Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:00 am BST

PDB ID	:	1IS2
Title	:	Crystal Structure of Peroxisomal Acyl-CoA Oxidase-II from Rat Liver
Authors	:	Nakajima, Y.; Miyahara, I.; Hirotsu, K.
Deposited on	:	2001-11-07
Resolution	:	2.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

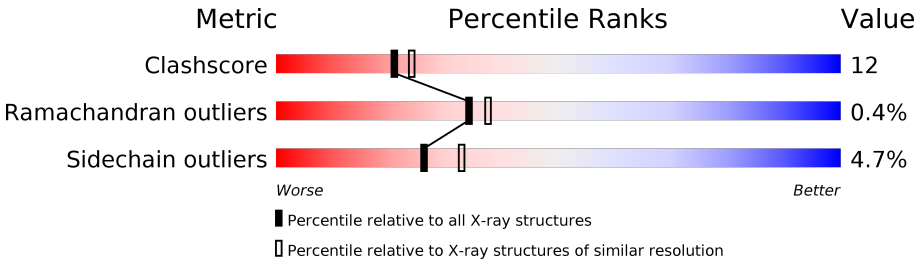
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 on 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	661	75% 20% • •
1	B	661	67% 25% • 5%

2 Entry composition

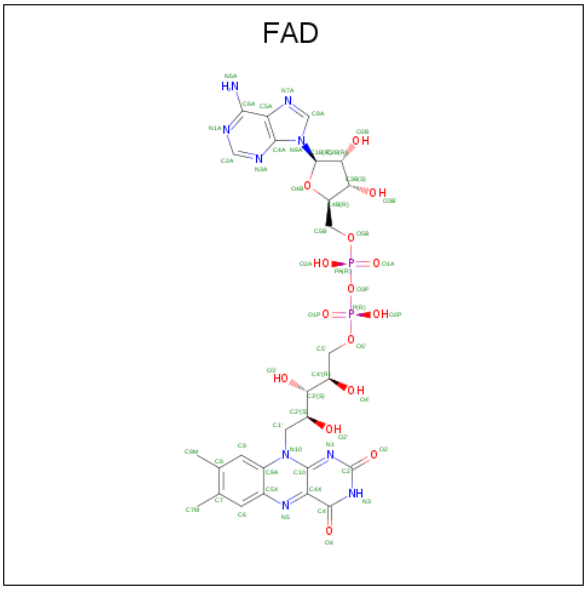
There are 3 unique types of molecules in this entry. The entry contains 10488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 acyl-CoA oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	0	0	0
			5028	3202	867	933	26			
1	B	629	Total	C	N	O	S	0	0	0
			4911	3127	851	909	24			

- 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	241	Total O 241 241	0	0
3	B	202	Total O 202 202	0	0

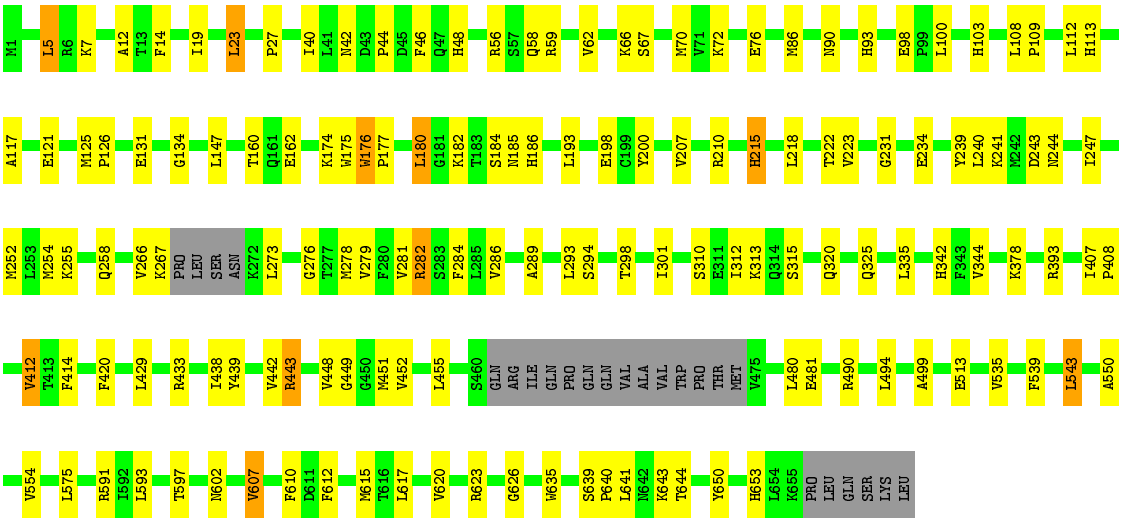
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

