Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 03:44 AM EST

PDB ID	:	3MDD
Title	:	CRYSTAL STRUCTURES OF MEDIUM CHAIN ACYL-COA DEHYDROGENASE FROM PIG LIVER MITOCHONDRIA WITH AND WITHOUT SUBSTRATE
Authors	:	Kim, J.-J.P.; Wang, M.; Paschke, R.
Deposited on	:	1994-07-13
Resolution	:	2.40 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:

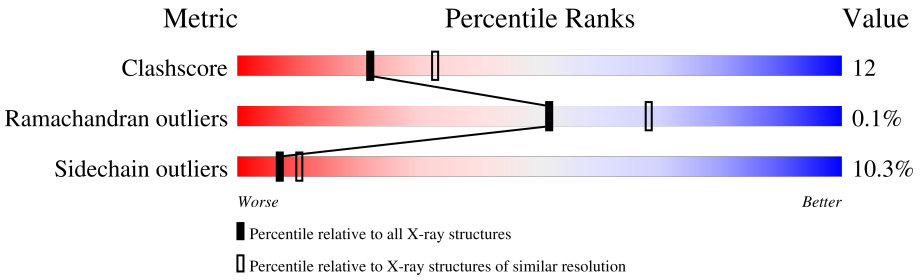
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	385	72% 25% ·
1	B	385	69% 26% · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6236 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.

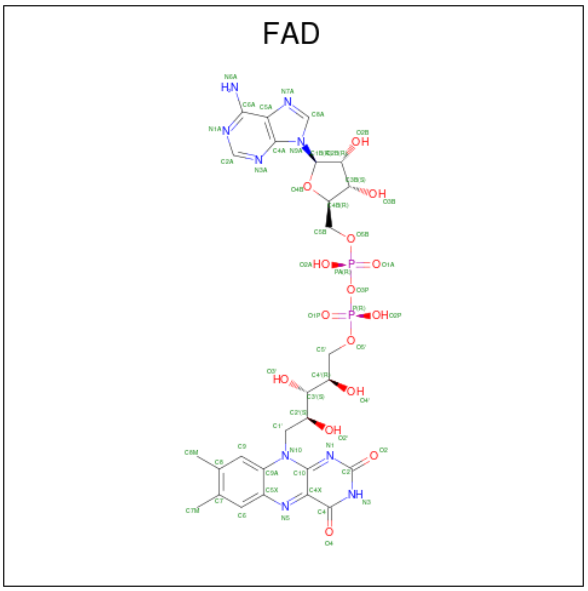
- Molecule 1 is a protein called MEDIUM CHAIN ACYL-COA DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2982	1891	514	563	14			
1	B	385	Total	C	N	O	S	0	0	0
			2982	1891	514	563	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLU	LYS	conflict	UNP P41367
A	258	PRO	SER	conflict	UNP P41367
A	280	GLU	GLY	conflict	UNP P41367
A	306	GLU	ASP	conflict	UNP P41367
B	15	GLU	LYS	conflict	UNP P41367
B	258	PRO	SER	conflict	UNP P41367
B	280	GLU	GLY	conflict	UNP P41367
B	306	GLU	ASP	conflict	UNP P41367

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	95	Total	O	0	0
			95	95		
3	B	71	Total	O	0	0
			71	71		

