N169 A173 Y176 F177 L178 R181 S182 D183 P184 D185 P186 K187 N191 K192 A193 F194 F197 I198 I206 Q207 I208 G209 R210 L213 N214 M215 G216 Q217 R218 C219 R223 G224 I225 V226 F227 E228 D229 V230

K231 V232 P233 K234 E235 N236 V237 L238 I239 G240 D241 M249 F252 D253 K254 T255 R256 P257 A263 V264 G265 L266 A267 Q268 R269 L279 K282 T283 F284 L287 L288 H291 Q292 A293 I294 S295 A299 E300 M303 K304 V305 E306 L307 A308 R309 M310 S311 Y312 Q313 A316

W317 E318 V319 R323 R324 N325 T326 Y327 A332 K333 A344 T345 V348 L351 F356 V362 E363 K364 L365 M366 R367 D368 A369 K370 I371 Y372 Q373 I374 Y375 E376 G377 T378 I381 Q382 R383 L384 E389 H390 I391 D392 K393 N396

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	169.59Å 169.59Å 151.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.75	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.75)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.221 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12184	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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

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	0.49	0/3048	0.86	15/4107 (0.4%)
1	B	1.42	2/3048 (0.1%)	1.79	18/4107 (0.4%)
1	C	0.74	4/3048 (0.1%)	1.01	10/4107 (0.2%)
1	D	0.68	4/3048 (0.1%)	0.84	11/4107 (0.3%)
All	All	0.90	10/12192 (0.1%)	1.19	54/16428 (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	3
1	B	0	2
1	C	0	3
1	D	0	8
All	All	0	16

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	PHE	CD2-CE2	69.95	2.79	1.39
1	C	284	PHE	CG-CD1	23.19	1.73	1.38
1	C	284	PHE	CG-CD2	-16.62	1.13	1.38
1	B	324	ARG	C-N	-14.74	1.00	1.34
1	D	214	ASN	C-N	-8.39	1.14	1.34

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	284	PHE	CE1-CZ-CE2	-65.95	1.28	120.00
1	B	284	PHE	CG-CD2-CE2	-55.57	59.67	120.80
1	B	284	PHE	CZ-CE2-CD2	-49.75	60.40	120.10
1	C	284	PHE	CB-CG-CD2	31.16	142.61	120.80
1	C	284	PHE	CB-CG-CD1	-24.65	103.54	120.80

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASN	Mainchain
1	A	229	ASP	Mainchain
1	A	230	VAL	Mainchain
1	B	285	GLY	Mainchain
1	B	29	LYS	Mainchain

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	2993	0	2982	123	0
1	B	2993	0	2981	116	0
1	C	2993	0	2981	118	0
1	D	2993	0	2981	146	0
2	A	53	0	31	6	0
2	B	53	0	31	1	0
2	C	53	0	31	5	0
2	D	53	0	31	1	0
All	All	12184	0	12049	472	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 472 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:D:137:GLU:HB2	1:D:138:PRO:CD	1.72	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:GLU:CB	1:D:138:PRO:HD2	1.90	1.01
1:A:197:PHE:HB3	1:A:237:VAL:HA	1.41	0.99
1:C:208:ILE:HG22	1:C:209:GLY:H	1.27	0.98
1:B:284:PHE:CZ	1:B:284:PHE:CD2	2.42	0.98

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	385/396 (97%)	343 (89%)	38 (10%)	4 (1%)	15	27
1	B	385/396 (97%)	349 (91%)	34 (9%)	2 (0%)	29	47
1	C	385/396 (97%)	355 (92%)	29 (8%)	1 (0%)	41	60
1	D	385/396 (97%)	347 (90%)	33 (9%)	5 (1%)	12	21
All	All	1540/1584 (97%)	1394 (90%)	134 (9%)	12 (1%)	19	34

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	GLY
1	B	326	THR
1	D	16	PHE
1	A	145	ALA
1	C	208	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	304/311 (98%)	268 (88%)	36 (12%)	5	8
1	B	304/311 (98%)	283 (93%)	21 (7%)	15	27
1	C	304/311 (98%)	281 (92%)	23 (8%)	13	23
1	D	304/311 (98%)	278 (91%)	26 (9%)	10	18
All	All	1216/1244 (98%)	1110 (91%)	106 (9%)	10	18

