Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 06:51 PM JST

PDB ID	:	8W7F
Title	:	Structure of Drosophila melanogaster L-2-hydroxyglutarate dehydrogenase bound with FAD and a sulfate ion
Authors	:	Yang, J.; Chen, X.; Jin, S.; Ding, J.
Deposited on	:	2023-08-30
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

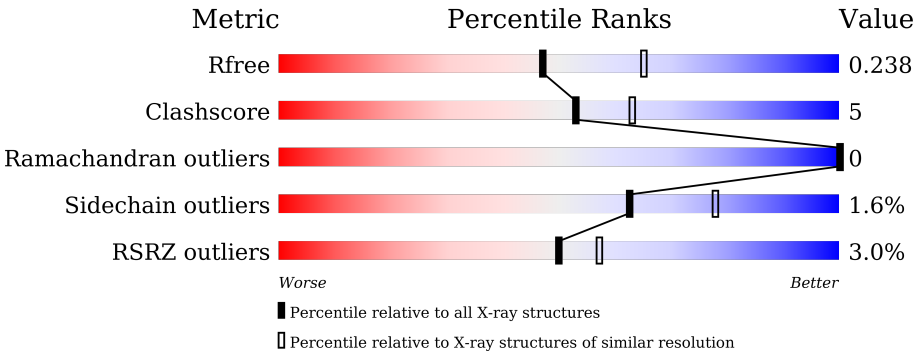
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	415	4% 88% 11%
1	B	415	2% 86% 13%
1	C	415	2% 84% 13%
1	D	415	4% 88% 11%

2 Entry composition

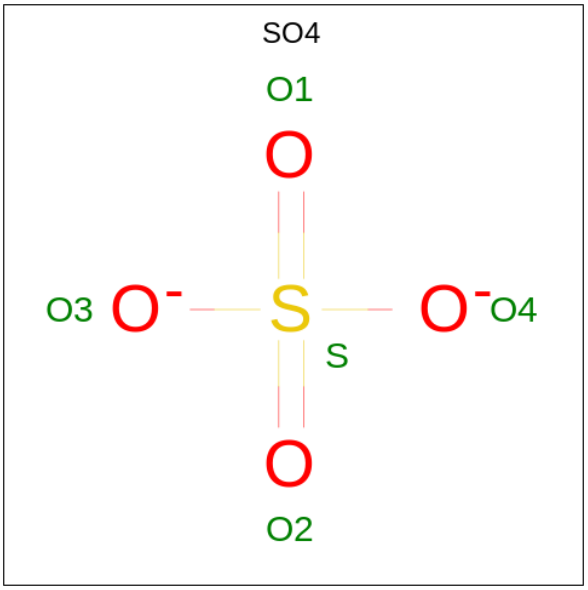
There are 5 unique types of molecules in this entry. The entry contains 13348 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FI05204p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3098	1982	527	573	16			
1	B	412	Total	C	N	O	S	0	0	0
			3124	1995	536	577	16			
1	C	404	Total	C	N	O	S	0	0	0
			3104	1990	526	572	16			
1	D	412	Total	C	N	O	S	0	0	0
			3077	1970	520	571	16			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



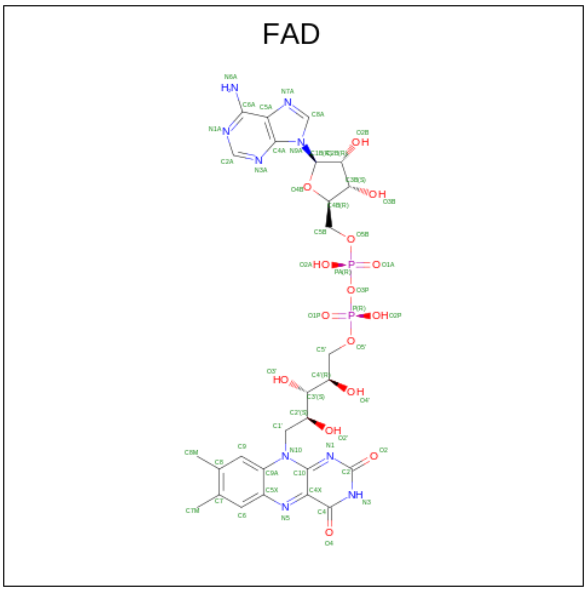
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			

Continued on next page...

Continued from previous page...

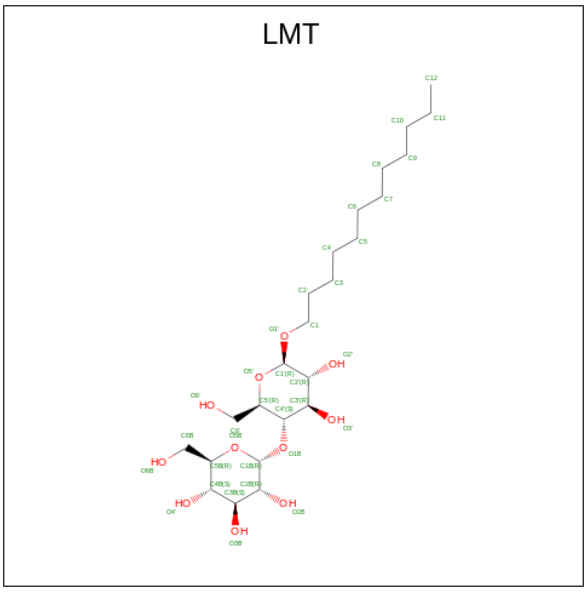
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	C	1	Total C O 35 24 11	0	0
4	D	1	Total C O 35 24 11	0	0

- Molecule 5 is water.

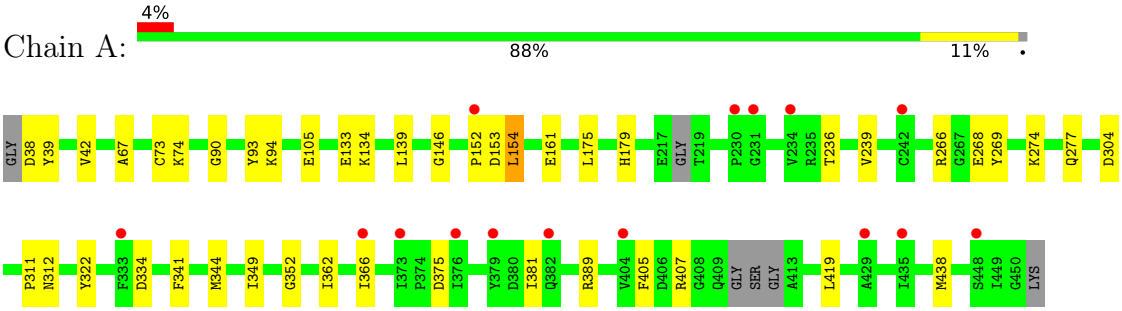
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	148	Total O 148 148	0	0
5	B	147	Total O 147 147	0	0
5	C	131	Total O 131 131	0	0
5	D	147	Total O 147 147	0	0

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.

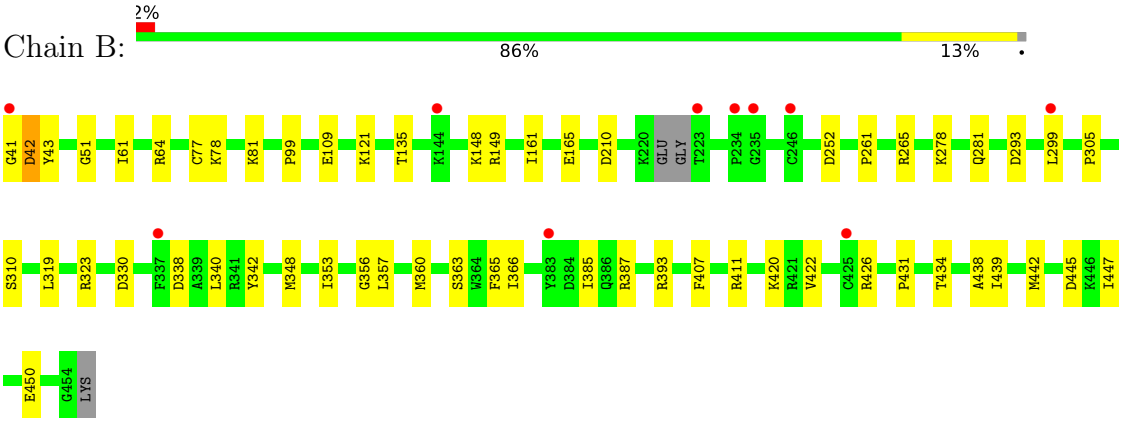
• Molecule 1: FI05204p

Chain A:



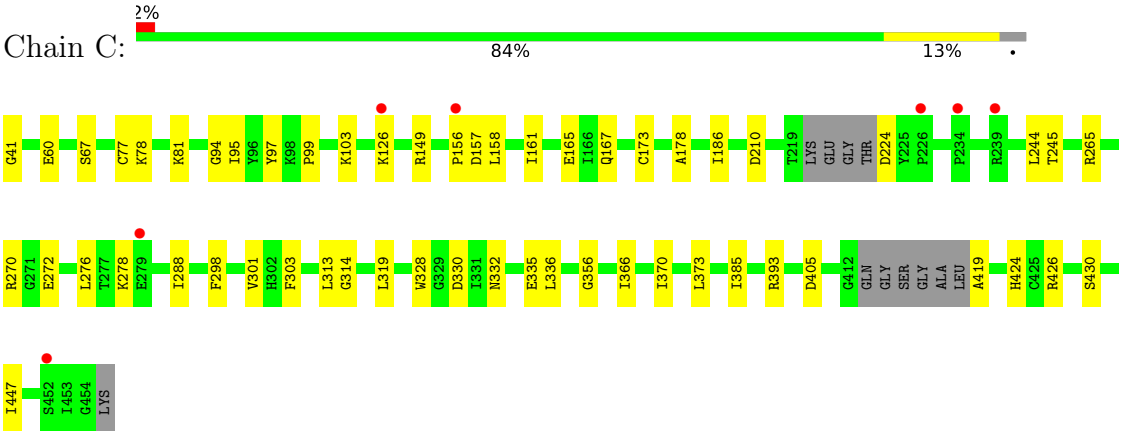
• Molecule 1: FI05204p

Chain B:



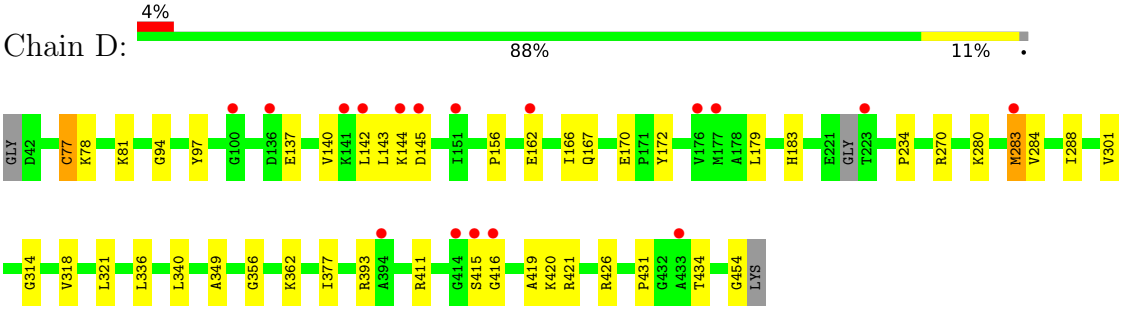
• Molecule 1: FI05204p

Chain C:



• Molecule 1: FI05204p

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.52Å 103.07Å 122.88Å 90.00° 114.63° 90.00°	Depositor
Resolution (Å)	33.26 – 2.30 33.26 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (33.26-2.30) 98.7 (33.26-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.204 , 0.238 0.204 , 0.238	Depositor DCC
R_{free} test set	1988 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13348	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1298e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, FAD, SO4

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	0.26	0/3167	0.45	1/4300 (0.0%)
1	B	0.25	0/3192	0.42	0/4326
1	C	0.26	0/3175	0.42	0/4302
1	D	0.26	0/3148	0.45	1/4282 (0.0%)
All	All	0.26	0/12682	0.43	2/17210 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	CYS	CA-CB-SG	-7.82	99.92	114.00
1	D	77	CYS	CA-CB-SG	-6.80	101.75	114.00

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	3098	0	3025	29	0
1	B	3124	0	3079	34	0
1	C	3104	0	3065	36	0
1	D	3077	0	2961	34	0
2	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
3	C	53	0	31	1	0
3	D	53	0	31	1	0
4	A	35	0	46	2	0
4	B	35	0	45	5	0
4	C	35	0	45	4	0
4	D	35	0	45	3	0
5	A	148	0	0	8	1
5	B	147	0	0	4	0
5	C	131	0	0	10	1
5	D	147	0	0	9	0
All	All	13348	0	12435	135	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 5.

All (135) 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:A:161:GLU:OE1	5:A:601:HOH:O	1.87	0.93
1:A:105:GLU:OE1	5:A:602:HOH:O	1.94	0.86
1:C:224:ASP:N	5:C:602:HOH:O	2.11	0.83
1:A:94:LYS:NZ	5:A:603:HOH:O	2.14	0.81
1:A:389:ARG:HG2	3:A:502:FAD:HM83	1.63	0.81
1:D:454:GLY:O	5:D:601:HOH:O	1.99	0.80
1:B:393:ARG:HG2	3:B:502:FAD:HM83	1.64	0.80
1:C:393:ARG:HG2	3:C:502:FAD:HM83	1.64	0.79
1:B:135:THR:OG1	5:B:601:HOH:O	2.03	0.76
1:D:142:LEU:O	5:D:602:HOH:O	2.02	0.75
1:D:166:ILE:N	5:D:603:HOH:O	2.20	0.75
1:D:393:ARG:HG2	3:D:502:FAD:HM83	1.70	0.73
1:A:38:ASP:N	5:A:605:HOH:O	2.22	0.73
1:B:356:GLY:HA3	4:B:503:LMT:H91	1.70	0.73
1:B:363:SER:O	1:B:387:ARG:NH2	2.21	0.72
1:C:60:GLU:OE1	5:C:601:HOH:O	2.07	0.72
1:A:352:GLY:HA3	4:A:503:LMT:H91	1.72	0.71
1:D:143:LEU:HD11	1:D:179:LEU:HB2	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ALA:N	5:C:606:HOH:O	2.25	0.68
1:B:161:ILE:HG12	1:B:165:GLU:HB2	1.76	0.67
1:B:293:ASP:OD2	5:B:602:HOH:O	2.12	0.67
1:A:366:ILE:HD11	1:A:381:ILE:HG12	1.76	0.67
1:C:245:THR:HB	1:C:424:HIS:HA	1.79	0.64
1:B:61:ILE:HG13	1:B:447:ILE:HD11	1.79	0.64
1:B:422:VAL:O	5:B:603:HOH:O	2.15	0.63
1:C:99:PRO:HD3	1:C:149:ARG:HG2	1.81	0.63
1:B:366:ILE:HG21	1:B:385:ILE:HD11	1.81	0.62
1:C:210:ASP:OD1	5:C:603:HOH:O	2.16	0.62
1:A:304:ASP:HB2	1:D:234:PRO:HB2	1.82	0.61
1:A:42:VAL:HG12	1:A:67:ALA:HB3	1.83	0.61
1:C:103:LYS:NZ	1:C:405:ASP:OD2	2.28	0.60
1:D:362:LYS:NZ	5:D:606:HOH:O	2.32	0.60
1:A:139:LEU:HD11	1:A:175:LEU:HB2	1.84	0.59
1:C:270:ARG:NH1	1:C:272:GLU:OE2	2.36	0.59
1:A:389:ARG:NH2	5:A:611:HOH:O	2.36	0.58
1:C:332:ASN:HB3	1:C:335:GLU:HB2	1.86	0.57
1:C:161:ILE:HG12	1:C:165:GLU:HB3	1.86	0.57
1:C:78:LYS:HE3	1:C:81:LYS:HD3	1.87	0.57
1:C:393:ARG:NH2	5:C:615:HOH:O	2.37	0.56
1:D:280:LYS:HB3	1:D:283:MET:HE2	1.87	0.56
1:C:356:GLY:HA3	4:C:503:LMT:H91	1.89	0.55
1:D:419:ALA:O	1:D:421:ARG:N	2.39	0.54
1:C:67:SER:O	5:C:604:HOH:O	2.18	0.54
1:B:99:PRO:HD3	1:B:149:ARG:HG2	1.90	0.53
1:D:166:ILE:HG13	5:D:603:HOH:O	2.07	0.53
1:D:415:SER:H	1:D:416:GLY:HA3	1.75	0.52
1:B:64:ARG:NH1	1:B:445:ASP:OD1	2.38	0.52
1:C:265:ARG:NH1	5:C:618:HOH:O	2.43	0.52
1:B:42:ASP:HB3	1:B:43:TYR:CD2	2.45	0.51
1:B:265:ARG:NH1	1:B:338:ASP:HB3	2.24	0.51
1:B:357:LEU:HA	1:B:360:MET:HE3	1.90	0.51
1:B:431:PRO:HG2	1:B:434:THR:HB	1.91	0.51
1:D:349:ALA:HB2	4:D:503:LMT:H122	1.92	0.51
1:A:268:GLU:H	1:A:312:ASN:HB2	1.75	0.51
1:C:366:ILE:HG21	1:C:385:ILE:HD11	1.93	0.51
1:B:78:LYS:HE2	1:B:81:LYS:HG3	1.92	0.50
1:B:319:LEU:HD22	4:B:503:LMT:H123	1.93	0.50
1:B:252:ASP:OD1	1:B:323:ARG:NH2	2.44	0.49
1:B:407:PHE:HZ	1:B:439:ILE:HG23	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLY:HA3	1:A:154:LEU:HD12	1.94	0.49
1:B:411:ARG:NH1	1:B:450:GLU:OE2	2.46	0.49
1:C:370:ILE:HD11	1:C:385:ILE:HG12	1.95	0.48
1:D:137:GLU:O	1:D:140:VAL:HG22	2.13	0.48
1:D:356:GLY:HA3	4:D:503:LMT:H91	1.95	0.48
1:D:415:SER:N	1:D:416:GLY:HA3	2.28	0.48
1:C:95:ILE:HG12	1:C:158:LEU:HD11	1.96	0.48
1:A:349:ILE:HD12	1:B:365:PHE:HE2	1.78	0.48
1:A:266:ARG:NH2	1:A:322:TYR:O	2.47	0.48
1:B:442:MET:HB3	1:B:442:MET:HE2	1.75	0.48
1:C:244:LEU:HD13	1:C:447:ILE:HD11	1.95	0.47
1:D:78:LYS:HE2	1:D:81:LYS:HD2	1.97	0.47
1:A:269:TYR:CZ	1:A:311:PRO:HB3	2.50	0.47
1:B:261:PRO:O	1:B:426:ARG:NH2	2.41	0.47
1:B:51:GLY:HA3	3:B:502:FAD:O1P	2.15	0.47
1:D:145:ASP:HB2	5:D:602:HOH:O	2.15	0.47
1:A:74:LYS:NZ	5:A:615:HOH:O	2.44	0.46
1:A:405:PHE:HB3	1:A:419:LEU:HD11	1.97	0.46
1:A:152:PRO:HA	1:A:153:ASP:HA	1.54	0.46
1:B:348:MET:SD	4:B:503:LMT:H82	2.56	0.46
1:C:126:LYS:HD2	1:C:186:ILE:HD11	1.97	0.46
1:C:126:LYS:NZ	5:C:607:HOH:O	2.28	0.45
1:C:41:GLY:N	5:C:620:HOH:O	2.50	0.45
1:B:121:LYS:HA	1:B:121:LYS:HD3	1.83	0.45
4:B:503:LMT:H1'	4:B:503:LMT:H21	1.61	0.44
1:D:162:GLU:C	5:D:603:HOH:O	2.56	0.44
1:A:90:GLY:HA2	1:A:93:TYR:CE2	2.53	0.44
1:A:341:PHE:O	1:A:344:MET:HG3	2.18	0.44
1:D:431:PRO:HG2	1:D:434:THR:HB	2.00	0.44
1:C:301:VAL:HG13	1:C:314:GLY:HA2	2.00	0.44
1:C:156:PRO:HA	1:C:157:ASP:HA	1.57	0.43
1:D:156:PRO:HB2	1:D:183:HIS:ND1	2.34	0.43
1:D:167:GLN:HA	1:D:170:GLU:O	2.17	0.43
1:C:167:GLN:NE2	1:C:173:CYS:O	2.52	0.43
1:C:161:ILE:HG22	1:C:178:ALA:O	2.19	0.43
1:D:426:ARG:HB3	5:D:646:HOH:O	2.18	0.43
1:D:170:GLU:HG2	1:D:288:ILE:HD11	2.01	0.43
1:D:94:GLY:HA2	1:D:97:TYR:CE2	2.54	0.43
1:D:411:ARG:HH21	1:D:420:LYS:H	1.66	0.43
1:C:319:LEU:HD22	4:C:503:LMT:H123	2.00	0.43
1:D:172:TYR:CG	1:D:283:MET:HG3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:MET:HG2	1:D:377:ILE:HD13	1.99	0.43
1:A:133:GLU:HG3	5:A:721:HOH:O	2.17	0.43
1:A:274:LYS:HA	1:A:277:GLN:HG3	2.01	0.42
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.86	0.42
4:A:503:LMT:H121	4:A:503:LMT:H92	1.84	0.42
1:D:270:ARG:HB3	1:D:318:VAL:HG23	2.01	0.42
1:D:321:LEU:HD22	1:D:336:LEU:HD12	2.01	0.42
1:D:362:LYS:NZ	5:D:622:HOH:O	2.52	0.42
1:B:340:LEU:C	1:B:342:TYR:H	2.22	0.42
1:C:366:ILE:HD13	1:C:366:ILE:HA	1.87	0.42
1:D:301:VAL:HG13	1:D:314:GLY:HA2	2.02	0.42
1:D:284:VAL:HG12	1:D:377:ILE:HD11	2.02	0.42
1:B:278:LYS:HA	1:B:281:GLN:HG3	2.02	0.41
1:B:353:ILE:HA	4:B:503:LMT:H102	2.01	0.41
1:C:313:LEU:HD13	1:C:373:LEU:HD13	2.02	0.41
1:B:41:GLY:HA3	1:B:42:ASP:HA	1.67	0.41
1:C:288:ILE:HB	1:C:303:PHE:HB2	2.02	0.41
1:D:283:MET:HG2	1:D:377:ILE:HG21	2.02	0.41
1:B:161:ILE:CG1	1:B:165:GLU:HB2	2.45	0.41
1:B:305:PRO:HA	1:B:310:SER:O	2.20	0.41
4:C:503:LMT:H1'	4:C:503:LMT:H21	1.66	0.41
1:B:109:GLU:HG2	1:B:438:ALA:HB2	2.01	0.41
1:A:42:VAL:HG23	1:A:239:VAL:HG13	2.03	0.41
1:A:375:ASP:HB2	5:A:730:HOH:O	2.20	0.41
1:A:39:TYR:O	1:A:236:THR:HA	2.21	0.41
1:A:362:ILE:HG21	1:A:381:ILE:HD11	2.03	0.41
4:D:503:LMT:H1'	4:D:503:LMT:H21	1.79	0.41
1:B:299:LEU:O	5:B:604:HOH:O	2.22	0.40
1:C:276:LEU:HD23	1:C:276:LEU:HA	1.95	0.40
1:C:426:ARG:HB3	5:C:653:HOH:O	2.21	0.40
1:D:336:LEU:HG	1:D:340:LEU:HD12	2.02	0.40
1:A:152:PRO:O	1:A:179:HIS:ND1	2.31	0.40
1:C:94:GLY:HA2	1:C:97:TYR:CE2	2.56	0.40
1:C:158:LEU:HA	1:C:158:LEU:HD23	1.86	0.40
1:C:298:PHE:HD2	4:C:503:LMT:H31	1.86	0.40