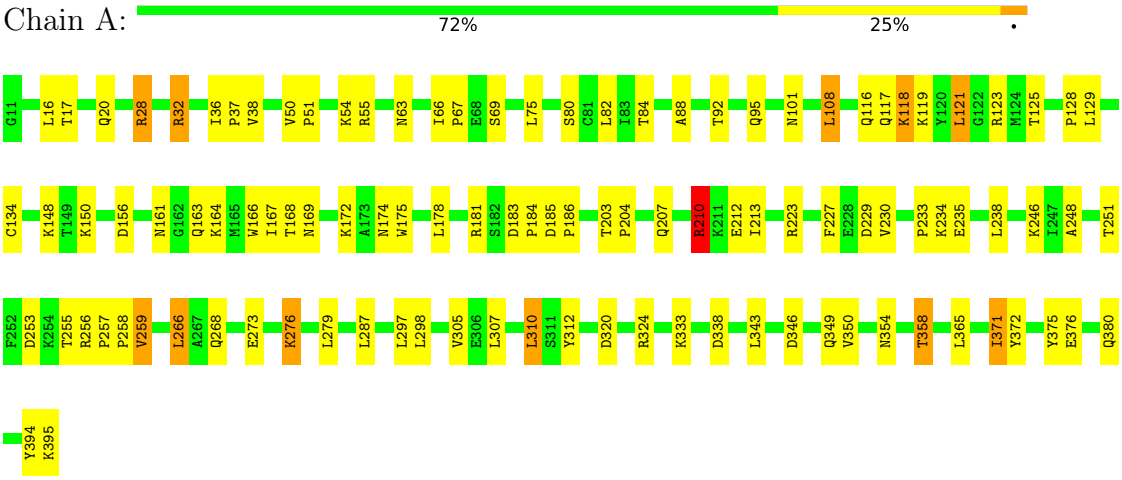
3 Residue-property plots (i)

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.

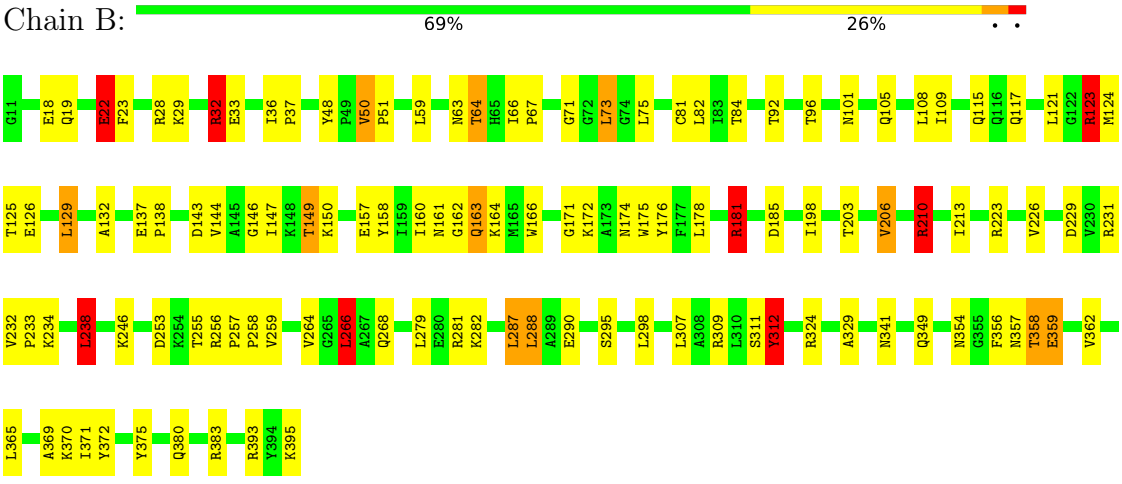
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain A:



• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	128.82Å 136.13Å 106.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6236	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.77	0/3039	1.14	10/4101 (0.2%)
1	B	0.81	3/3039 (0.1%)	1.14	9/4101 (0.2%)
All	All	0.79	3/6078 (0.0%)	1.14	19/8202 (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	B	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	SER	C-N	7.46	1.51	1.34
1	B	22	GLU	C-N	6.50	1.49	1.34
1	B	146	GLY	C-N	5.53	1.46	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	223	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	28	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	383	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	210	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	32	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	32	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	320	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	393	ARG	NE-CZ-NH1	6.05	123.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	123	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	A	223	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	28	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	181	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	338	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	210	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	181	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	324	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	311	SER	C-N-CA	-5.21	108.67	121.70
1	B	143	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	253	ASP	CB-CG-OD1	5.07	122.87	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	149	THR	Mainchain
1	B	264	VAL	Mainchain
1	B	266	LEU	Mainchain
1	B	312	TYR	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	2982	0	2974	60	0
1	B	2982	0	2974	93	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	95	0	0	1	0
3	B	71	0	0	0	0
All	All	6236	0	6010	143	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 12.

