wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 08:35 AM EDT

PDB ID	:	5NCC
Title	:	Structure of Fatty acid Photodecarboxylase in complex with FAD and palmitic acid
Authors	:	Arnoux, P.; Sorigue, D.; Beisson, F.; Pignol, D.
Deposited on	:	2017-03-03
Resolution	:	3.12 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 (i)) were used in the production of this report:

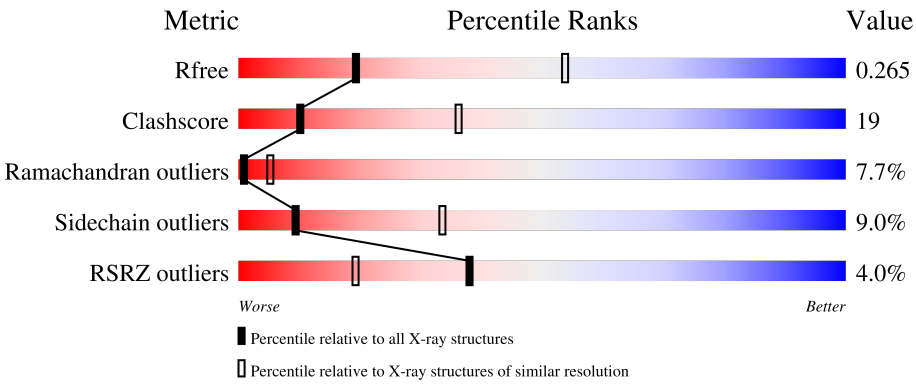
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.12 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}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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% 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	594	60% 28% 8%
1	B	594	2% 61% 28% 6%
1	C	594	2% 61% 27% 7%
1	D	594	2% 60% 28% 7%
1	E	594	10% 59% 29% 8%

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Mol	Chain	Length	Quality of chain
1	F	594	7% 63% 25% 8%

2 Entry composition (i)

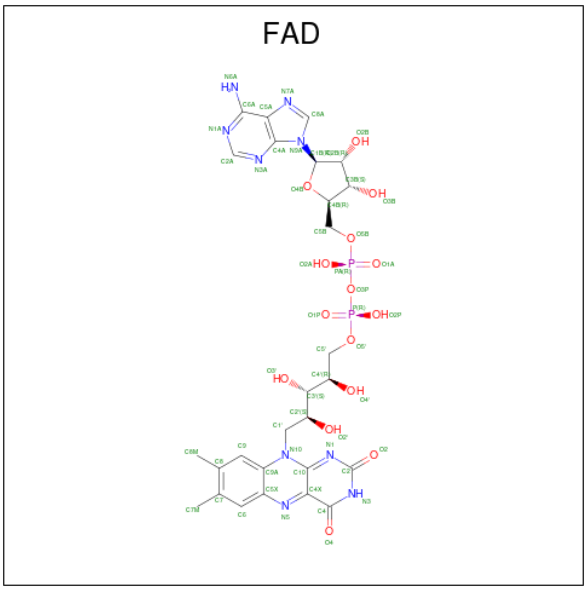
There are 3 unique types of molecules in this entry. The entry contains 26184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fatty acid Photodecarboxylase.

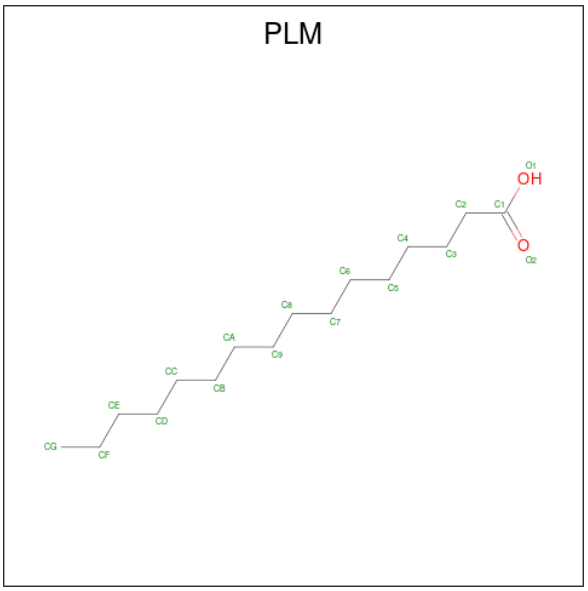
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	578	4299	2685	769	830	15	0	0	0
1	B	578	4299	2685	769	830	15	0	0	0
1	C	578	4299	2685	769	830	15	0	0	0
1	D	578	4299	2685	769	830	15	0	0	0
1	E	578	4299	2685	769	830	15	0	0	0
1	F	578	4299	2685	769	830	15	0	0	0

- 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
2	C	1	53	27	9	15	2	0	0
2	D	1	53	27	9	15	2	0	0
2	E	1	53	27	9	15	2	0	0
2	F	1	53	27	9	15	2	0	0

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



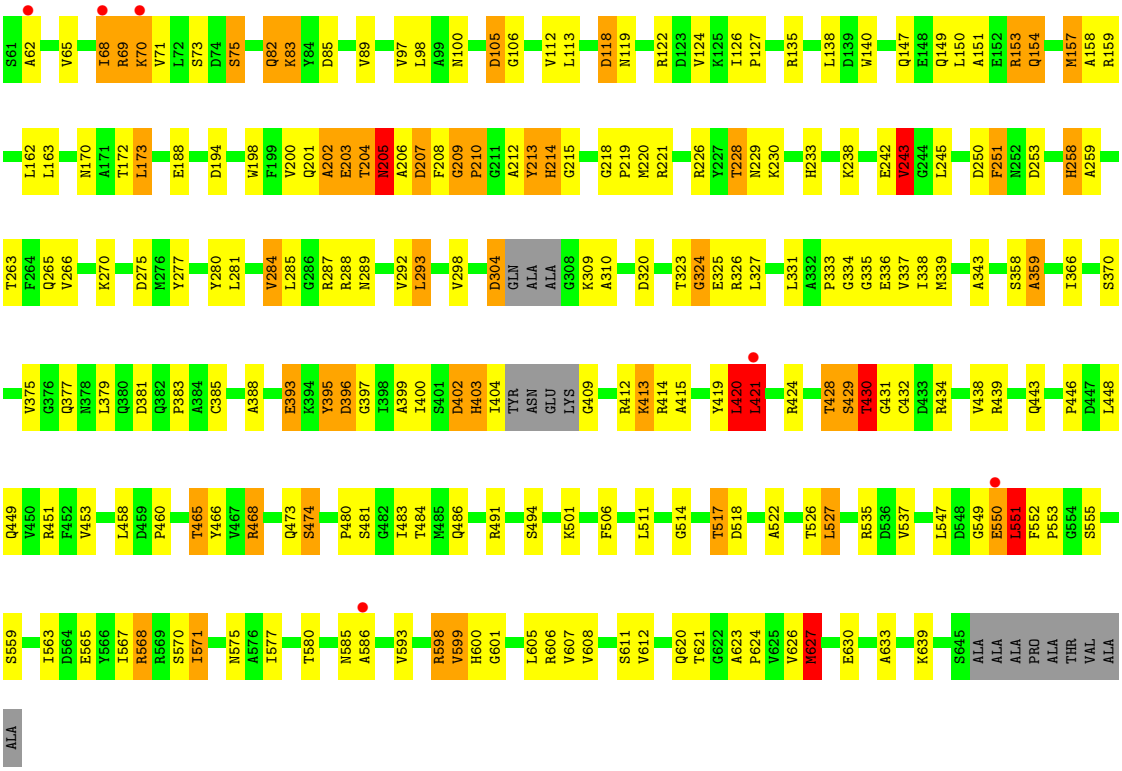
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	18	16	2	0	0
3	B	1	18	16	2	0	0
3	C	1	18	16	2	0	0
3	D	1	18	16	2	0	0

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 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.

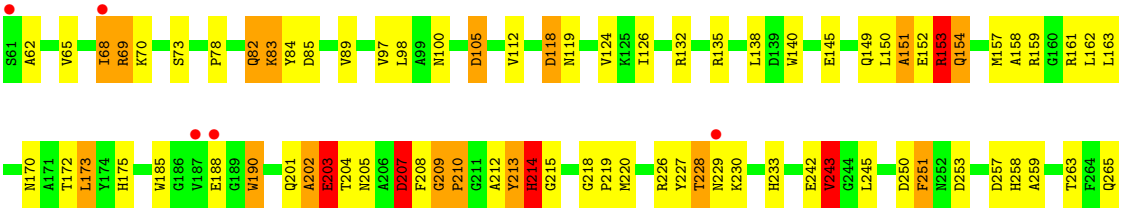
• Molecule 1: Fatty acid Photodecarboxylase

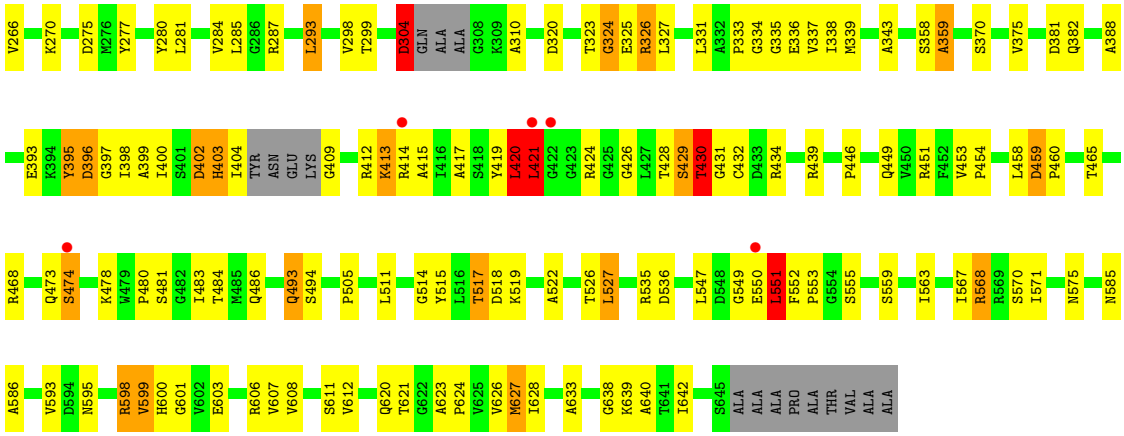
Chain A:



• Molecule 1: Fatty acid Photodecarboxylase

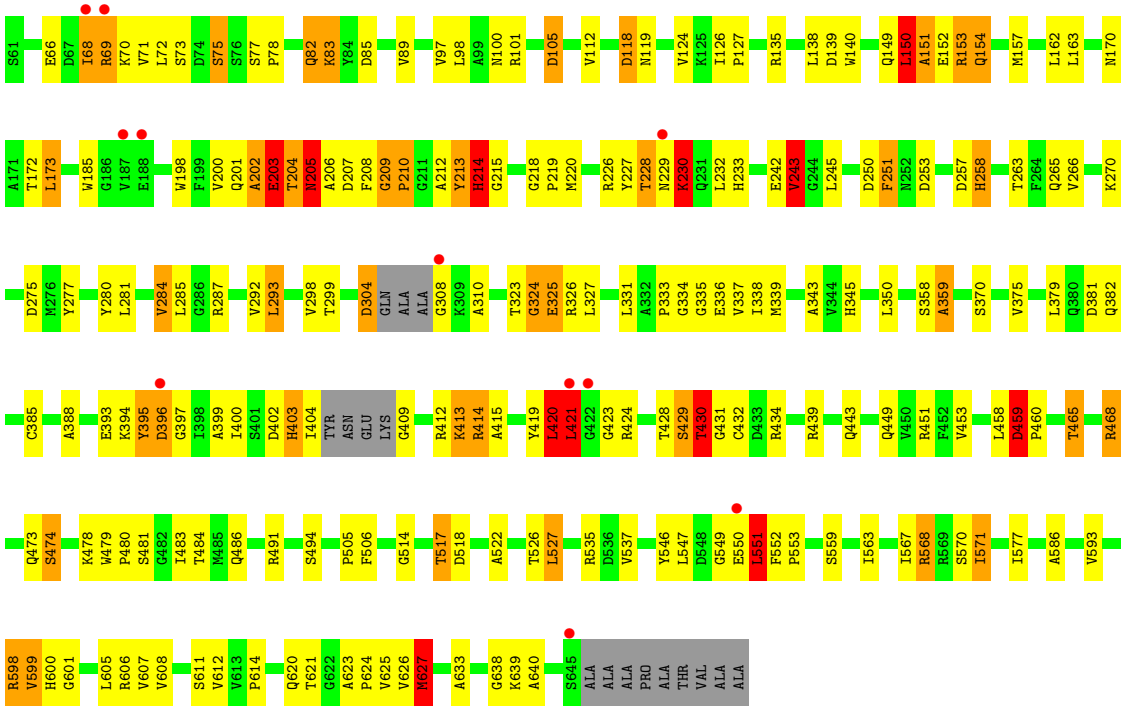
Chain B:





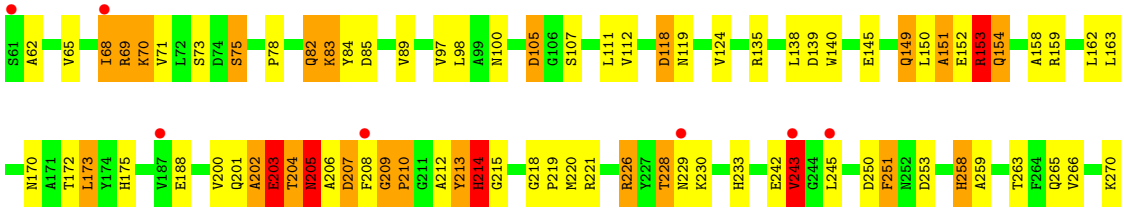
- Molecule 1: Fatty acid Photodecarboxylase

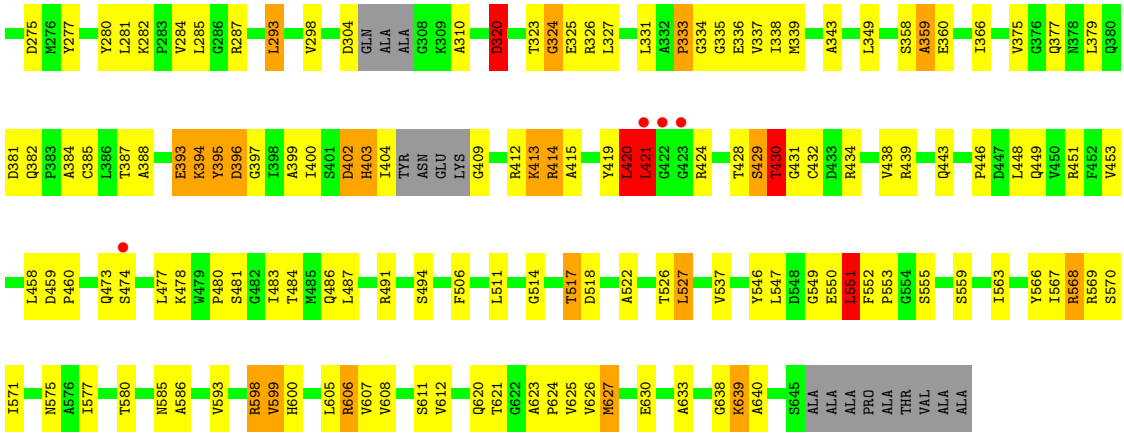
Chain C:



- Molecule 1: Fatty acid Photodecarboxylase

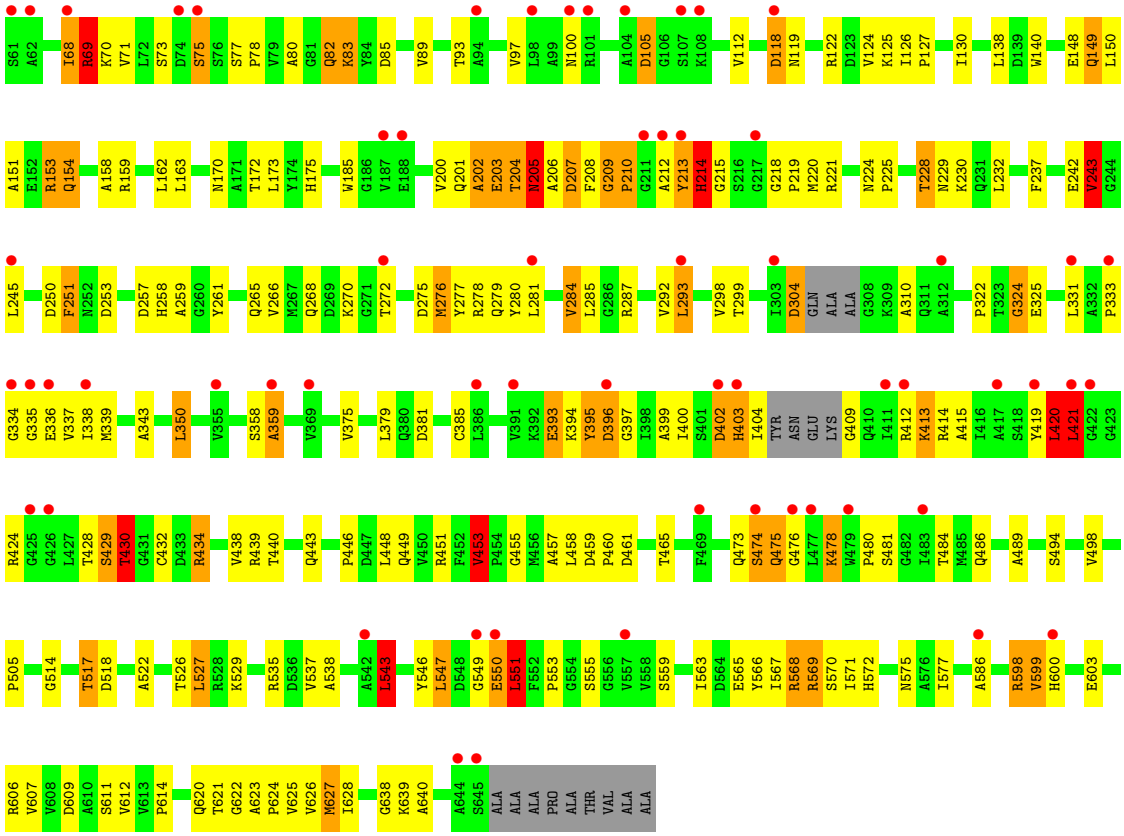
Chain D:





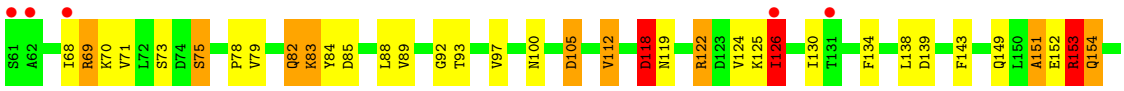
• Molecule 1: Fatty acid Photodecarboxylase