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)
5:A:712:HOH:O	5:C:699:HOH:O[3_545]	2.11	0.09

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	403/415 (97%)	388 (96%)	15 (4%)	0	100	100
1	B	408/415 (98%)	393 (96%)	15 (4%)	0	100	100
1	C	398/415 (96%)	381 (96%)	17 (4%)	0	100	100
1	D	408/415 (98%)	395 (97%)	13 (3%)	0	100	100
All	All	1617/1660 (97%)	1557 (96%)	60 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	319/343 (93%)	314 (98%)	5 (2%)	62	78
1	B	323/343 (94%)	317 (98%)	6 (2%)	57	73
1	C	325/343 (95%)	319 (98%)	6 (2%)	59	75
1	D	310/343 (90%)	307 (99%)	3 (1%)	76	87
All	All	1277/1372 (93%)	1257 (98%)	20 (2%)	62	78

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	LYS
1	A	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	334	ASP
1	A	407	ARG
1	A	438	MET
1	B	42	ASP
1	B	77	CYS
1	B	148	LYS
1	B	210	ASP
1	B	330	ASP
1	B	420	LYS
1	C	77	CYS
1	C	278	LYS
1	C	328	TRP
1	C	330	ASP
1	C	336	LEU
1	C	430	SER
1	D	77	CYS
1	D	144	LYS
1	D	283	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

12 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	$\#\|Z\| > 2$
3	FAD	C	502	-	53,58,58	0.48	0	68,89,89	0.54	1 (1%)
3	FAD	D	502	-	53,58,58	0.46	0	68,89,89	0.54	2 (2%)
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.12	0
4	LMT	C	503	-	36,36,36	1.16	5 (13%)	47,47,47	0.97	2 (4%)
2	SO4	B	501	-	4,4,4	0.15	0	6,6,6	0.06	0
3	FAD	A	502	-	53,58,58	0.46	0	68,89,89	0.54	1 (1%)
4	LMT	A	503	-	36,36,36	1.15	5 (13%)	47,47,47	0.97	3 (6%)
4	LMT	D	503	-	36,36,36	1.16	5 (13%)	47,47,47	0.97	3 (6%)
2	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.07	0
3	FAD	B	502	-	53,58,58	0.47	0	68,89,89	0.52	1 (1%)
2	SO4	D	501	-	4,4,4	0.12	0	6,6,6	0.06	0
4	LMT	B	503	-	36,36,36	1.16	5 (13%)	47,47,47	0.96	2 (4%)

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	C	502	-	-	4/30/50/50	0/6/6/6
4	LMT	C	503	-	-	7/21/61/61	0/2/2/2
3	FAD	A	502	-	-	7/30/50/50	0/6/6/6
4	LMT	A	503	-	-	7/21/61/61	0/2/2/2
4	LMT	D	503	-	-	7/21/61/61	0/2/2/2
3	FAD	B	502	-	-	6/30/50/50	0/6/6/6
3	FAD	D	502	-	-	3/30/50/50	0/6/6/6
4	LMT	B	503	-	-	6/21/61/61	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	LMT	O3'-C3'	-2.74	1.36	1.43
4	C	503	LMT	O3'-C3'	-2.65	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	LMT	O3'-C3'	-2.61	1.36	1.43
4	A	503	LMT	O3'-C3'	-2.52	1.37	1.43
4	C	503	LMT	O3B-C3B	-2.48	1.37	1.43
4	C	503	LMT	O2'-C2'	-2.47	1.37	1.43
4	D	503	LMT	O2B-C2B	-2.43	1.37	1.43
4	A	503	LMT	O2B-C2B	-2.39	1.37	1.43
4	D	503	LMT	O3B-C3B	-2.38	1.37	1.43
4	A	503	LMT	O3B-C3B	-2.38	1.37	1.43
4	A	503	LMT	O2'-C2'	-2.34	1.37	1.43
4	B	503	LMT	O2'-C2'	-2.32	1.37	1.43
4	B	503	LMT	O3B-C3B	-2.31	1.37	1.43
4	B	503	LMT	O2B-C2B	-2.28	1.37	1.43
4	D	503	LMT	O4'-C4B	-2.25	1.37	1.43
4	D	503	LMT	O2'-C2'	-2.24	1.37	1.43
4	C	503	LMT	O2B-C2B	-2.24	1.37	1.43
4	B	503	LMT	O4'-C4B	-2.23	1.37	1.43
4	A	503	LMT	O4'-C4B	-2.23	1.37	1.43
4	C	503	LMT	O4'-C4B	-2.08	1.38	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	503	LMT	C3'-C4'-C5'	-2.63	104.90	110.93
4	A	503	LMT	C3'-C4'-C5'	-2.60	104.95	110.93
4	C	503	LMT	C3'-C4'-C5'	-2.53	105.12	110.93
4	D	503	LMT	C3'-C4'-C5'	-2.34	105.56	110.93
3	D	502	FAD	C5A-C6A-N6A	2.33	123.89	120.35
3	C	502	FAD	C5A-C6A-N6A	2.30	123.85	120.35
4	A	503	LMT	C1'-O5'-C5'	-2.30	109.18	113.69
3	A	502	FAD	C5A-C6A-N6A	2.29	123.83	120.35
4	D	503	LMT	C1'-O5'-C5'	-2.26	109.26	113.69
3	B	502	FAD	C5A-C6A-N6A	2.23	123.75	120.35
4	B	503	LMT	C1'-O5'-C5'	-2.21	109.36	113.69
3	D	502	FAD	P-O3P-PA	-2.19	125.32	132.83
4	D	503	LMT	C3B-C4B-C5B	-2.14	106.42	110.24
4	C	503	LMT	C1'-O5'-C5'	-2.10	109.57	113.69
4	A	503	LMT	C3B-C4B-C5B	-2.06	106.57	110.24