All (143) 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:B:137:GLU:OE2	1:B:149:THR:HG23	1.69	0.91
1:B:161:ASN:HD21	1:B:229:ASP:H	1.23	0.82
1:A:63:ASN:HD21	1:A:101:ASN:HD22	1.26	0.81
1:B:32:ARG:HA	1:B:36:ILE:HD12	1.63	0.81
1:B:50:VAL:HG13	1:B:51:PRO:HD3	1.63	0.80
1:B:268:GLN:HE21	1:B:309:ARG:HH22	1.27	0.80
1:A:380:GLN:HE22	1:B:349:GLN:HE21	1.27	0.80
1:B:63:ASN:HD21	1:B:101:ASN:HD22	1.28	0.79
1:B:161:ASN:ND2	1:B:229:ASP:H	1.79	0.79
1:A:174:ASN:HD22	1:A:175:TRP:HD1	1.32	0.78
1:B:117:GLN:HA	1:B:121:LEU:HD13	1.68	0.75
1:A:161:ASN:ND2	1:A:229:ASP:H	1.86	0.73
1:A:349:GLN:HE21	1:B:380:GLN:HE22	1.38	0.71
1:A:358:THR:HB	1:B:213:ILE:O	1.92	0.70
1:A:213:ILE:O	1:B:358:THR:HB	1.92	0.70
1:A:123:ARG:HH11	1:A:174:ASN:HD21	1.40	0.70
1:B:73:LEU:HB3	1:B:75:LEU:HD13	1.75	0.68
1:B:380:GLN:NE2	1:B:380:GLN:H	1.92	0.67
1:B:108:LEU:HD13	1:B:198:ILE:HD11	1.77	0.66
1:B:266:LEU:C	1:B:266:LEU:HD12	2.17	0.65
1:B:256:ARG:HB3	1:B:329:ALA:HB1	1.79	0.63
1:B:174:ASN:HD22	1:B:175:TRP:HD1	1.44	0.63
1:B:268:GLN:NE2	1:B:309:ARG:HH22	1.97	0.62
1:A:380:GLN:NE2	1:A:380:GLN:H	1.97	0.62
1:B:149:THR:HG21	1:B:164:LYS:HE2	1.83	0.60
1:B:158:TYR:HB2	1:B:232:VAL:HG13	1.81	0.60
1:B:157:GLU:OE1	1:B:231:ARG:HD2	2.02	0.60
1:A:255:THR:O	1:A:258:PRO:HD2	2.04	0.58
1:B:108:LEU:HG	1:B:121:LEU:HD11	1.86	0.57
1:B:109:ILE:HG12	1:B:121:LEU:HD21	1.86	0.57
1:B:123:ARG:HE	1:B:174:ASN:HD21	1.50	0.57
1:A:380:GLN:HE22	1:B:349:GLN:NE2	1.99	0.56
1:A:354:ASN:HD22	1:B:166:TRP:HZ2	1.53	0.56
1:A:349:GLN:NE2	1:B:380:GLN:HE22	2.04	0.56
1:A:255:THR:O	1:A:259:VAL:HG12	2.05	0.56
1:B:108:LEU:HG	1:B:121:LEU:CD1	2.36	0.56
1:A:50:VAL:HB	1:A:51:PRO:HD3	1.88	0.55
1:A:161:ASN:HD21	1:A:229:ASP:H	1.51	0.55
1:A:134:CYS:HA	1:A:167:ILE:HD12	1.87	0.55
1:B:253:ASP:OD2	1:B:324:ARG:HG3	2.06	0.55
1:A:256:ARG:HB3	1:A:257:PRO:HD3	1.88	0.55
1:B:203:THR:O	1:B:206:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ARG:HB3	1:B:288:LEU:HD22	1.89	0.54
1:A:273:GLU:HA	1:A:276:LYS:HZ2	1.72	0.54
1:A:268:GLN:HE21	1:A:305:VAL:HG11	1.72	0.54
1:A:333:LYS:HE3	1:A:376:GLU:O	2.08	0.53