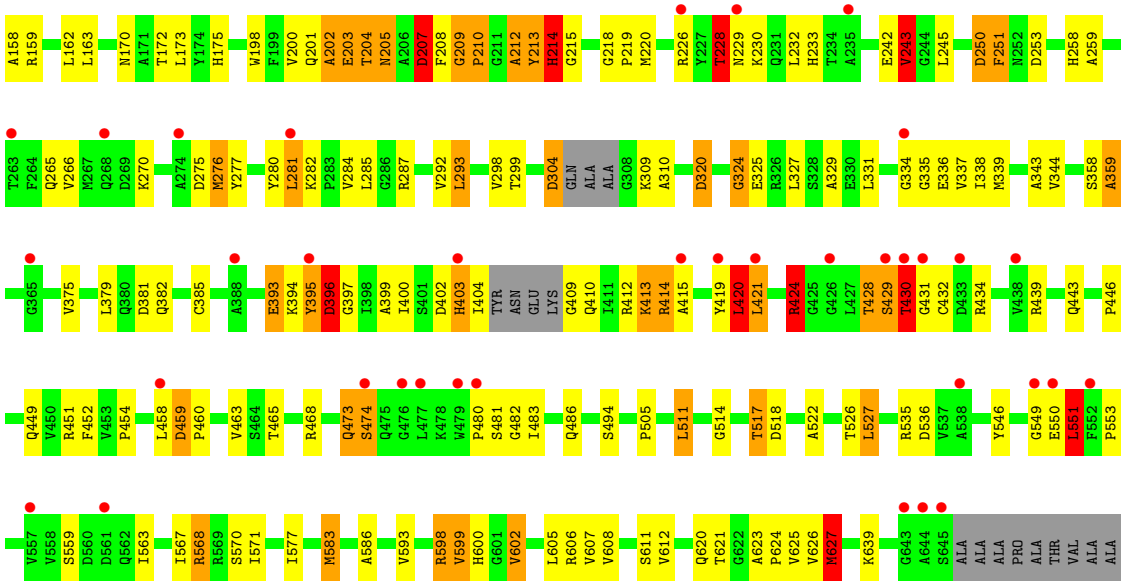
Chain E:



• Molecule 1: Fatty acid Photodecarboxylase

Chain F:




A158 R159 L162 L163 N170 A171 T172 L173 Y174 H175 W198 F199 V200 Q201 A202 E203 T204 N205 A206 D207 F208 G209 P210 G211 A212 Y213 H214 G215 G218 P219 M220 R226 Y227 T228 N229 K230 Q231 L232 H233 T234 A235 E242 V243 G244 L245 D250 F251 N252 D253 H258 A259
T263 F264 Q265 V266 M267 Q268 D269 K270 A274 D275 M276 Y277 Y280 L281 K282 P283 V284 L285 G286 R287 V292 L293 V298 T299 D304 GLN ALA ALA G308 K309 A310 D320 G324 E325 R326 L327 S328 A329 E330 L331 G334 G335 E336 V337 I338 M339 A343 V344 S358 A359
G365 V375 L379 Q380 D381 Q382 C385 A388 E393 K394 Y395 D396 G397 I398 A399 I400 S401 D402 H403 I404 TYR ASN GLU LYS G409 Q410 I411 R412 K413 R414 A415 Y419 L420 L421 R424 G425 G426 L427 T428 S429 T430 G431 C432 D433 R434 V438 R439 Q443 P446
Q449 Y450 R451 F452 Y453 P454 L458 D459 P460 V463 S464 T465 R468 Q473 S474 Q475 G476 L477 K478 W479 P480 S481 G482 I483 Q486 S494 P505 L511 G514 T517 D518 A522 T526 L527 R535 D536 V537 A538 Y546 G549 E550 L551 F552 P553
V557 V558 S559 D560 D561 Q562 I563 I567 R568 R569 S570 I571 I577 M583 A586 V593 R598 V599 H600 G601 V602 L605 R606 V607 V608 S611 V612 Q620 T621 G622 A623 P624 V625 V626 M627 K639 G643 A644 S645 ALA ALA ALA PRO ALA THR VAL ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.23Å 192.11Å 116.13Å 90.00° 113.28° 90.00°	Depositor
Resolution (Å)	49.07 – 3.12 49.07 – 3.12	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.07-3.12) 97.4 (49.07-3.12)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.225 , 0.278 0.227 , 0.265	Depositor DCC
R_{free} test set	5575 reflections (8.51%)	wwPDB-VP
Wilson B-factor (Å^2)	60.7	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.853 for H, K, L 0.147 for H, -K, -H-L	Depositor
Outliers	0 of 65516 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	26184	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, PLM

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	0.65	0/4383	0.92	11/5943 (0.2%)
1	B	0.64	2/4383 (0.0%)	0.93	13/5943 (0.2%)
1	C	0.63	0/4383	0.95	13/5943 (0.2%)
1	D	0.63	1/4383 (0.0%)	0.96	14/5943 (0.2%)
1	E	0.61	0/4383	0.93	12/5943 (0.2%)
1	F	0.60	0/4383	0.94	15/5943 (0.3%)
All	All	0.63	3/26298 (0.0%)	0.94	78/35658 (0.2%)

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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	3
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLU	CD-OE2	-5.82	1.19	1.25
1	B	326	ARG	CG-CD	-5.76	1.37	1.51
1	D	207	ASP	CB-CG	5.09	1.62	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	139	ASP	CB-CG-OD2	-16.25	103.68	118.30
1	D	139	ASP	CB-CG-OD1	13.49	130.44	118.30
1	C	420	LEU	CB-CG-CD2	12.72	132.63	111.00
1	C	150	LEU	CB-CG-CD2	-11.67	91.17	111.00
1	E	421	LEU	CB-CG-CD1	-10.60	92.98	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ASN	Peptide
1	A	608	VAL	Peptide
1	B	205	ASN	Peptide
1	B	608	VAL	Peptide
1	C	205	ASN	Peptide

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	4299	0	4238	169	0
1	B	4299	0	4238	156	1
1	C	4299	0	4238	172	0
1	D	4299	0	4238	171	1
1	E	4299	0	4238	167	0
1	F	4299	0	4238	162	0
2	A	53	0	31	5	0
2	B	53	0	31	4	0
2	C	53	0	31	9	0
2	D	53	0	31	8	0
2	E	53	0	31	7	0
2	F	53	0	31	5	0
3	A	18	0	31	7	0
3	B	18	0	31	4	0
3	C	18	0	31	3	0
3	D	18	0	31	3	0
All	All	26184	0	25738	980	1

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 980 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:E:453:VAL:HG12	1:E:484:THR:HB	1.26	1.18
1:C:395:TYR:CD1	1:C:478:LYS:NZ	2.12	1.17
1:C:400:ILE:HD11	1:C:481:SER:HB2	1.33	1.08
1:C:400:ILE:HD11	1:C:481:SER:CB	1.83	1.07
1:C:429:SER:HB3	1:C:430:THR:HA	1.38	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:LYS:NZ	1:D:107:SER:O[1_454]	2.04	0.16

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	572/594 (96%)	463 (81%)	65 (11%)	44 (8%)	1	5
1	B	572/594 (96%)	461 (81%)	67 (12%)	44 (8%)	1	5
1	C	572/594 (96%)	464 (81%)	64 (11%)	44 (8%)	1	5
1	D	572/594 (96%)	465 (81%)	63 (11%)	44 (8%)	1	5
1	E	572/594 (96%)	463 (81%)	65 (11%)	44 (8%)	1	5
1	F	572/594 (96%)	466 (82%)	63 (11%)	43 (8%)	1	5
All	All	3432/3564 (96%)	2782 (81%)	387 (11%)	263 (8%)	1	5

5 of 263 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	173	LEU
1	A	202	ALA
1	A	229	ASN
1	A	242	GLU

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	446/455 (98%)	405 (91%)	41 (9%)	9	32
1	B	446/455 (98%)	410 (92%)	36 (8%)	11	38
1	C	446/455 (98%)	409 (92%)	37 (8%)	11	37
1	D	446/455 (98%)	406 (91%)	40 (9%)	9	33
1	E	446/455 (98%)	400 (90%)	46 (10%)	7	26
1	F	446/455 (98%)	404 (91%)	42 (9%)	8	32
All	All	2676/2730 (98%)	2434 (91%)	242 (9%)	9	33

5 of 242 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	75	SER
1	F	320	ASP
1	D	429	SER
1	F	304	ASP
1	F	551	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	119	ASN
1	E	585	ASN
1	E	175	HIS
1	E	279	GLN

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Mol	Chain	Res	Type
1	F	119	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)

10 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	A	701	-	53,58,58	1.54	7 (13%)	68,89,89	1.44	13 (19%)
2	FAD	B	701	-	53,58,58	1.53	10 (18%)	68,89,89	1.77	17 (25%)
2	FAD	C	701	-	53,58,58	1.41	7 (13%)	68,89,89	1.72	15 (22%)
3	PLM	A	702	-	17,17,17	0.67	0	17,17,17	0.77	0
3	PLM	B	702	-	17,17,17	0.72	0	17,17,17	0.77	1 (5%)
2	FAD	D	701	-	53,58,58	1.28	7 (13%)	68,89,89	1.58	13 (19%)
2	FAD	F	701	-	53,58,58	1.46	8 (15%)	68,89,89	1.50	13 (19%)
3	PLM	C	702	-	17,17,17	0.57	0	17,17,17	1.06	1 (5%)
3	PLM	D	702	-	17,17,17	0.63	0	17,17,17	0.76	0
2	FAD	E	701	-	53,58,58	1.42	10 (18%)	68,89,89	1.41	10 (14%)