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	FAD	C5B-O5B-PA-O2A
3	A	502	FAD	P-O3P-PA-O5B
3	A	502	FAD	O4B-C4B-C5B-O5B
3	B	502	FAD	P-O3P-PA-O5B
3	C	502	FAD	P-O3P-PA-O5B
4	A	503	LMT	C2-C1-O1'-C1'
4	C	503	LMT	C2-C1-O1'-C1'
3	C	502	FAD	O4B-C4B-C5B-O5B
3	D	502	FAD	O4B-C4B-C5B-O5B
4	D	503	LMT	O1'-C1-C2-C3
4	C	503	LMT	O1'-C1-C2-C3
4	A	503	LMT	O1'-C1-C2-C3
3	A	502	FAD	C3B-C4B-C5B-O5B
4	C	503	LMT	C7-C8-C9-C10
4	D	503	LMT	C11-C10-C9-C8
4	B	503	LMT	C7-C8-C9-C10
4	D	503	LMT	C7-C8-C9-C10
4	C	503	LMT	C11-C10-C9-C8
4	C	503	LMT	O5B-C5B-C6B-O6B
4	A	503	LMT	C11-C10-C9-C8
4	A	503	LMT	C7-C8-C9-C10
4	B	503	LMT	C11-C10-C9-C8
4	C	503	LMT	C2-C3-C4-C5
4	D	503	LMT	C1-C2-C3-C4
4	B	503	LMT	C2-C3-C4-C5
4	B	503	LMT	C1-C2-C3-C4
3	B	502	FAD	O4B-C4B-C5B-O5B
4	C	503	LMT	C1-C2-C3-C4
4	D	503	LMT	C9-C10-C11-C12
4	B	503	LMT	C2-C1-O1'-C1'
4	D	503	LMT	C2-C1-O1'-C1'
4	A	503	LMT	C4-C5-C6-C7
3	D	502	FAD	P-O3P-PA-O5B
4	D	503	LMT	C2-C3-C4-C5
3	A	502	FAD	C5B-O5B-PA-O3P
3	A	502	FAD	C5B-O5B-PA-O1A
4	A	503	LMT	C1-C2-C3-C4
3	B	502	FAD	N10-C1'-C2'-O2'
4	B	503	LMT	O1'-C1-C2-C3
4	A	503	LMT	C5-C6-C7-C8
3	B	502	FAD	PA-O3P-P-O2P
3	C	502	FAD	C3B-C4B-C5B-O5B
3	D	502	FAD	C3B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	502	FAD	C5'-O5'-P-O3P
3	C	502	FAD	C5B-O5B-PA-O3P
3	B	502	FAD	C3B-C4B-C5B-O5B
3	A	502	FAD	PA-O3P-P-O2P

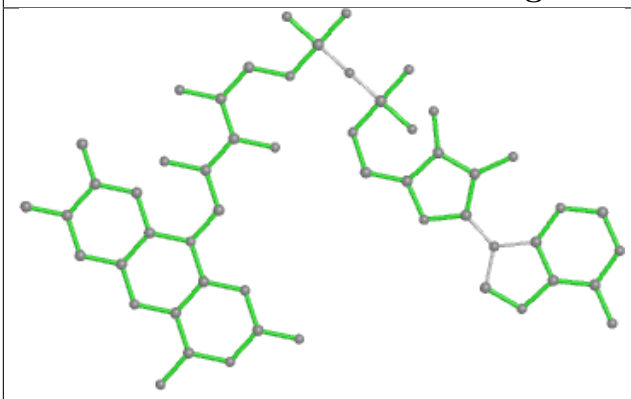
There are no ring outliers.

8 monomers are involved in 19 short contacts:

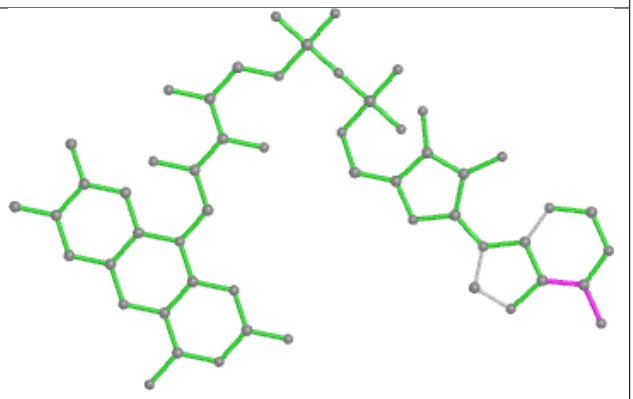
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	FAD	1	0
3	D	502	FAD	1	0
4	C	503	LMT	4	0
3	A	502	FAD	1	0
4	A	503	LMT	2	0
4	D	503	LMT	3	0
3	B	502	FAD	2	0
4	B	503	LMT	5	0

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.