1:B:18:GLU:O	1:B:22:GLU:HG2	2.09	0.53
1:A:63:ASN:ND2	1:A:101:ASN:HD22	2.01	0.53
1:A:166:TRP:HZ2	1:B:354:ASN:HD22	1.55	0.53
1:B:255:THR:O	1:B:259:VAL:HG13	2.08	0.53
1:A:17:THR:H	1:A:20:GLN:HE21	1.56	0.53
1:B:266:LEU:HD12	1:B:266:LEU:O	2.09	0.53
1:B:150:LYS:HE3	1:B:161:ASN:HB2	1.89	0.53
1:B:124:MET:HE3	1:B:175:TRP:HE1	1.75	0.52
1:B:138:PRO:HG2	1:B:163:GLN:HG2	1.92	0.52
1:B:132:ALA:HB3	1:B:176:TYR:HD1	1.74	0.52
1:A:32:ARG:HA	1:A:36:ILE:HD12	1.91	0.52
1:B:178:LEU:C	1:B:178:LEU:HD13	2.30	0.52
1:B:312:TYR:CD1	1:B:312:TYR:C	2.83	0.52
1:B:64:THR:HG23	1:B:75:LEU:HB2	1.92	0.52
1:B:255:THR:O	1:B:258:PRO:HD2	2.09	0.52
1:B:257:PRO:HB2	1:B:258:PRO:HD3	1.92	0.52
1:A:28:ARG:O	1:A:32:ARG:HG3	2.11	0.50
1:A:181:ARG:NH2	1:A:185:ASP:O	2.45	0.50
1:A:108:LEU:HD13	1:A:121:LEU:HD13	1.95	0.49
1:A:233:PRO:HB2	1:A:235:GLU:HG2	1.95	0.49
1:B:92:THR:O	1:B:96:THR:HG23	2.12	0.49
1:B:123:ARG:NE	1:B:174:ASN:HD21	2.11	0.48
1:B:287:LEU:HB2	1:B:290:GLU:HG3	1.94	0.48
1:A:227:PHE:HD2	1:A:230:VAL:HG21	1.78	0.48
1:B:171:GLY:C	1:B:172:LYS:HD2	2.34	0.48
1:B:160:ILE:HD11	1:B:232:VAL:HG11	1.96	0.48
1:A:255:THR:C	1:A:258:PRO:HD2	2.34	0.48
1:B:380:GLN:H	1:B:380:GLN:HE21	1.62	0.47
1:B:117:GLN:O	1:B:121:LEU:HB2	2.14	0.47
1:A:16:LEU:HD21	1:A:82:LEU:HD21	1.97	0.47
1:A:36:ILE:HB	1:A:37:PRO:HD3	1.97	0.47
1:B:19:GLN:HG2	1:B:23:PHE:CE2	2.49	0.47
1:B:50:VAL:CG1	1:B:51:PRO:HD3	2.40	0.46
1:B:124:MET:HE2	1:B:129:LEU:HD23	1.98	0.46
1:B:256:ARG:HB3	1:B:257:PRO:HD3	1.96	0.46
1:B:256:ARG:HG2	1:B:329:ALA:O	2.16	0.46
1:B:48:TYR:CE2	1:B:172:LYS:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:HD21	1:B:369:ALA:HB2	1.98	0.45
1:A:266:LEU:CD1	1:A:365:LEU:HG	2.46	0.45
1:A:371:ILE:HG23	1:B:356:PHE:CD2	2.52	0.45
1:B:181:ARG:NH2	1:B:185:ASP:O	2.49	0.45
1:A:185:ASP:HA	1:A:186:PRO:HD3	1.82	0.45
1:B:123:ARG:HE	1:B:174:ASN:ND2	2.15	0.45
1:B:163:GLN:HB2	1:B:226:VAL:HG22	1.98	0.45
1:B:123:ARG:HA	1:B:126:GLU:HG3	1.99	0.45
1:B:341:ASN:HD21	1:B:370:LYS:HA	1.82	0.45
1:B:84:THR:HG21	1:B:258:PRO:O	2.17	0.44
1:A:166:TRP:HZ2	1:B:354:ASN:ND2	2.15	0.44
1:A:116:GLN:NE2	1:A:235:GLU:O	2.44	0.44