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	A	701	-	-	10/30/50/50	0/6/6/6
2	FAD	B	701	-	-	12/30/50/50	0/6/6/6
2	FAD	C	701	-	-	7/30/50/50	0/6/6/6
3	PLM	A	702	-	-	8/15/15/15	-
3	PLM	B	702	-	-	9/15/15/15	-
2	FAD	D	701	-	-	15/30/50/50	0/6/6/6
2	FAD	F	701	-	-	15/30/50/50	0/6/6/6
3	PLM	C	702	-	-	10/15/15/15	-
3	PLM	D	702	-	-	9/15/15/15	-
2	FAD	E	701	-	-	7/30/50/50	0/6/6/6

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FAD	C9A-C5X	5.84	1.51	1.41
2	F	701	FAD	C9A-C5X	5.34	1.50	1.41
2	E	701	FAD	C9A-C5X	5.20	1.49	1.41
2	B	701	FAD	C9A-C5X	5.09	1.49	1.41
2	C	701	FAD	C9A-C5X	4.66	1.49	1.41

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	FAD	N3A-C2A-N1A	-5.30	120.39	128.68
2	B	701	FAD	C4'-C3'-C2'	-4.72	103.54	113.36
2	B	701	FAD	N3A-C2A-N1A	-4.58	121.52	128.68
2	E	701	FAD	P-O3P-PA	-4.16	118.56	132.83
2	F	701	FAD	N3A-C2A-N1A	-4.05	122.34	128.68

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C5'-O5'-P-O2P
2	B	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	B	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	O4'-C4'-C5'-O5'

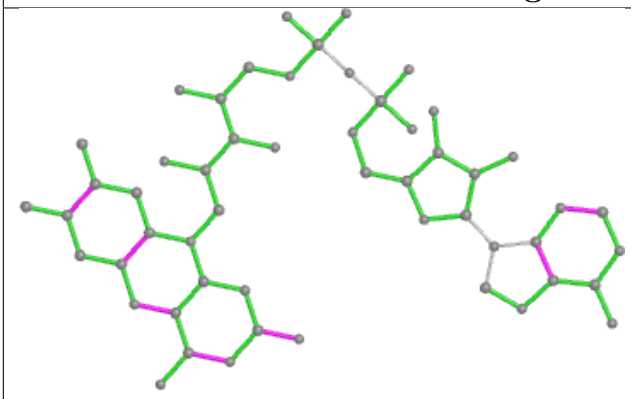
There are no ring outliers.

10 monomers are involved in 55 short contacts:

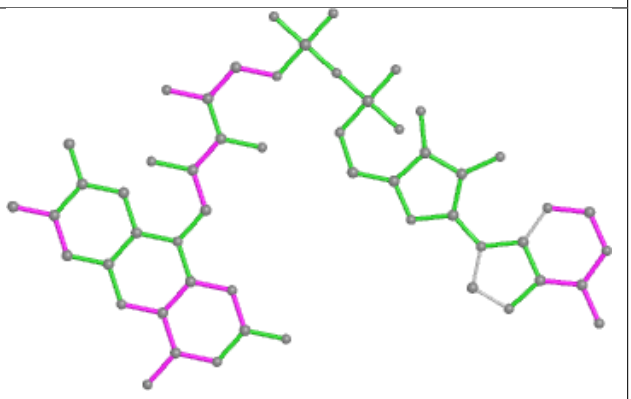
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAD	5	0
2	B	701	FAD	4	0
2	C	701	FAD	9	0
3	A	702	PLM	7	0
3	B	702	PLM	4	0
2	D	701	FAD	8	0
2	F	701	FAD	5	0
3	C	702	PLM	3	0
3	D	702	PLM	3	0
2	E	701	FAD	7	0

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.