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	41	GLU
1	C	221	ASP
1	D	269	ARG
1	C	103	LEU
1	C	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	161	ASN
1	D	373	GLN
1	B	268	GLN
1	C	396	ASN
1	B	174	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 monosaccharides 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	D	399	-	53,58,58	1.49	7 (13%)	68,89,89	2.02	15 (22%)
2	FAD	C	399	-	53,58,58	1.22	3 (5%)	68,89,89	1.60	11 (16%)
2	FAD	A	399	-	53,58,58	1.36	7 (13%)	68,89,89	1.63	12 (17%)
2	FAD	B	399	-	53,58,58	1.30	6 (11%)	68,89,89	1.82	12 (17%)

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	D	399	-	-	9/30/50/50	0/6/6/6
2	FAD	C	399	-	-	8/30/50/50	0/6/6/6
2	FAD	A	399	-	-	4/30/50/50	0/6/6/6
2	FAD	B	399	-	-	10/30/50/50	0/6/6/6

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	399	FAD	O4B-C1B	4.08	1.46	1.41
2	C	399	FAD	C9-C8	-3.96	1.33	1.39
2	D	399	FAD	C6-C7	-3.82	1.34	1.39
2	B	399	FAD	C4X-N5	3.80	1.38	1.30
2	A	399	FAD	C4X-N5	3.63	1.37	1.30

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	399	FAD	O4B-C1B-C2B	-5.99	98.17	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	399	FAD	O3'-C3'-C2'	-5.50	95.52	108.81
2	B	399	FAD	C9A-C5X-N5	5.28	128.17	122.43
2	C	399	FAD	C2B-C3B-C4B	-5.05	92.82	102.64
2	D	399	FAD	C9A-C5X-N5	4.76	127.61	122.43

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	399	FAD	C5B-O5B-PA-O3P
2	B	399	FAD	C5B-O5B-PA-O2A
2	B	399	FAD	C3'-C4'-C5'-O5'
2	B	399	FAD	O4'-C4'-C5'-O5'
2	C	399	FAD	C5B-O5B-PA-O1A

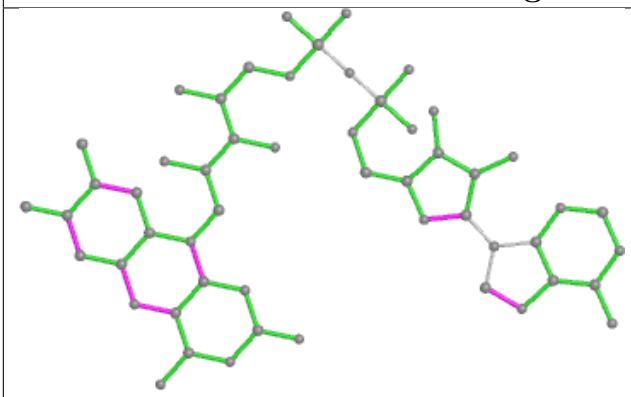
There are no ring outliers.

4 monomers are involved in 13 short contacts:

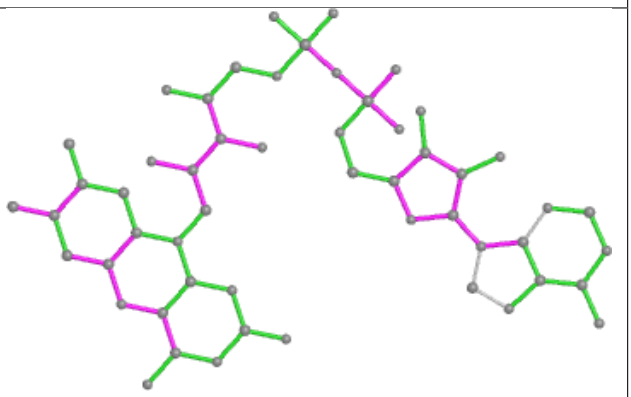
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	399	FAD	1	0
2	C	399	FAD	5	0
2	A	399	FAD	6	0
2	B	399	FAD	1	0

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 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.