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.60	0.44
1:A:297:LEU:HD11	1:A:346:ASP:HB3	2.00	0.44
1:B:108:LEU:CD1	1:B:198:ILE:HD11	2.47	0.44
1:B:357:ASN:OD1	1:B:359:GLU:HB2	2.18	0.44
1:B:144:VAL:O	1:B:147:ILE:HG12	2.17	0.44
1:A:178:LEU:C	1:A:178:LEU:HD13	2.38	0.44
1:A:174:ASN:ND2	1:A:175:TRP:HD1	2.09	0.44
1:B:255:THR:C	1:B:258:PRO:HD2	2.38	0.43
1:A:210:ARG:HD2	1:A:212:GLU:OE2	2.19	0.43
1:B:109:ILE:CG1	1:B:121:LEU:HD21	2.47	0.43
1:A:168:THR:O	1:A:169:ASN:HB2	2.19	0.43
2:A:399:FAD:H9	2:A:399:FAD:H1'2	1.78	0.43
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.78	0.43
1:B:117:GLN:CA	1:B:121:LEU:HD13	2.43	0.43
1:A:394:TYR:O	1:A:395:LYS:HD2	2.19	0.43
1:A:310:LEU:HD13	3:A:869:HOH:O	2.19	0.42
1:A:66:ILE:HA	1:A:67:PRO:HD3	1.89	0.42
1:A:117:GLN:O	1:A:121:LEU:HB2	2.19	0.42
1:A:118:LYS:HE2	1:A:119:LYS:N	2.34	0.42
1:B:266:LEU:C	1:B:266:LEU:CD1	2.88	0.42
1:B:36:ILE:HB	1:B:37:PRO:HD3	2.01	0.42
1:A:84:THR:HG21	1:A:258:PRO:O	2.19	0.42
1:A:256:ARG:O	1:A:259:VAL:HG13	2.19	0.42
1:B:287:LEU:HD12	1:B:287:LEU:HA	1.95	0.42
1:A:54:LYS:HE2	1:A:128:PRO:HG3	2.02	0.42
1:A:88:ALA:HB1	1:A:92:THR:HG22	2.02	0.42
1:B:232:VAL:HA	1:B:233:PRO:HD3	1.89	0.42
1:A:248:ALA:O	1:A:251:THR:HB	2.20	0.42
1:A:134:CYS:HB3	1:A:164:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:O	1:A:150:LYS:HG2	2.19	0.41
1:B:29:LYS:O	1:B:33:GLU:HB2	2.20	0.41
1:B:81:CYS:HB3	1:B:312:TYR:CE1	2.55	0.41
1:B:149:THR:HB	1:B:162:GLY:HA3	2.01	0.41
1:B:362:VAL:HA	1:B:365:LEU:HD22	2.02	0.41
1:B:28:ARG:O	1:B:32:ARG:CG	2.68	0.41
1:B:66:ILE:HA	1:B:67:PRO:HD3	1.83	0.41
1:A:210:ARG:NH1	1:B:359:GLU:OE1	2.51	0.41
1:B:71:GLY:HA3	1:B:125:THR:HG21	2.03	0.41
1:B:371:ILE:HD12	1:B:372:TYR:N	2.34	0.41
1:B:63:ASN:ND2	1:B:101:ASN:HD22	2.04	0.41
1:A:183:ASP:HA	1:A:184:PRO:HD2	1.90	0.41
1:B:50:VAL:N	1:B:51:PRO:CD	2.84	0.41
1:B:63:ASN:HB3	1:B:66:ILE:CD1	2.51	0.41
1:B:210:ARG:O	1:B:223:ARG:HG2	2.21	0.41
1:A:203:THR:HA	1:A:204:PRO:HD3	1.97	0.41
1:B:257:PRO:CB	1:B:258:PRO:HD3	2.52	0.40
1:A:333:LYS:NZ	1:A:372:TYR:O	2.49	0.40
1:B:63:ASN:ND2	1:B:105:GLN:OE1	2.54	0.40