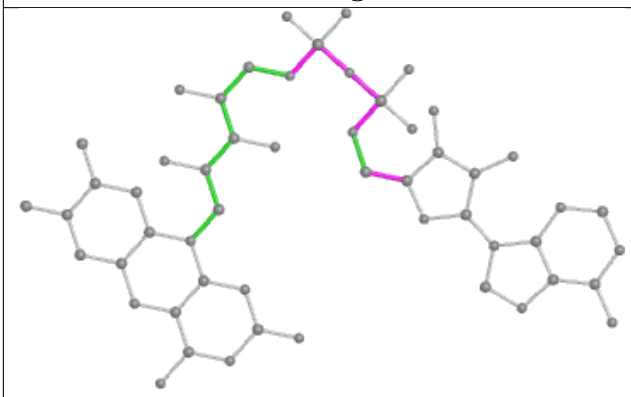
Ligand FAD A 701



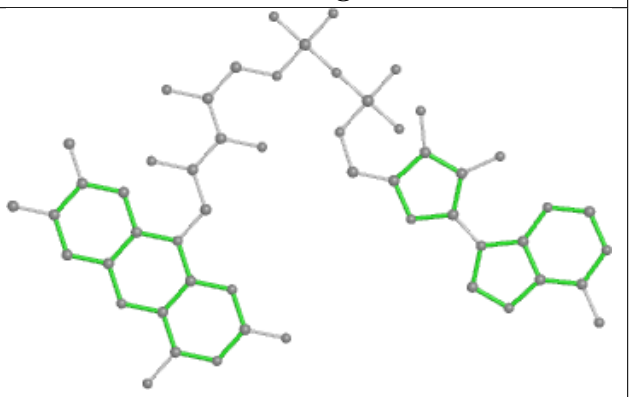
Bond lengths



Bond angles

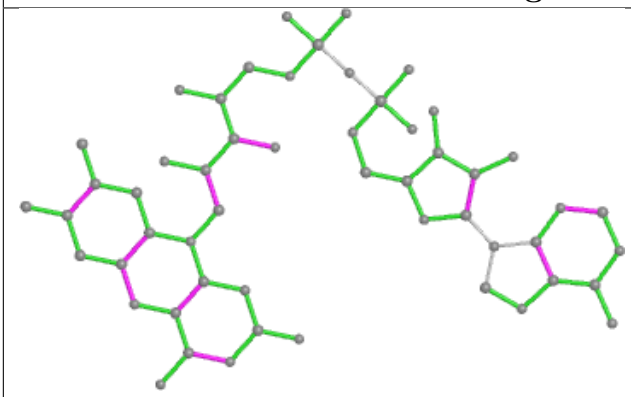


Torsions

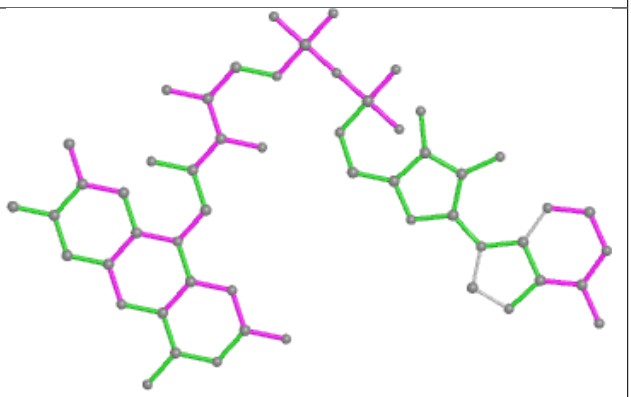


Rings

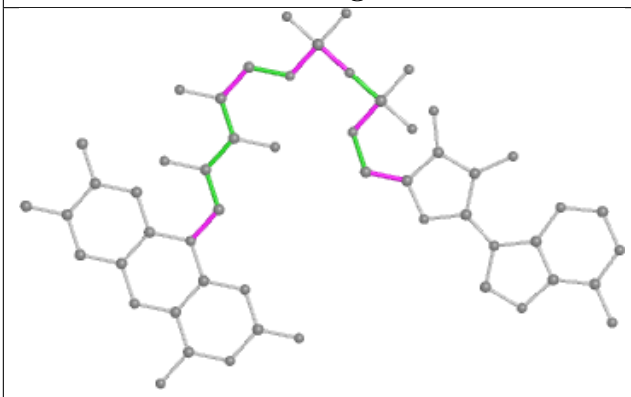
Ligand FAD B 701



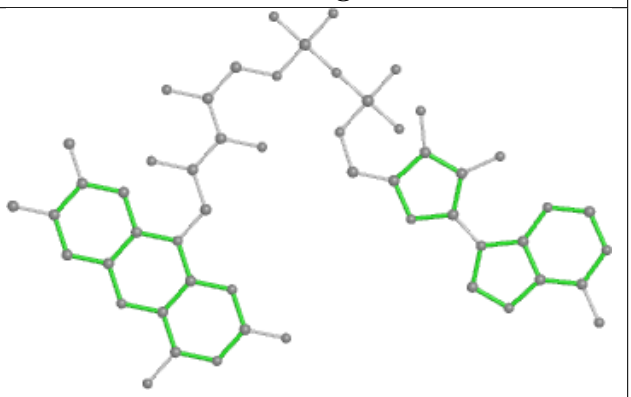
Bond lengths



Bond angles

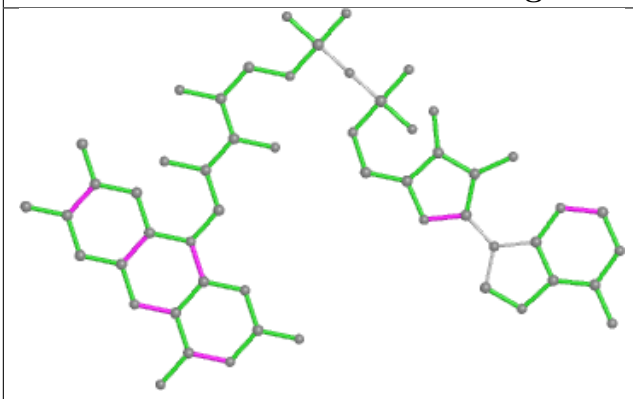


Torsions

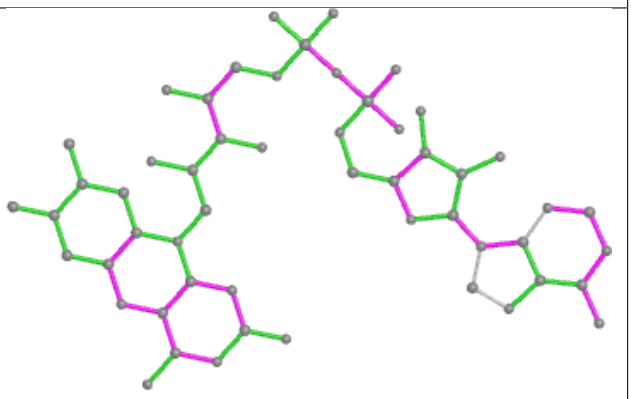


Rings

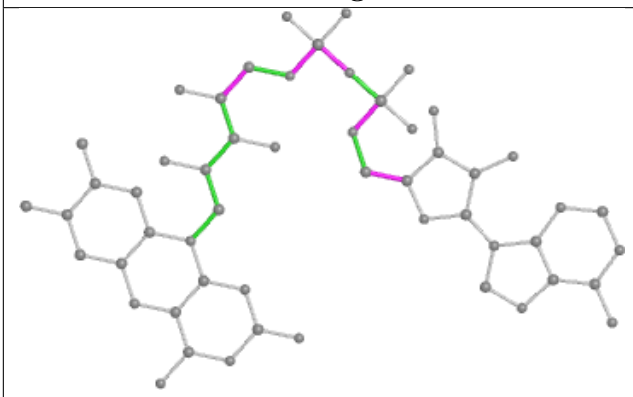
Ligand FAD C 701



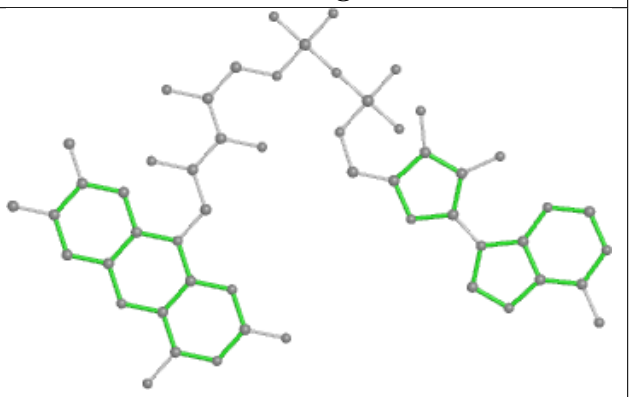
Bond lengths



Bond angles

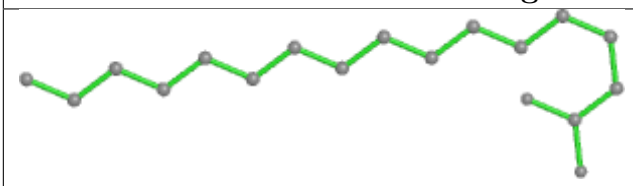


Torsions

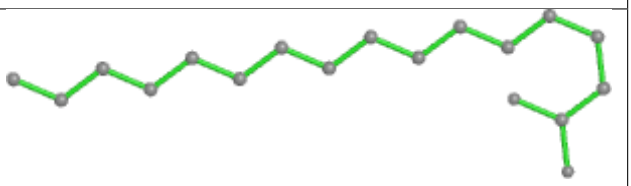


Rings

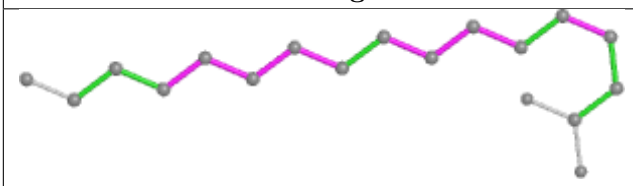
Ligand PLM A 702



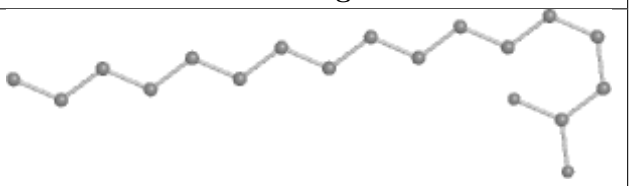
Bond lengths



Bond angles

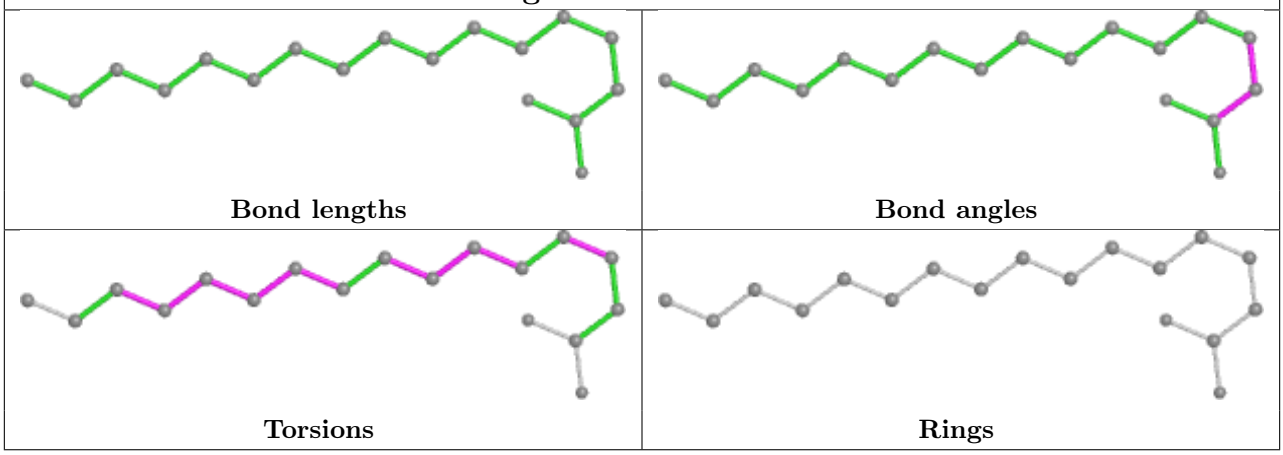


Torsions

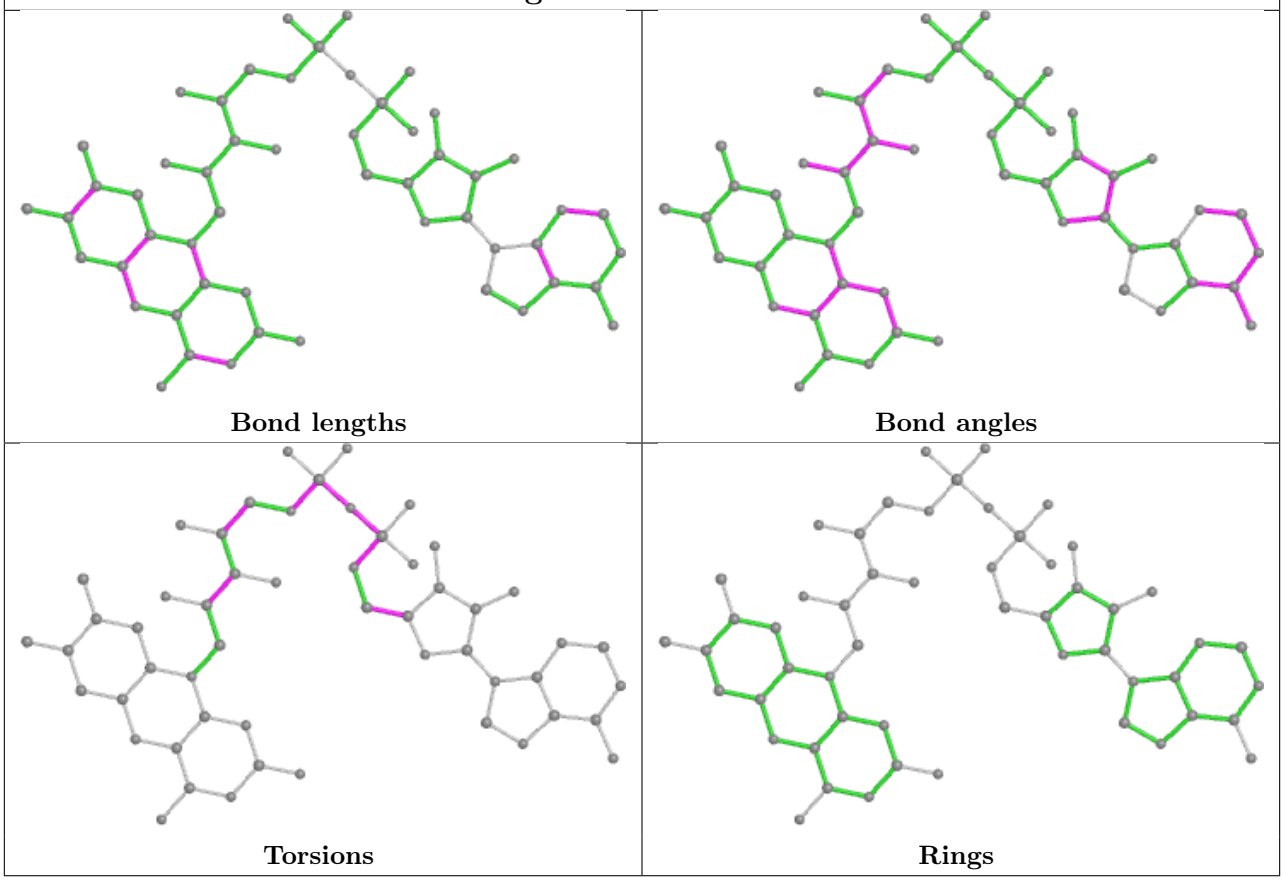


Rings

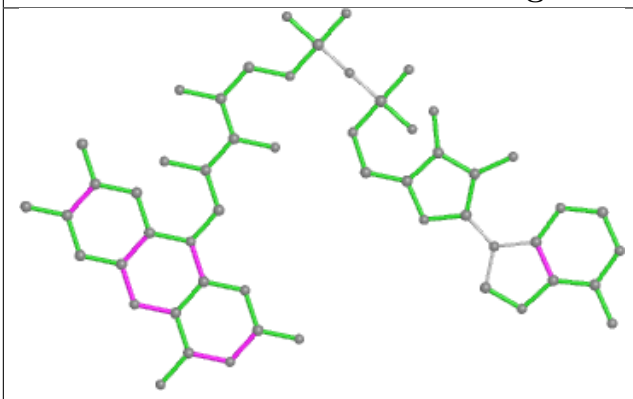
Ligand PLM B 702



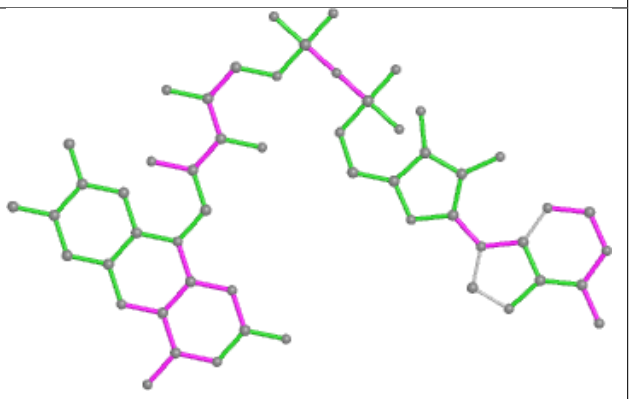
Ligand FAD D 701



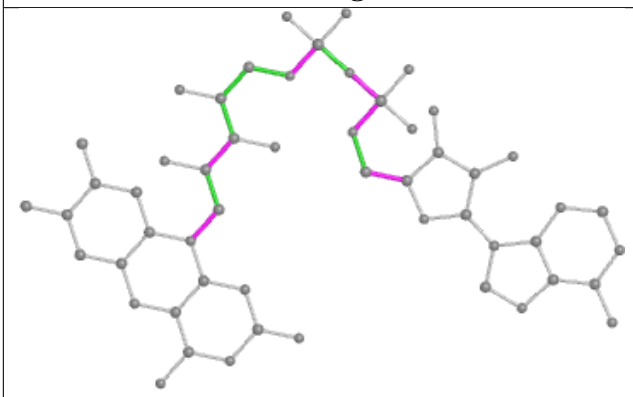
Ligand FAD F 701



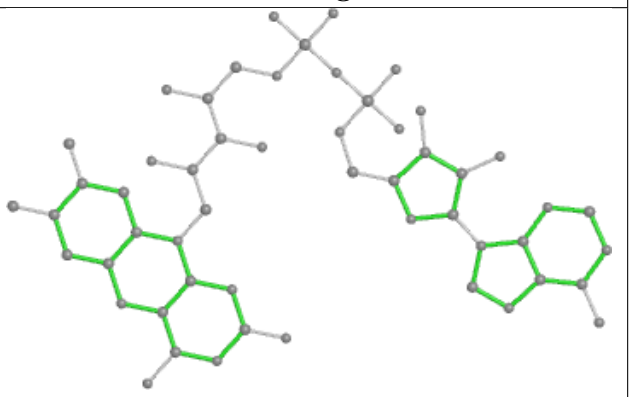