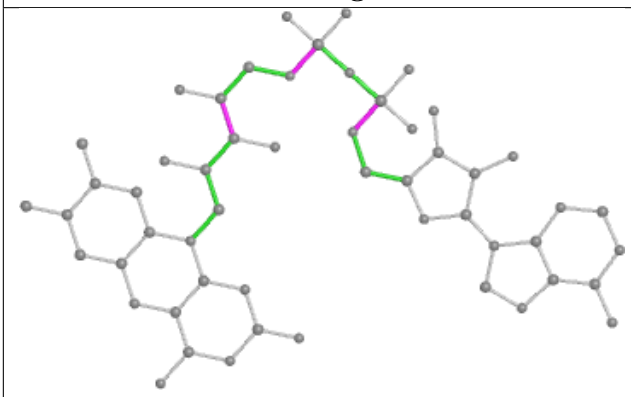
Ligand FAD D 399



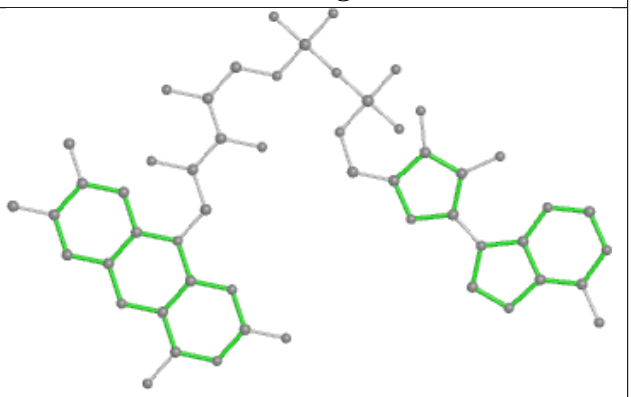
Bond lengths



Bond angles

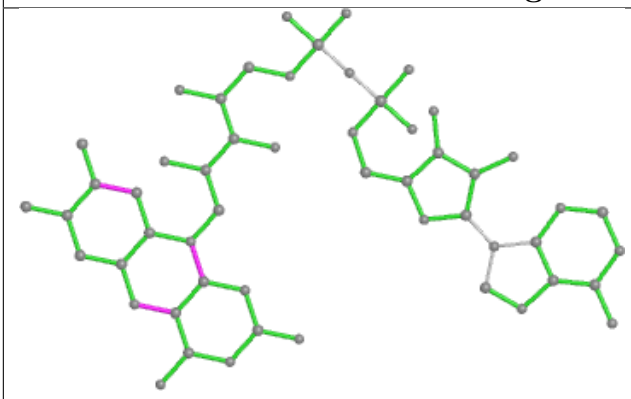


Torsions

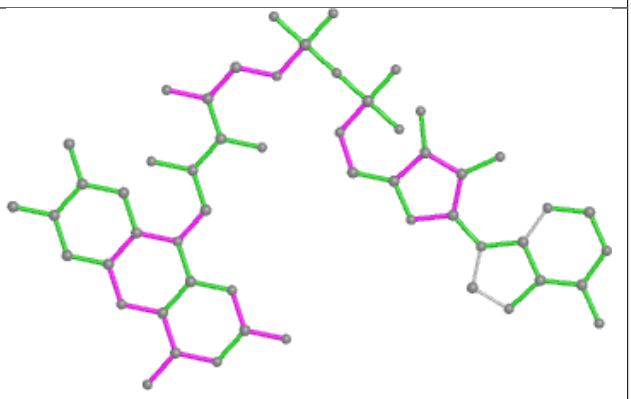


Rings

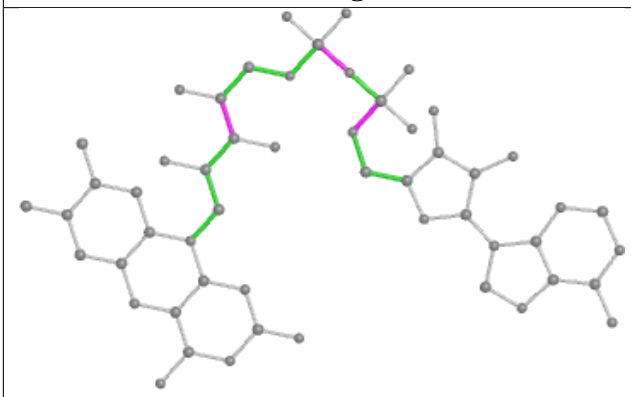
Ligand FAD C 399