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	383/385 (100%)	369 (96%)	14 (4%)	0	100	100
1	B	383/385 (100%)	370 (97%)	12 (3%)	1 (0%)	41	55
All	All	766/770 (100%)	739 (96%)	26 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	LEU

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	301/301 (100%)	269 (89%)	32 (11%)	6 9
1	B	301/301 (100%)	271 (90%)	30 (10%)	7 11
All	All	602/602 (100%)	540 (90%)	62 (10%)	7 10

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	55	ARG
1	A	69	SER
1	A	75	LEU
1	A	80	SER
1	A	95	GLN
1	A	108	LEU
1	A	118	LYS
1	A	121	LEU
1	A	125	THR
1	A	129	LEU
1	A	156	ASP
1	A	163	GLN
1	A	172	LYS
1	A	207	GLN
1	A	210	ARG
1	A	234	LYS
1	A	246	LYS
1	A	259	VAL
1	A	266	LEU
1	A	276	LYS
1	A	279	LEU
1	A	287	LEU

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Mol	Chain	Res	Type
1	A	298	LEU
1	A	307	LEU
1	A	310	LEU
1	A	312	TYR
1	A	343	LEU
1	A	350	VAL
1	A	358	THR
1	A	371	ILE
1	A	375	TYR
1	B	22	GLU
1	B	32	ARG
1	B	50	VAL
1	B	59	LEU
1	B	64	THR
1	B	73	LEU
1	B	82	LEU
1	B	115	GLN
1	B	123	ARG
1	B	129	LEU
1	B	163	GLN
1	B	181	ARG
1	B	206	VAL
1	B	210	ARG
1	B	234	LYS
1	B	238	LEU
1	B	246	LYS
1	B	266	LEU
1	B	279	LEU
1	B	282	LYS
1	B	287	LEU
1	B	288	LEU
1	B	295	SER
1	B	298	LEU
1	B	307	LEU
1	B	312	TYR
1	B	358	THR
1	B	359	GLU
1	B	375	TYR
1	B	395	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	63	ASN
1	A	105	GLN
1	A	161	ASN
1	A	169	ASN
1	A	174	ASN
1	A	217	GLN
1	A	268	GLN
1	A	313	GLN
1	A	341	ASN
1	A	354	ASN
1	A	373	GLN
1	A	380	GLN
1	B	20	GLN
1	B	63	ASN
1	B	105	GLN
1	B	117	GLN
1	B	161	ASN
1	B	169	ASN
1	B	174	ASN
1	B	236	ASN
1	B	268	GLN
1	B	313	GLN
1	B	341	ASN
1	B	354	ASN
1	B	373	GLN
1	B	380	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	399	-	53,58,58	1.13	1 (1%)	68,89,89	1.22	7 (10%)
2	FAD	B	399	-	53,58,58	1.12	2 (3%)	68,89,89	1.20	7 (10%)

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	399	-	-	0/30/50/50	0/6/6/6
2	FAD	B	399	-	-	0/30/50/50	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	399	FAD	C4X-N5	5.51	1.41	1.30
2	A	399	FAD	C4X-N5	5.47	1.41	1.30
2	B	399	FAD	C5X-N5	-2.03	1.35	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	399	FAD	C1'-N10-C9A	-4.10	113.68	120.51
2	A	399	FAD	C1'-N10-C9A	-3.75	114.26	120.51
2	A	399	FAD	P-O3P-PA	-3.43	121.04	132.83
2	B	399	FAD	P-O3P-PA	-3.03	122.44	132.83
2	A	399	FAD	O5'-C5'-C4'	3.00	117.36	109.36
2	B	399	FAD	O5'-C5'-C4'	2.93	117.18	109.36
2	A	399	FAD	C10-N1-C2	2.38	121.67	116.90
2	A	399	FAD	C10-C4X-N5	-2.22	120.15	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	399	FAD	C5A-C6A-N6A	2.18	123.66	120.35
2	B	399	FAD	C4-N3-C2	-2.10	121.77	125.64
2	A	399	FAD	C4X-C10-N1	-2.09	119.88	124.73
2	B	399	FAD	C10-N1-C2	2.07	121.05	116.90
2	B	399	FAD	C10-C4X-N5	-2.07	120.47	124.86
2	B	399	FAD	C4X-C10-N1	-2.06	119.95	124.73