Bond lengths



Bond angles

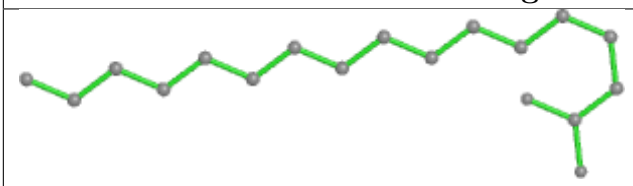


Torsions

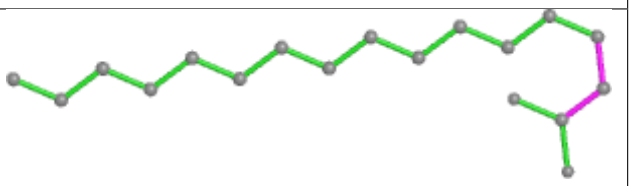


Rings

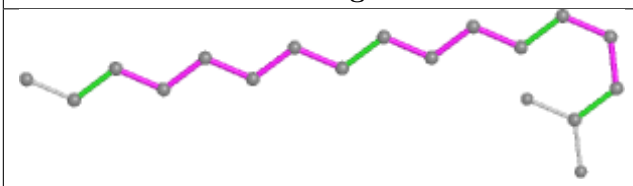
Ligand PLM C 702



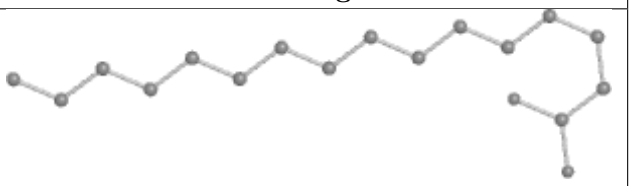
Bond lengths



Bond angles

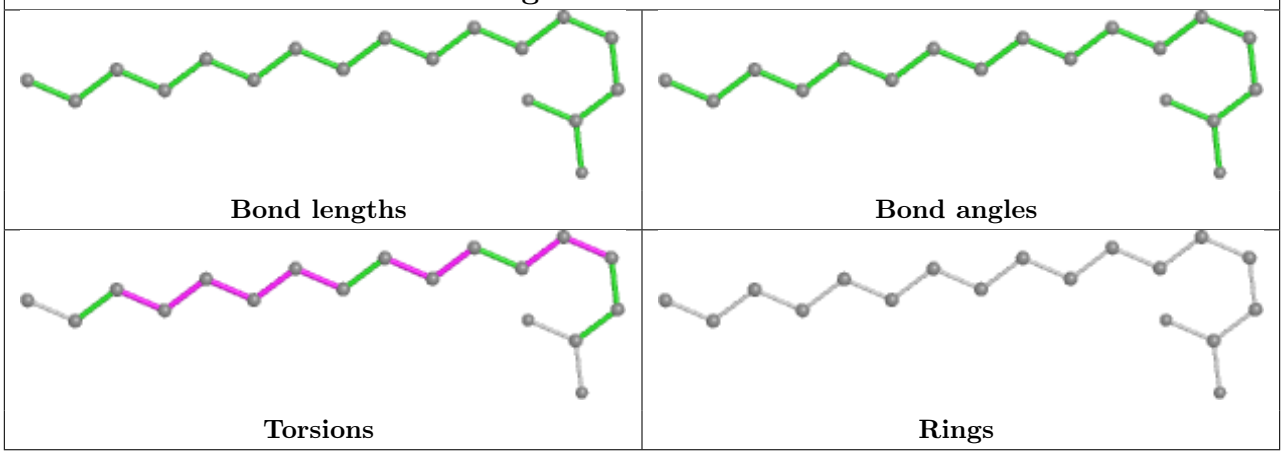


Torsions

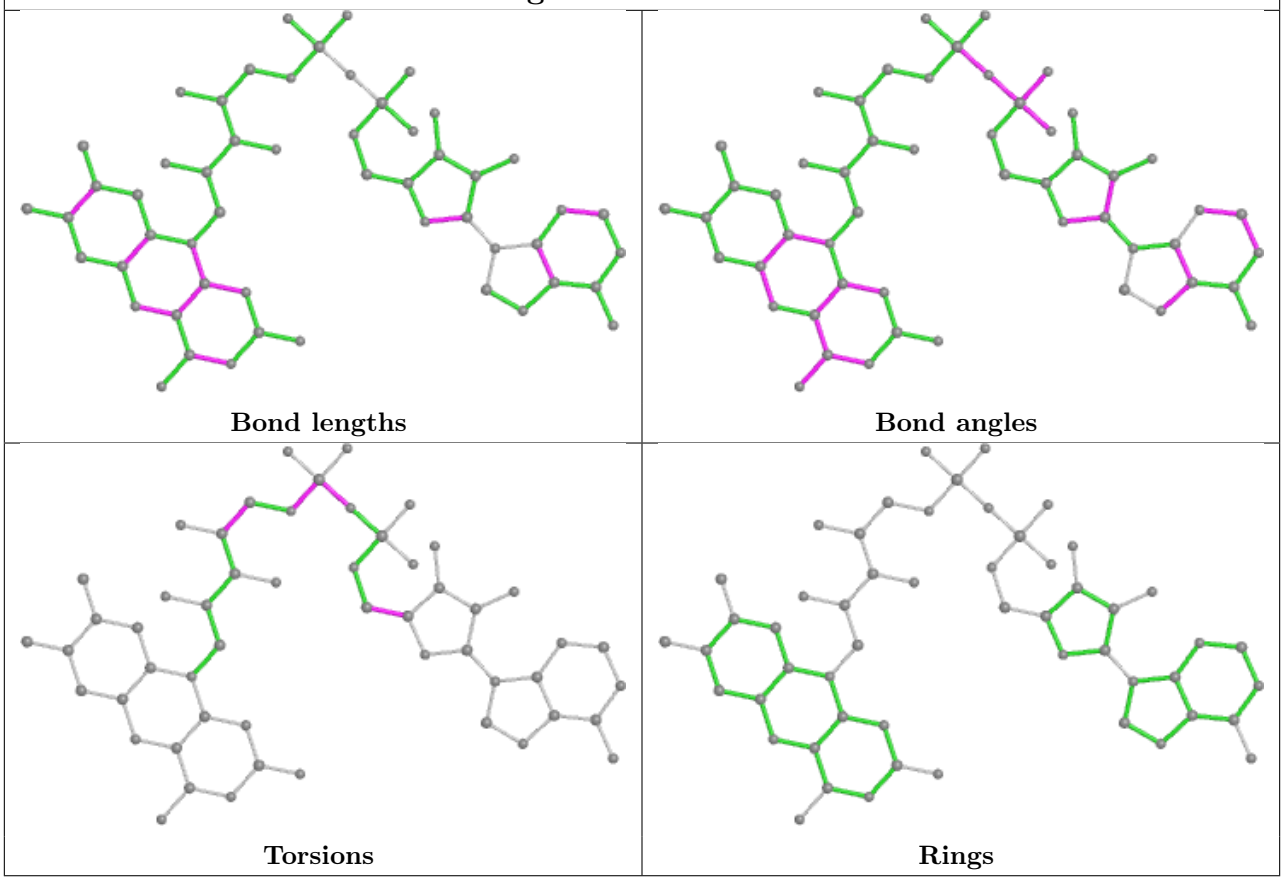


Rings

Ligand PLM D 702



Ligand FAD E 701



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	578/594 (97%)	-0.23	6 (1%)	82	69	20, 41, 74, 102	0
1	B	578/594 (97%)	-0.17	10 (1%)	70	50	21, 43, 77, 119	0
1	C	578/594 (97%)	-0.21	11 (1%)	66	47	22, 44, 79, 114	0
1	D	578/594 (97%)	-0.12	11 (1%)	66	47	24, 48, 78, 132	0
1	E	578/594 (97%)	0.63	61 (10%)	6	2	46, 90, 127, 152	0
1	F	578/594 (97%)	0.51	41 (7%)	16	6	47, 86, 123, 170	0
All	All	3468/3564 (97%)	0.07	140 (4%)	38	19	20, 54, 112, 170	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	419	TYR	6.2
1	E	426	GLY	5.4
1	F	480	PRO	5.4
1	F	229	ASN	5.3
1	E	335	GLY	5.2

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 monosaccharides in this entry.

6.4 Ligands (i)

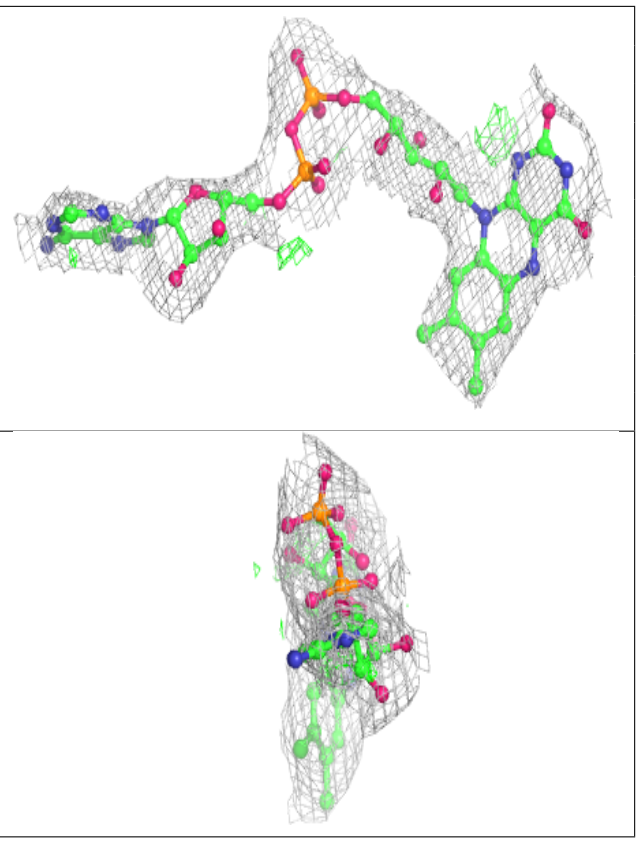
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	E	701	53/53	0.91	0.24	57,85,122,126	0