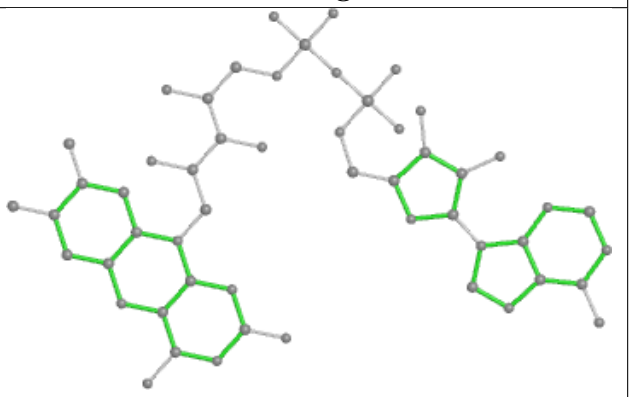
Bond lengths



Bond angles

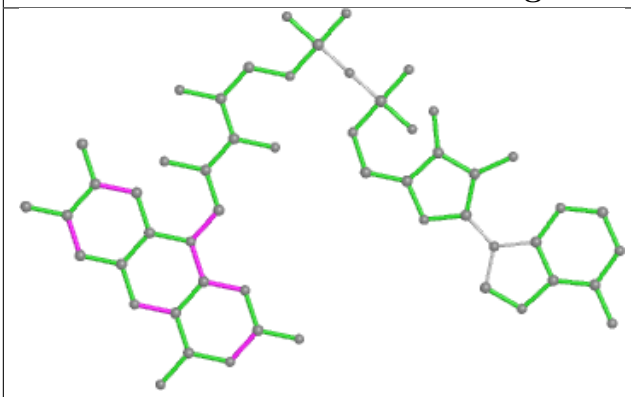


Torsions

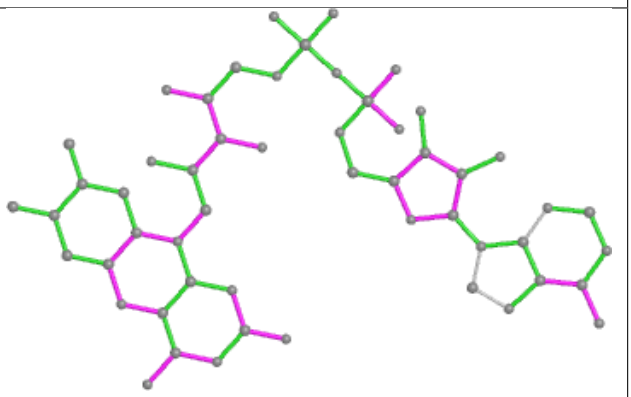


Rings

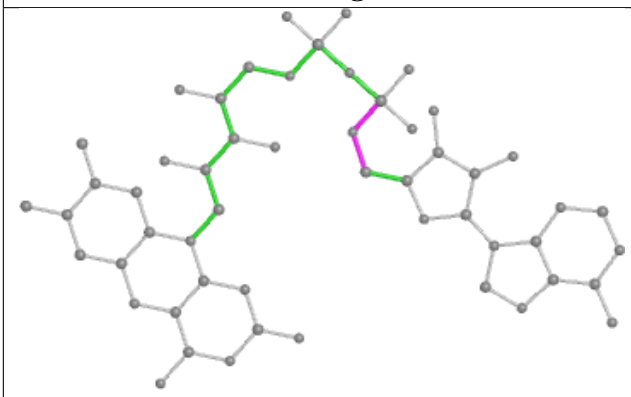
Ligand FAD A 399



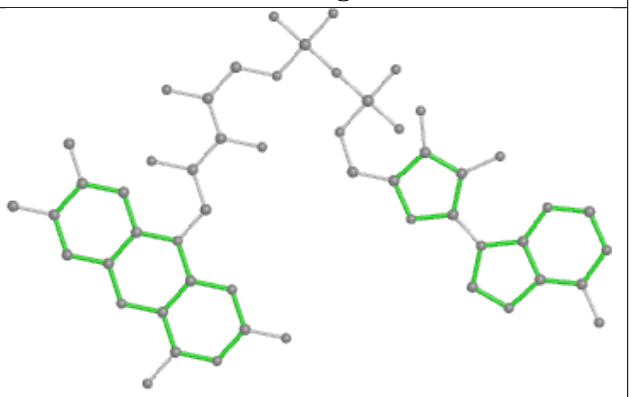
Bond lengths



Bond angles

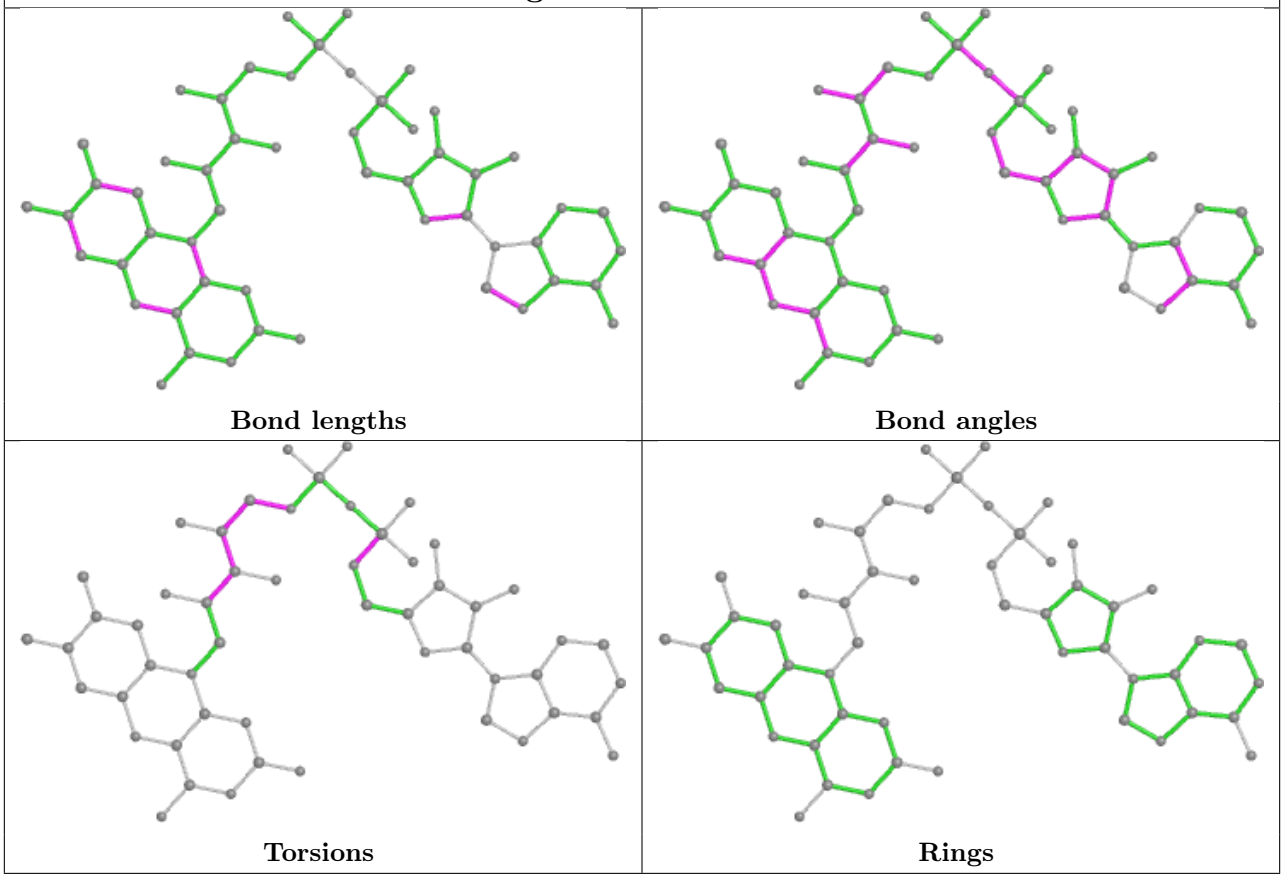


Torsions



Rings

Ligand FAD B 399



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
1	D	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	226:VAL	C	227:PHE	N	1.18
1	D	214:ASN	C	215:MET	N	1.14
1	B	324:ARG	C	325:ASN	N	1.00

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.