There are no chirality outliers.

There are no torsion outliers.

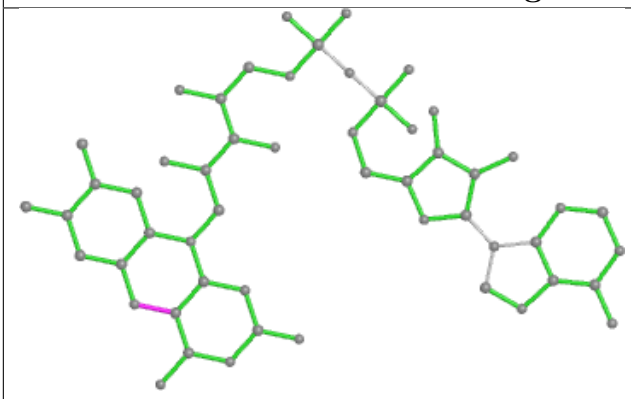
There are no ring outliers.

1 monomer is involved in 1 short contact:

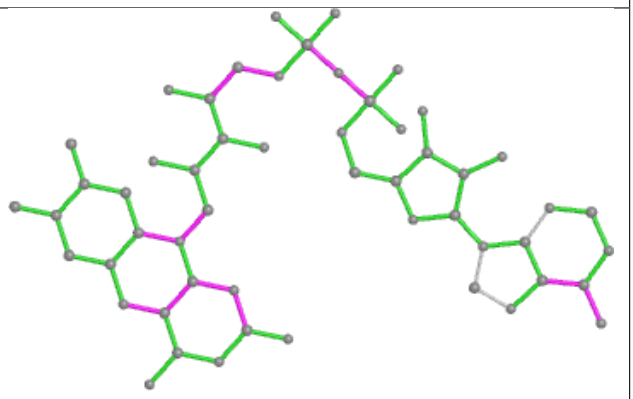
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	399	FAD	1	0

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.