3	PLM	B	702	18/18	0.91	0.40	31,50,56,58	0
3	PLM	A	702	18/18	0.92	0.25	26,34,43,44	0
2	FAD	F	701	53/53	0.95	0.18	52,65,74,82	0
3	PLM	C	702	18/18	0.95	0.23	29,41,45,45	0
3	PLM	D	702	18/18	0.95	0.24	28,32,35,36	0
2	FAD	A	701	53/53	0.96	0.20	26,35,43,44	0
2	FAD	B	701	53/53	0.96	0.20	23,30,42,53	0
2	FAD	D	701	53/53	0.96	0.19	26,33,41,44	0
2	FAD	C	701	53/53	0.97	0.20	21,32,43,46	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.

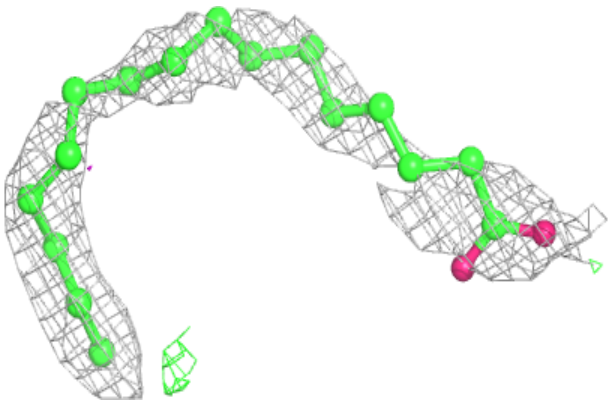
Electron density around FAD E 701:

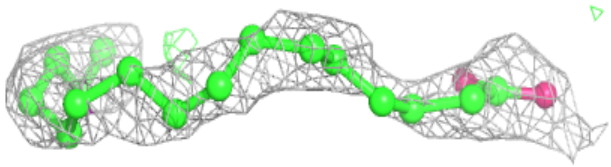
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

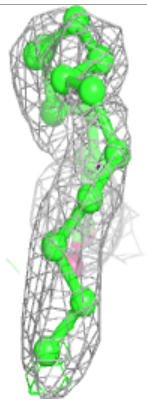


Electron density around PLM B 702:

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

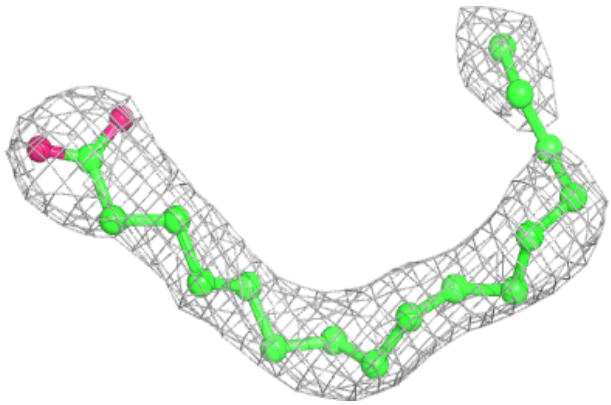


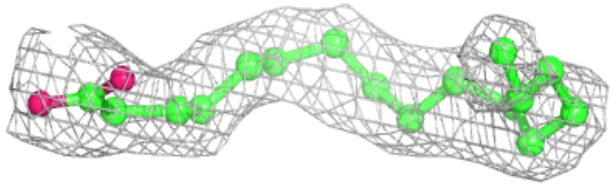


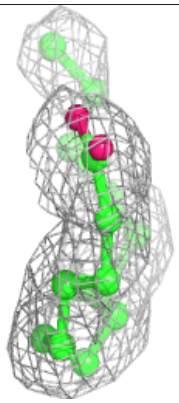


Electron density around PLM A 702:

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

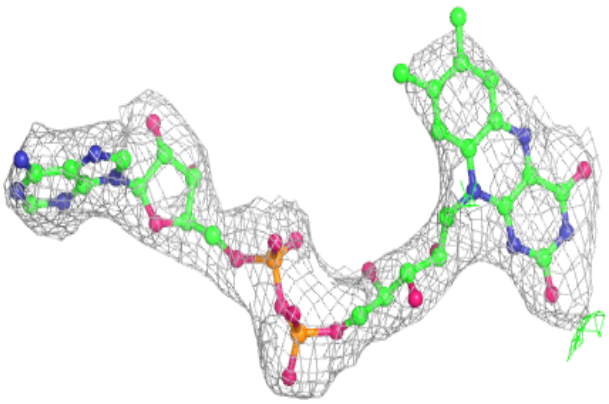


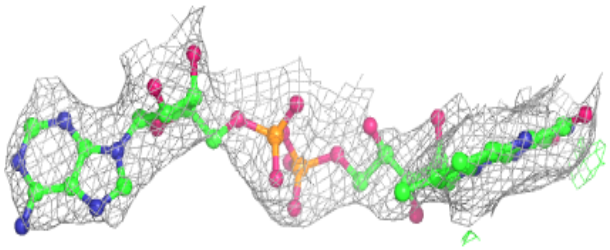


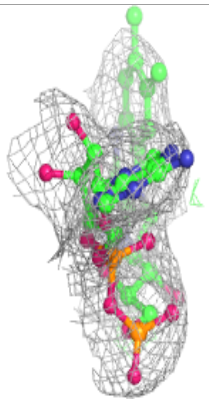


Electron density around FAD F 701:

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

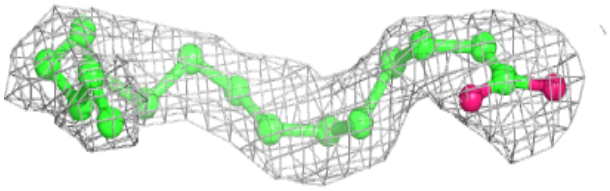


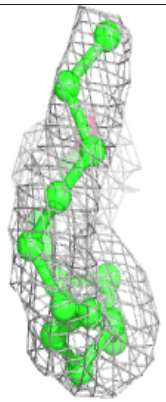




Electron density around PLM C 702:

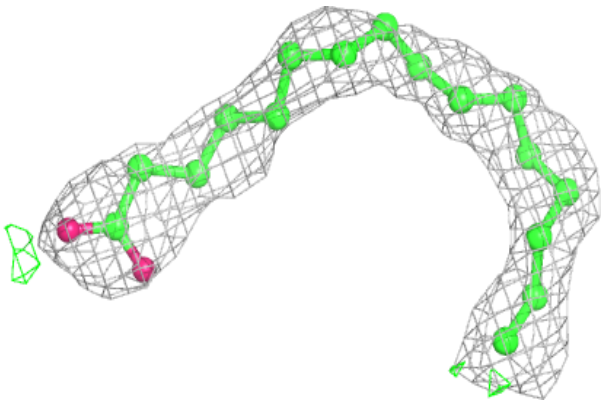
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

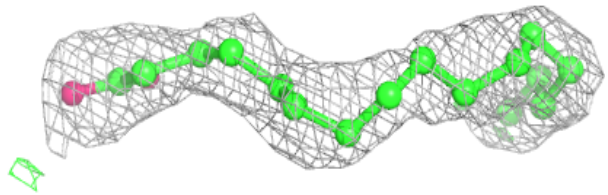


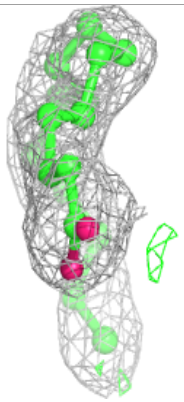


Electron density around PLM D 702:

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

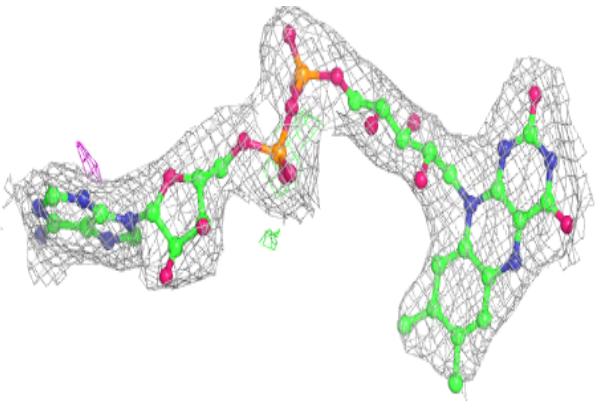


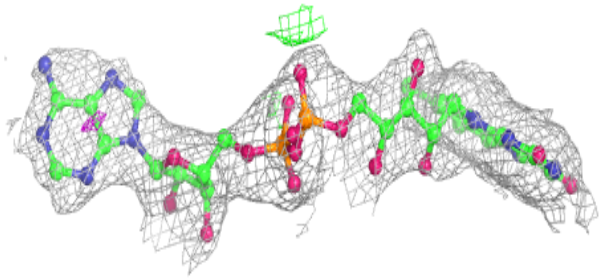


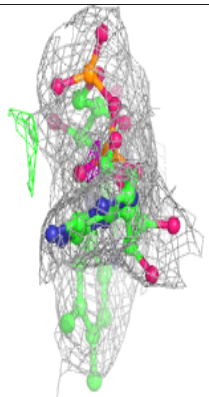


Electron density around FAD A 701:

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

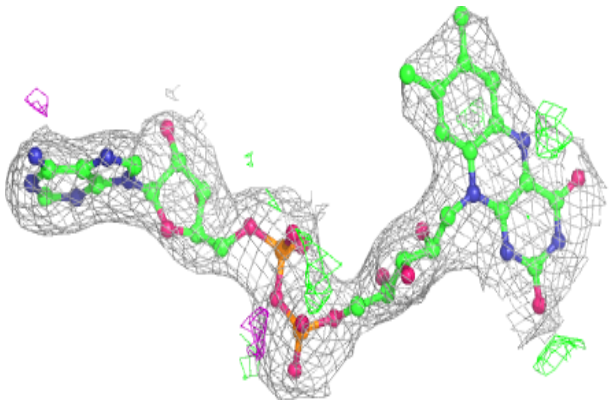


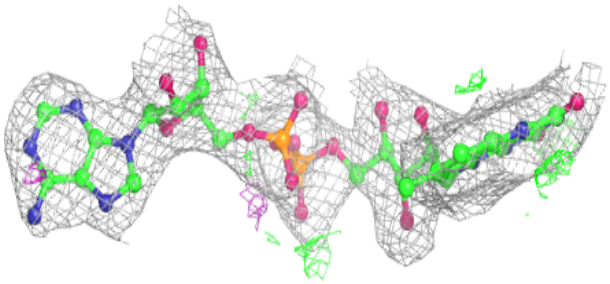


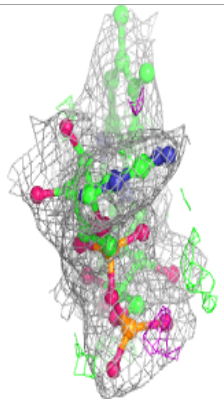


Electron density around FAD B 701:

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

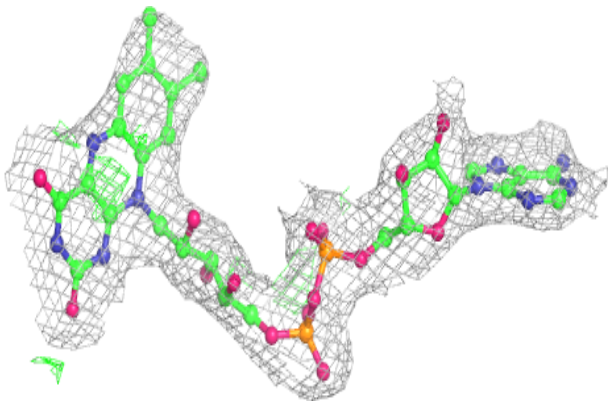


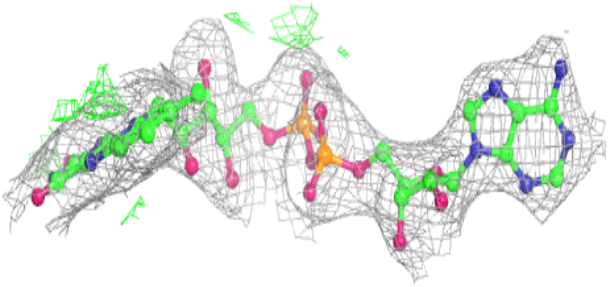


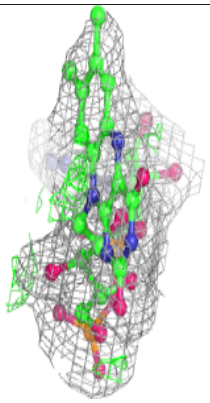


Electron density around FAD D 701:

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

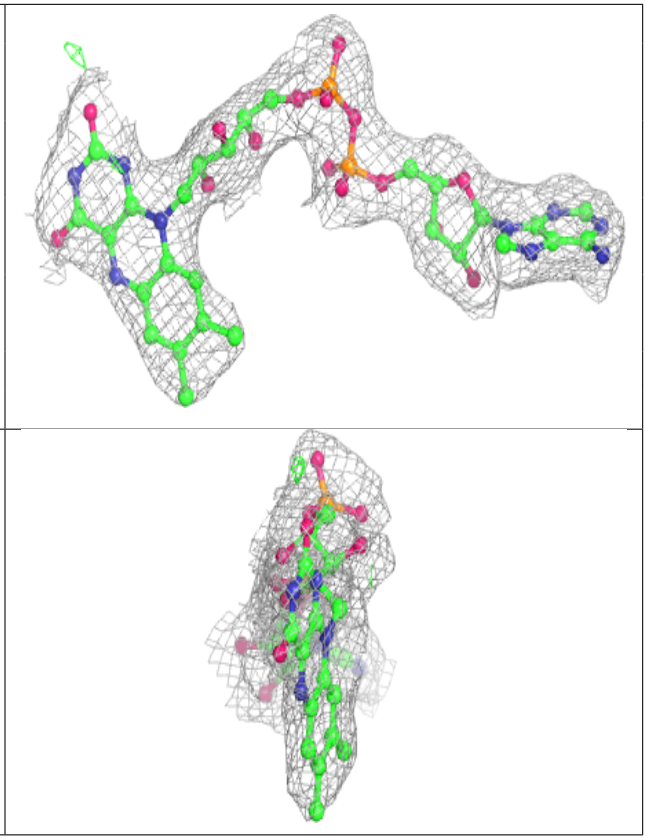






Electron density around FAD C 701:

$2mF_o$-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.