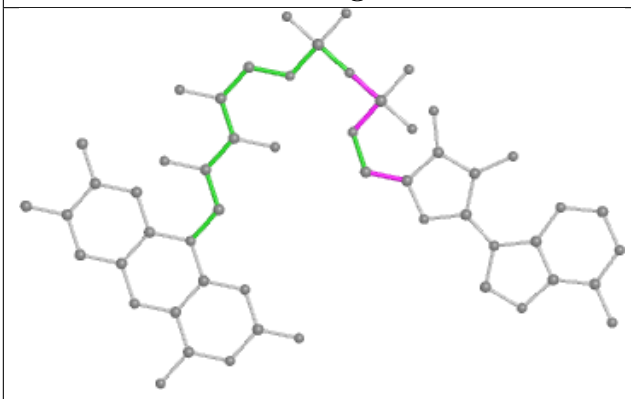
Ligand FAD C 502



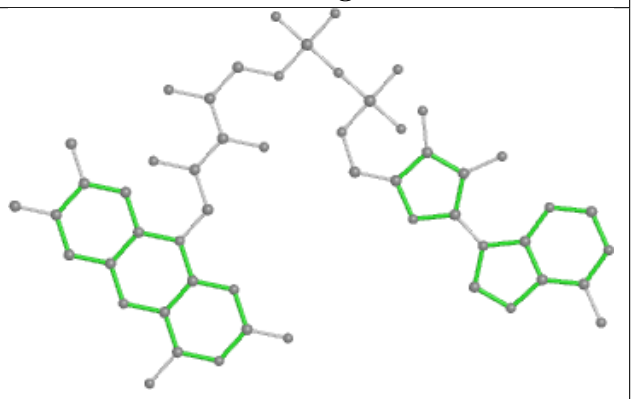
Bond lengths



Bond angles

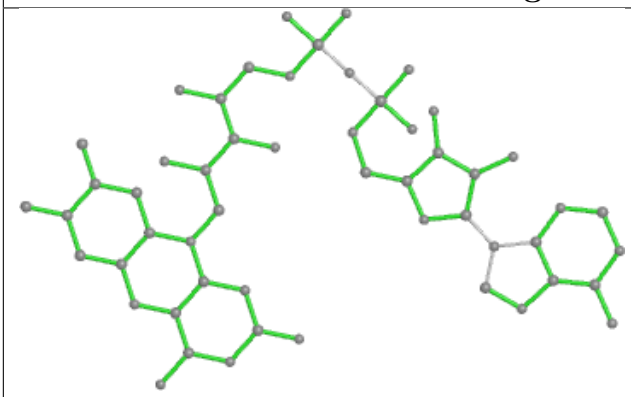


Torsions

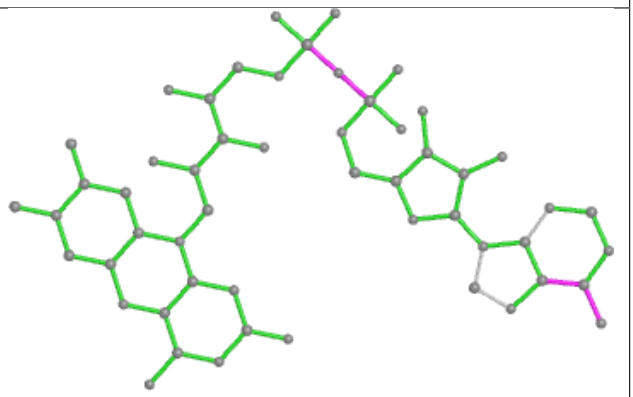


Rings

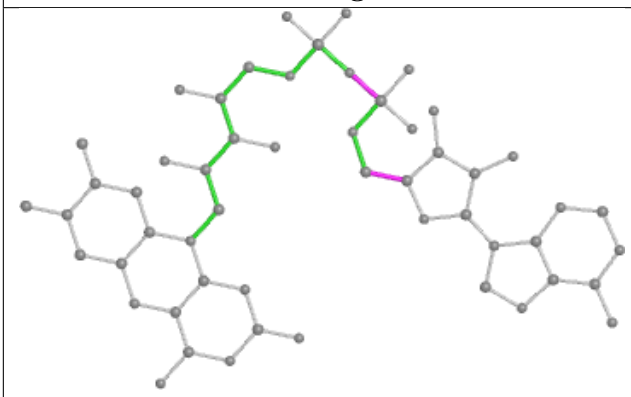
Ligand FAD D 502



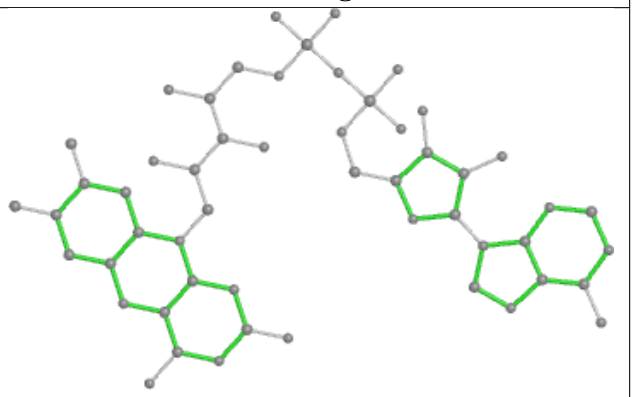
Bond lengths



Bond angles

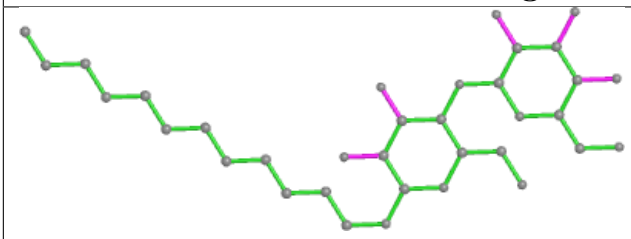


Torsions

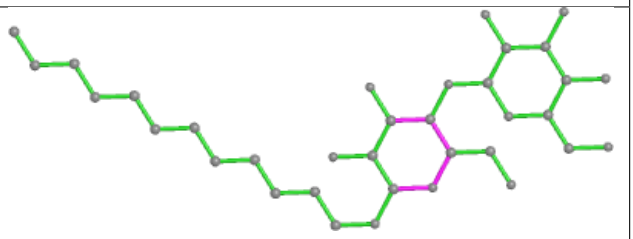


Rings

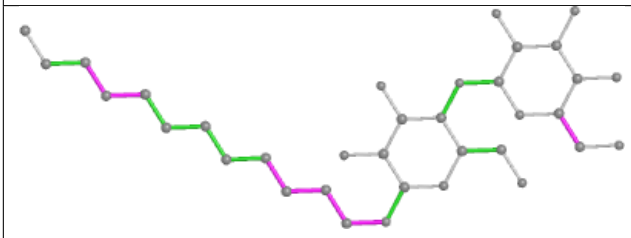
Ligand LMT C 503



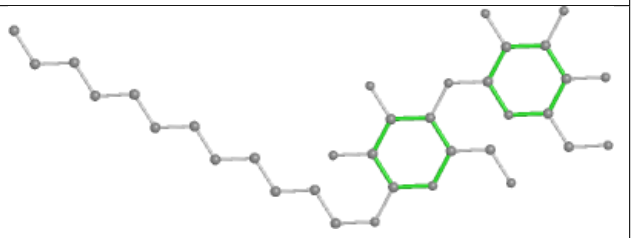
Bond lengths



Bond angles

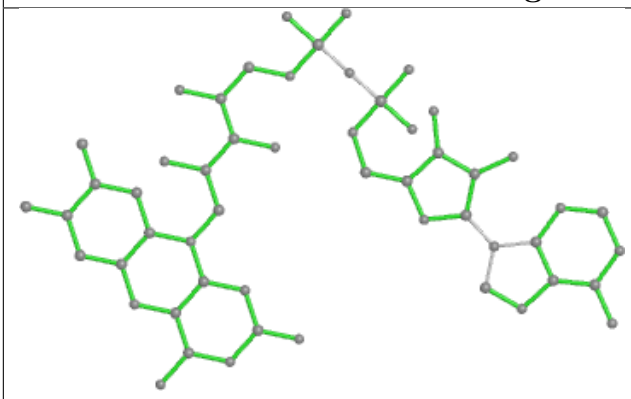


Torsions

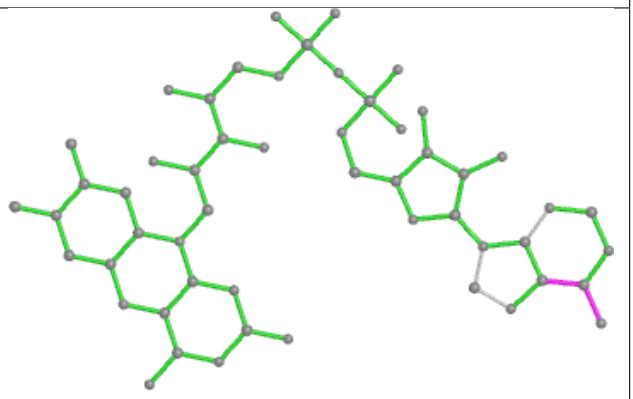


Rings

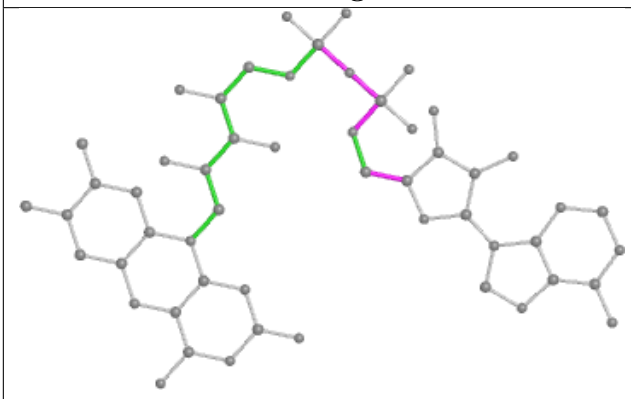
Ligand FAD A 502



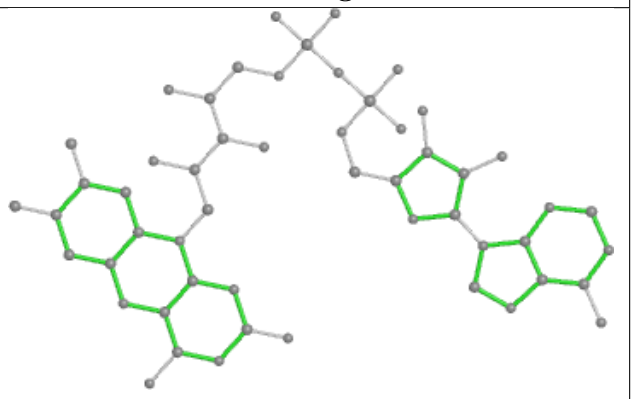
Bond lengths



Bond angles

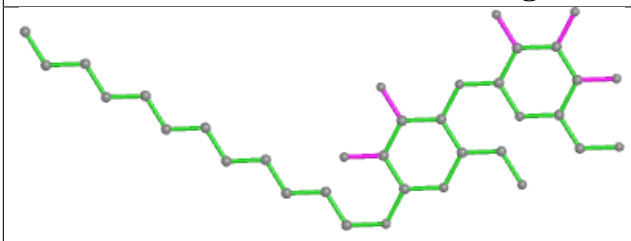


Torsions

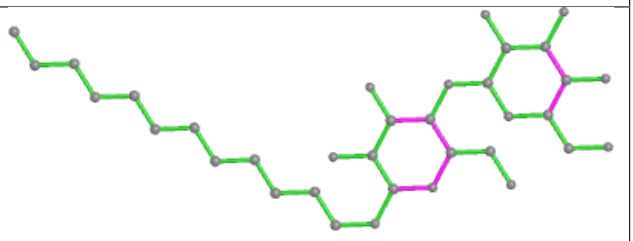


Rings

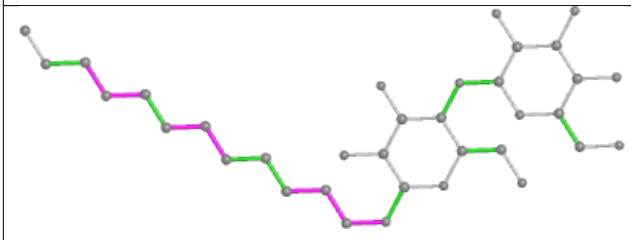
Ligand LMT A 503



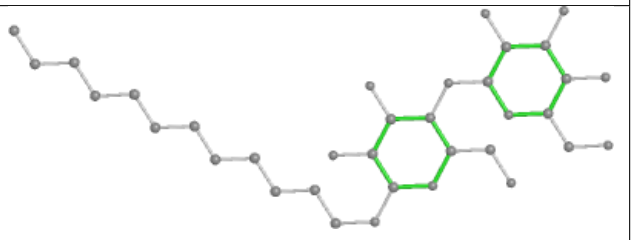
Bond lengths



Bond angles

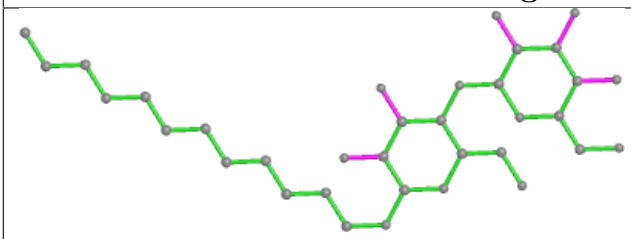


Torsions

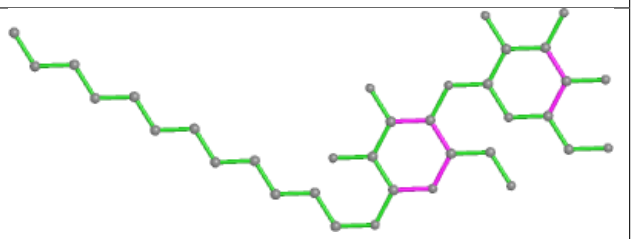


Rings

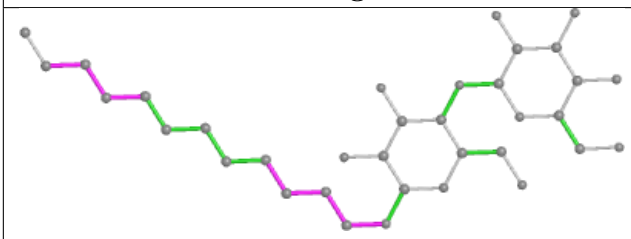
Ligand LMT D 503



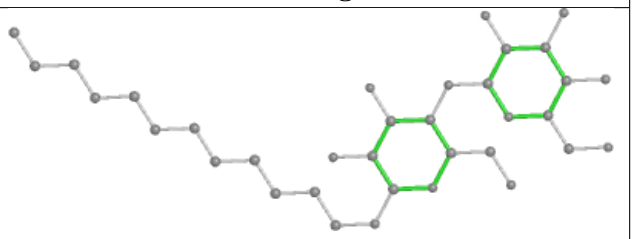
Bond lengths



Bond angles

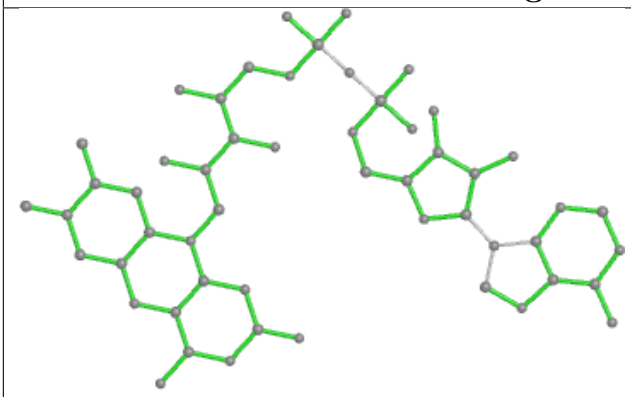


Torsions

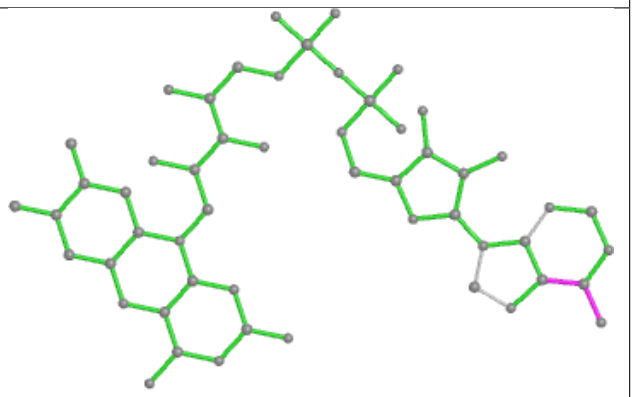


Rings

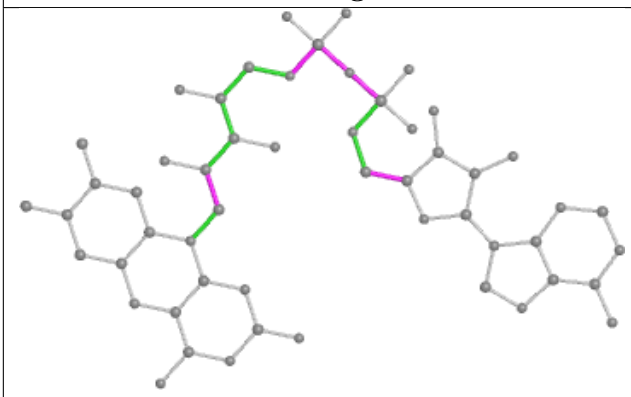
Ligand FAD B 502



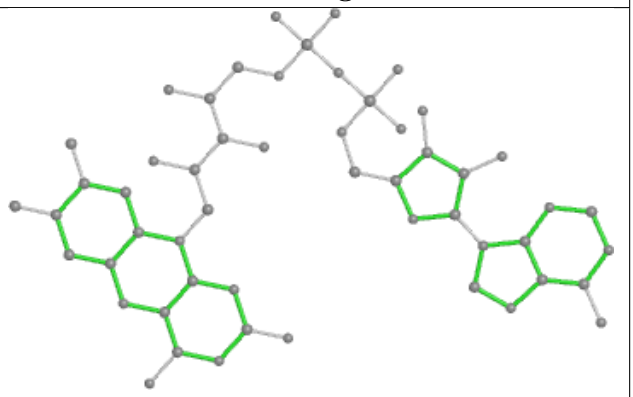
Bond lengths



Bond angles

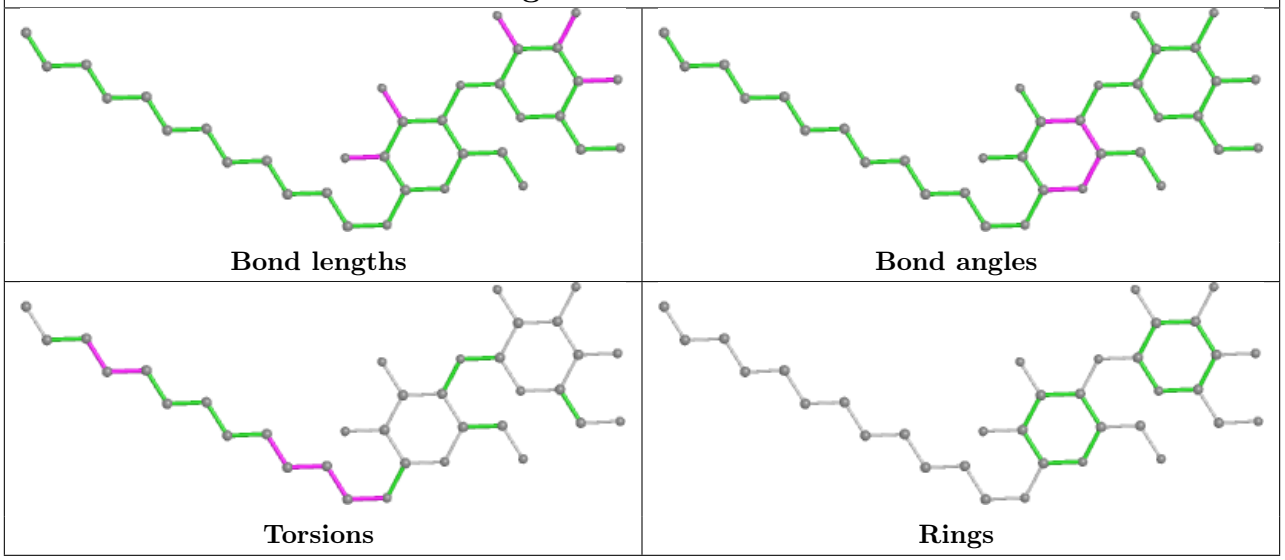


Torsions



Rings

Ligand LMT B 503



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

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, 95^{th} 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	409/415 (98%)	0.16	15 (3%) 41 48	30, 46, 62, 78	0
1	B	412/415 (99%)	0.10	10 (2%) 59 66	30, 45, 63, 81	0