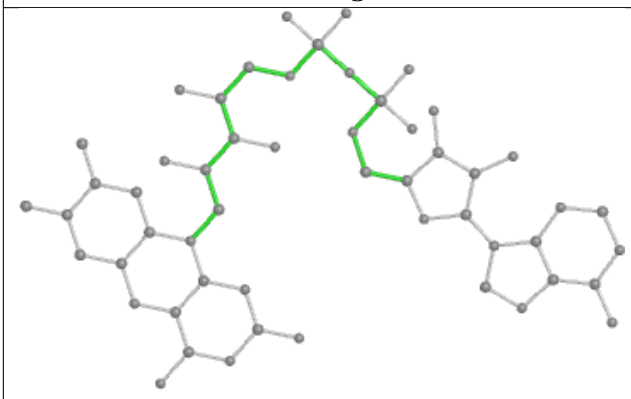
Ligand FAD A 399



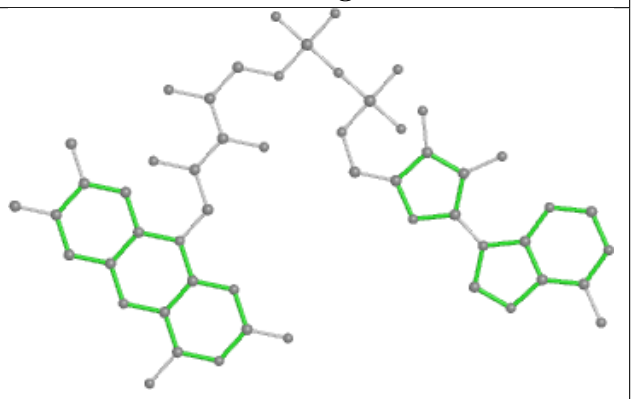
Bond lengths



Bond angles

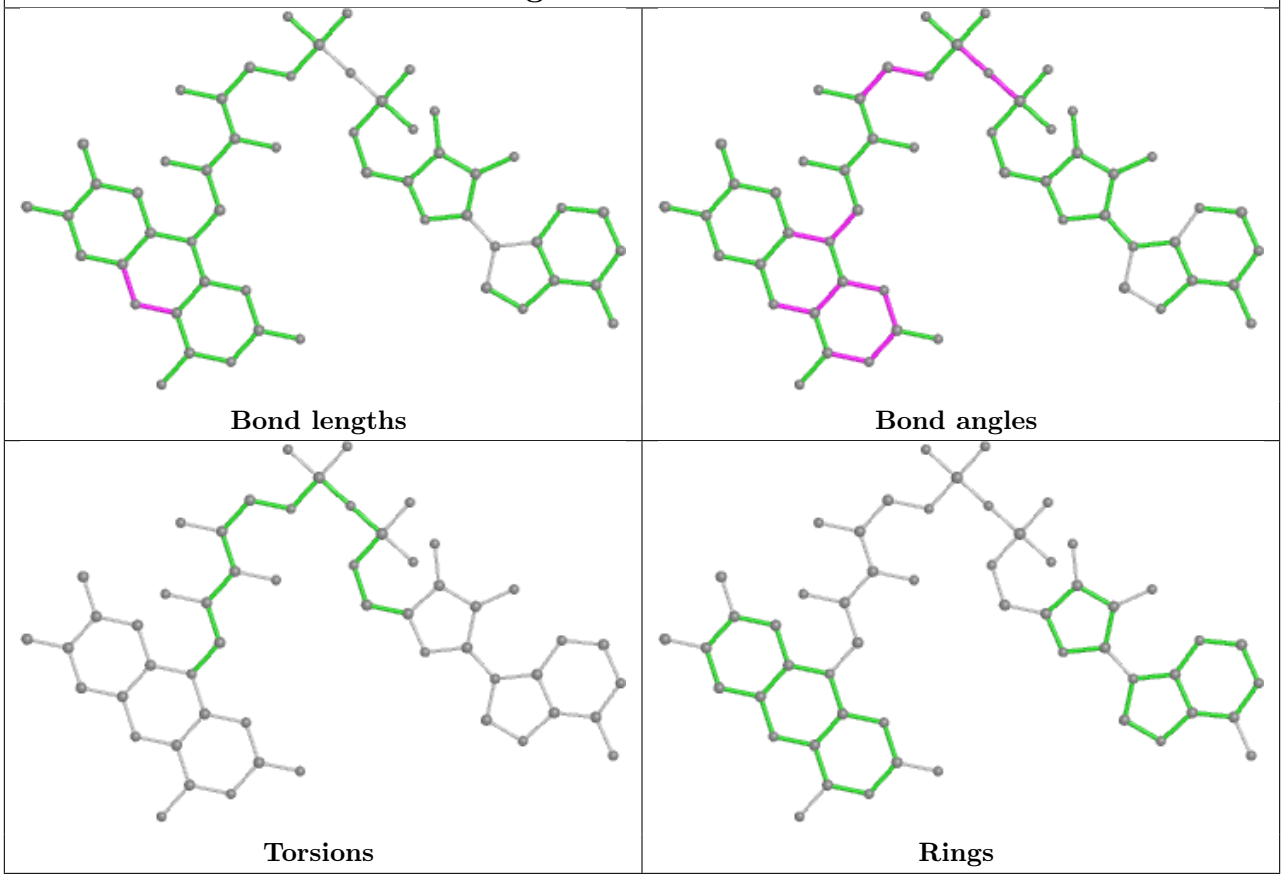


Torsions



Rings

Ligand FAD B 399



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.