1	C	404/415 (97%)	0.10	7 (1%) 70 76	33, 46, 63, 76	0
1	D	412/415 (99%)	0.13	17 (4%) 37 44	30, 45, 65, 77	0
All	All	1637/1660 (98%)	0.12	49 (2%) 50 57	30, 46, 64, 81	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	SER	4.5
1	D	414	GLY	3.8
1	B	41	GLY	3.6
1	A	379	TYR	3.5
1	C	452	SER	3.4
1	A	448	SER	3.2
1	A	230	PRO	3.0
1	D	151	ILE	2.9
1	A	376	ILE	2.9
1	B	425	CYS	2.8
1	D	141	LYS	2.8
1	C	226	PRO	2.7
1	D	177	MET	2.7
1	B	234	PRO	2.5
1	B	383	TYR	2.5
1	B	337	PHE	2.4
1	D	176	VAL	2.4
1	C	126	LYS	2.4
1	A	435	ILE	2.4
1	B	235	GLY	2.4
1	D	100	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	144	LYS	2.4
1	D	433	ALA	2.4
1	A	366	ILE	2.4
1	C	279	GLU	2.3
1	D	394	ALA	2.3
1	D	223	THR	2.3
1	D	145	ASP	2.3
1	B	144	LYS	2.3
1	D	162	GLU	2.3
1	A	242	CYS	2.3
1	A	231	GLY	2.3
1	C	239	ARG	2.3
1	B	223	THR	2.2
1	D	416	GLY	2.2
1	A	152	PRO	2.2
1	D	283	MET	2.2
1	A	234	VAL	2.2
1	A	382	GLN	2.2
1	B	246	CYS	2.1
1	D	142	LEU	2.1
1	C	234	PRO	2.1
1	A	333	PHE	2.1
1	D	136	ASP	2.1
1	A	373	ILE	2.0
1	C	156	PRO	2.0
1	B	299	LEU	2.0
1	A	404	VAL	2.0
1	A	429	ALA	2.0

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,

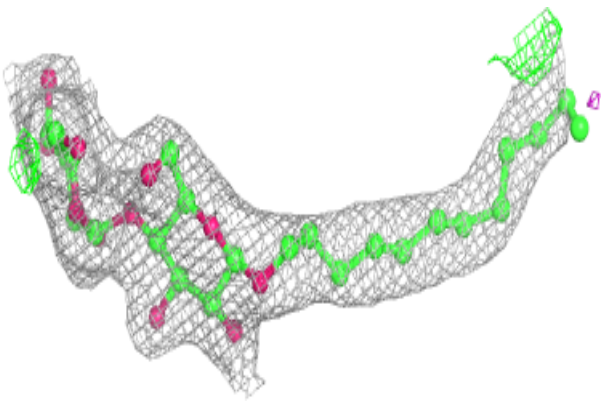
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

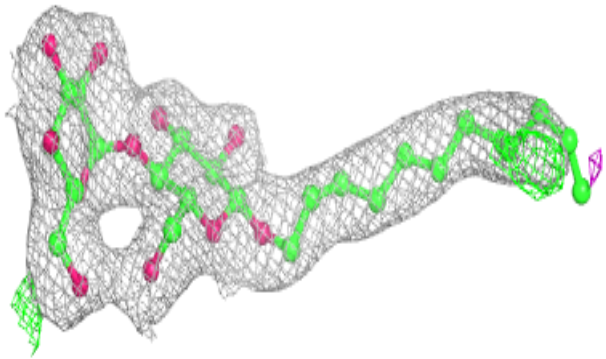
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LMT	B	503	35/35	0.93	0.15	41,45,64,72	0
4	LMT	C	503	35/35	0.93	0.16	40,49,57,71	0
4	LMT	D	503	35/35	0.93	0.14	42,49,65,78	0
4	LMT	A	503	35/35	0.94	0.14	40,49,58,67	0
3	FAD	C	502	53/53	0.94	0.21	25,35,47,60	0
3	FAD	A	502	53/53	0.95	0.18	26,36,44,57	0
3	FAD	D	502	53/53	0.95	0.20	26,33,38,47	0
3	FAD	B	502	53/53	0.96	0.19	25,36,41,49	0
2	SO4	A	501	5/5	0.99	0.16	31,36,40,47	0
2	SO4	B	501	5/5	0.99	0.12	36,37,40,47	0
2	SO4	C	501	5/5	0.99	0.20	40,40,43,47	0
2	SO4	D	501	5/5	0.99	0.19	37,38,39,43	0

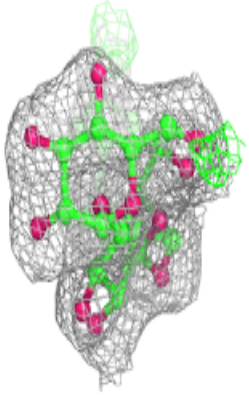
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT B 503:

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

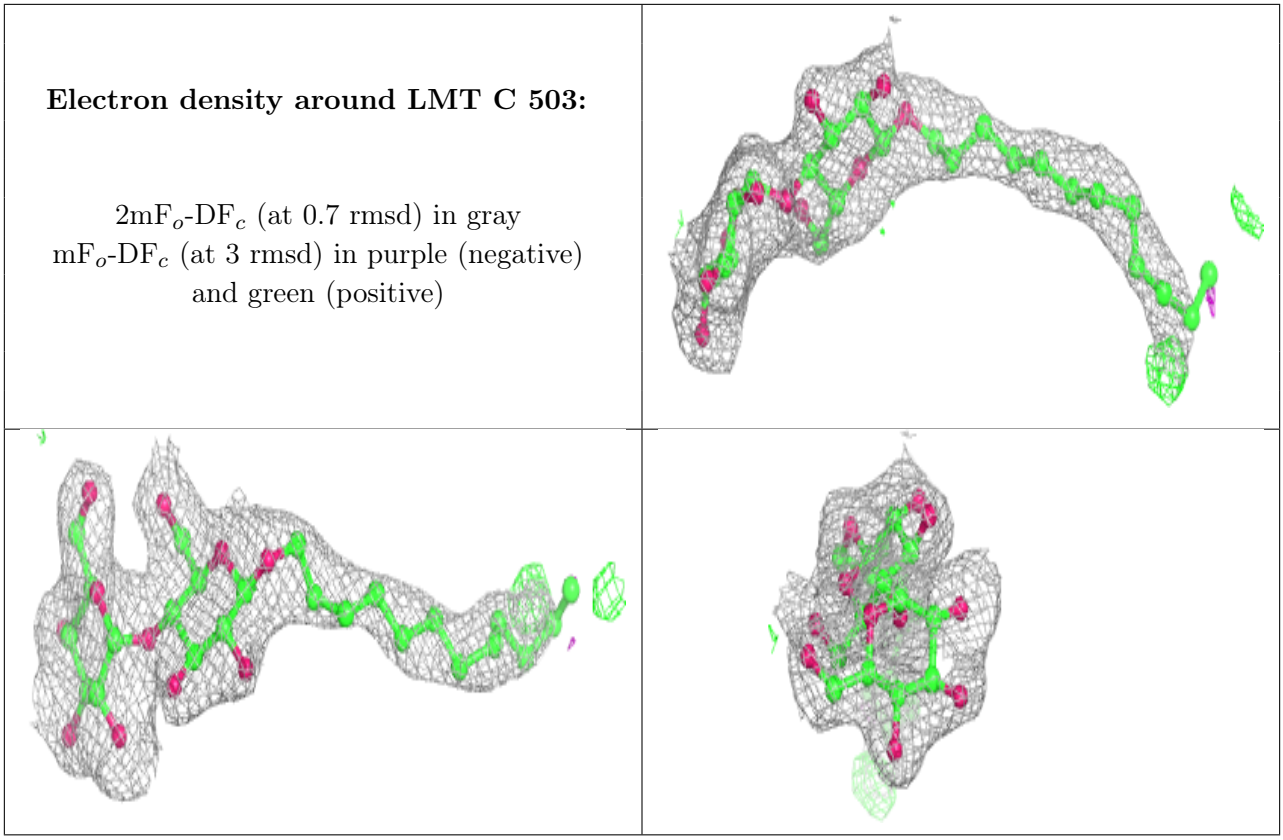






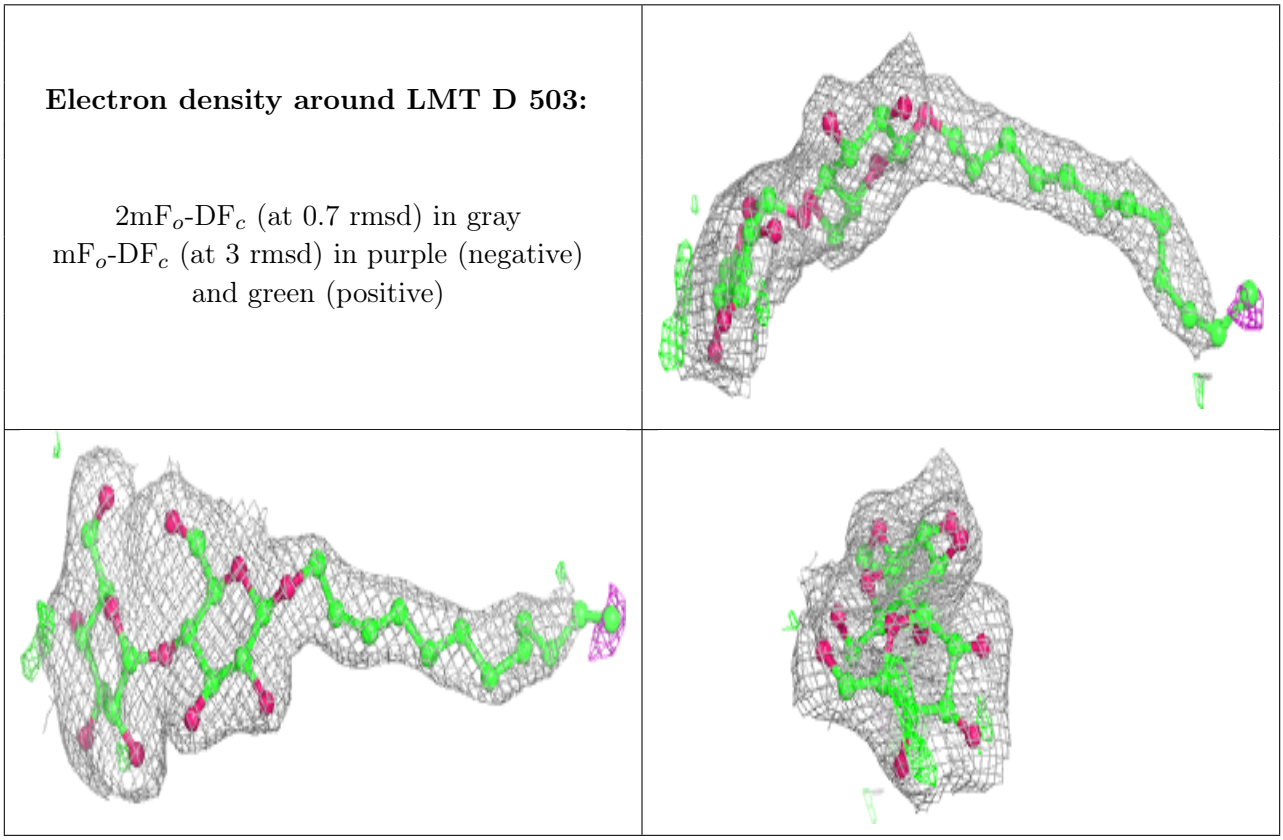
Electron density around LMT C 503:

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



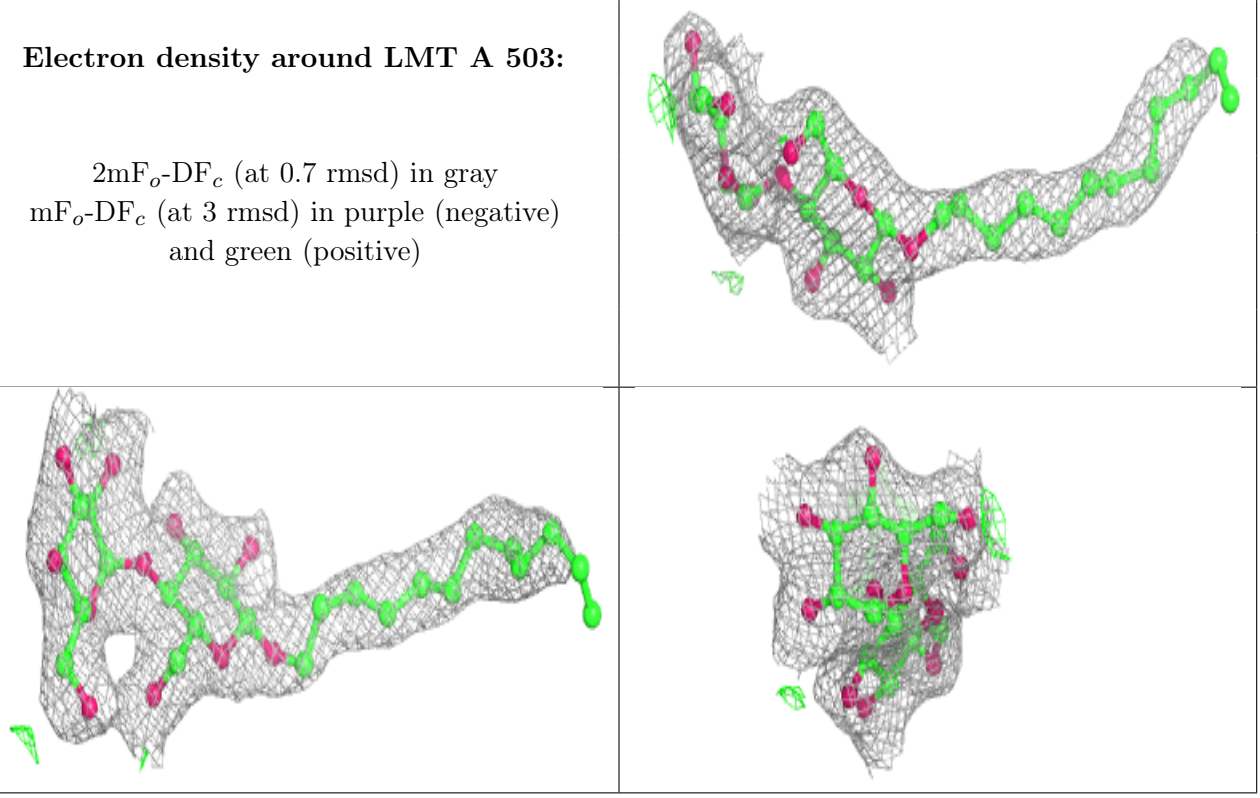
Electron density around LMT D 503:

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



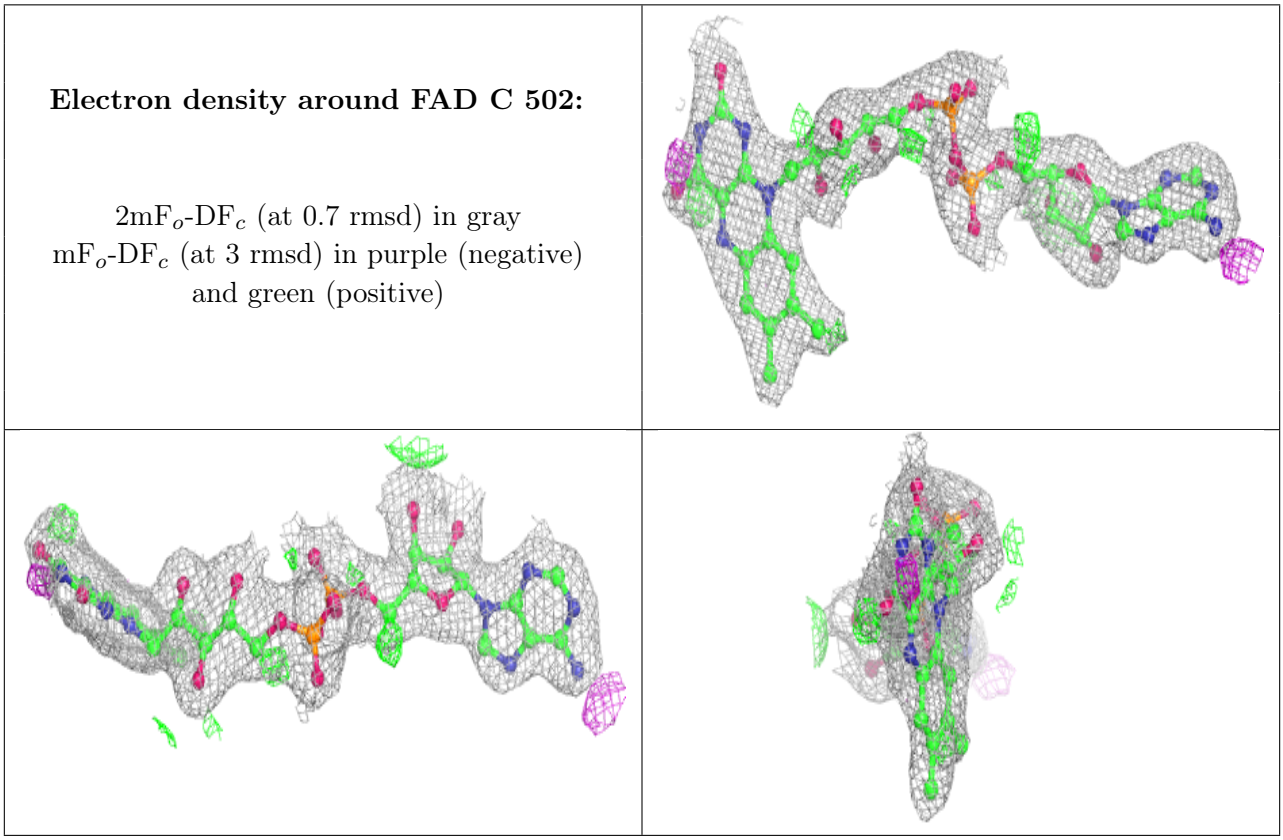
Electron density around LMT A 503:

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



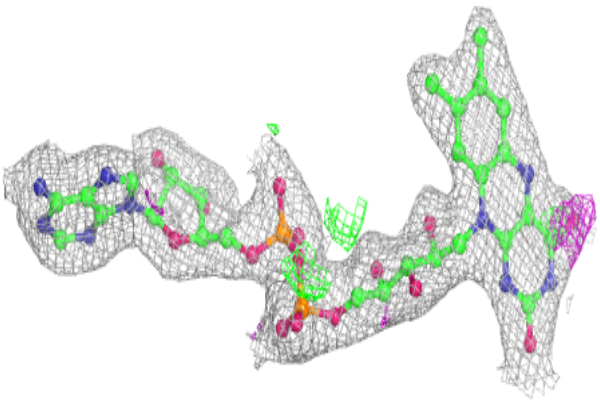
Electron density around FAD C 502:

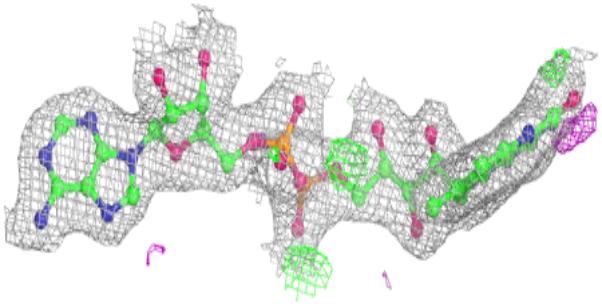
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

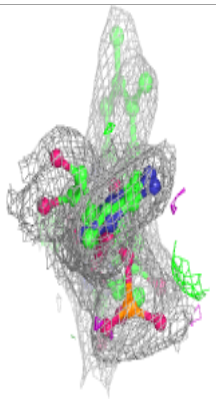


Electron density around FAD A 502:

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

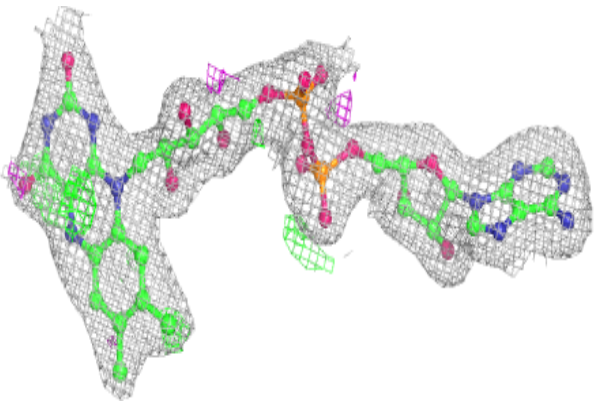


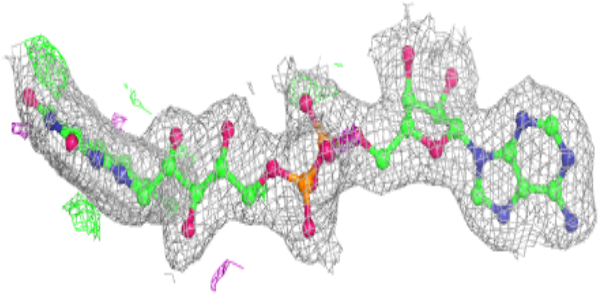


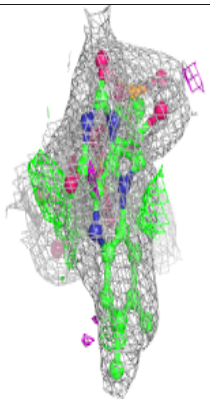


Electron density around FAD D 502:

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

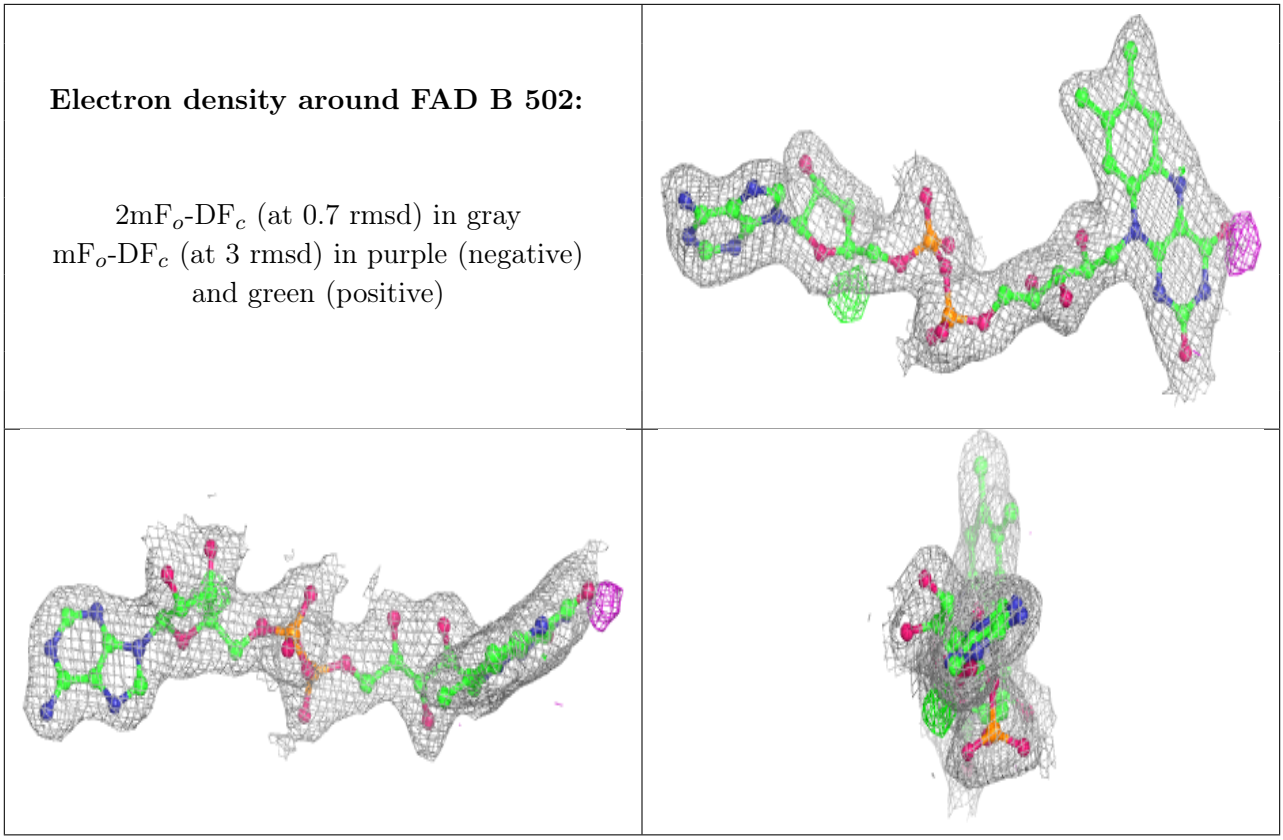






Electron density around FAD B 502:

$2mF_o$-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.