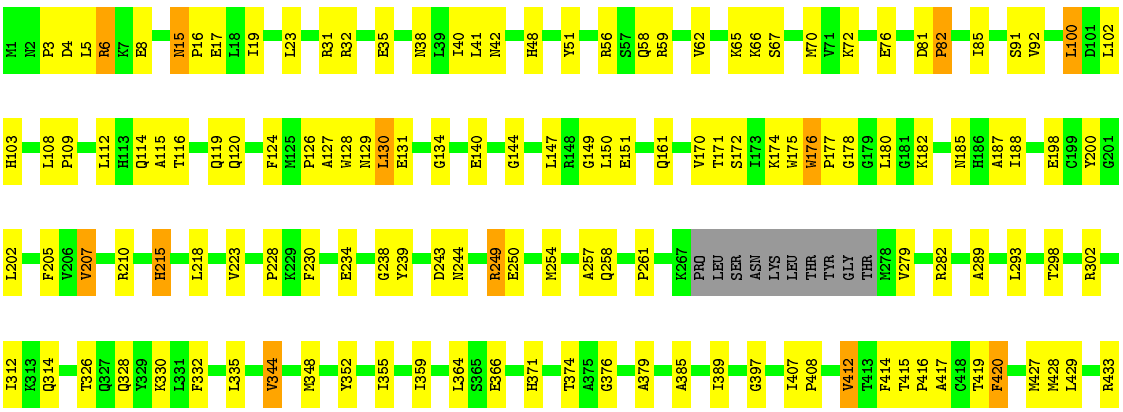
- Molecule 1: acyl-CoA oxidase

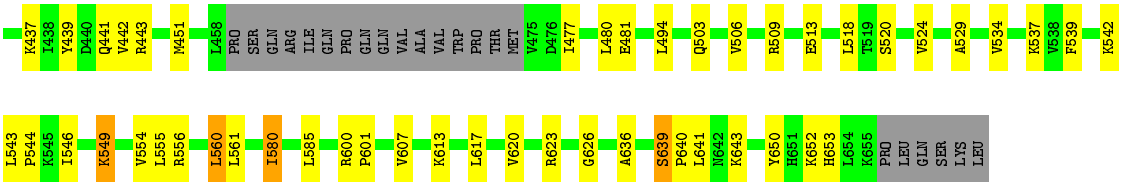
Chain A:



- Molecule 1: acyl-CoA oxidase

Chain B:




K437
I438
Y439
D440
Q441
V442
R443
M451
L458
PRO
SER
GLN
ARG
ILE
GLN
PRO
GLN
GLN
VAL
ALA
VAL
TRP
PRO
THR
MET
V475
D476
I477
L480
E481
L494
Q503
V506
R509
E513
L518
T519
S520
V524
A529
V534
K537
V538
F539
K542
L543
P544
K545
I546
K549
V554
L555
R556
L560
L561
I580
L585
R600
P601
V607
K613
L617
V620
R623
G626
A636
S639
P640
L641
N642
K643
Y650
H651
K652
H653
L654
K655
PRO
LEU
GLN
SER
LYS
LEU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.03Å 91.50Å 214.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	93.3 (10.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10488	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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	0.37	0/5141	0.59	0/6966
1	B	0.36	0/5018	0.59	0/6805
All	All	0.37	0/10159	0.59	0/13771

There are no bond length outliers.

There are no bond angle outliers.

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	5028	0	4974	109	0
1	B	4911	0	4837	140	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	241	0	0	6	0
3	B	202	0	0	4	0
All	All	10488	0	9873	243	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 (243) 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:549:LYS:HD3	1:B:549:LYS:H	1.05	1.18
1:B:549:LYS:CD	1:B:549:LYS:H	1.79	0.93
1:B:477:ILE:HD11	1:B:580:ILE:HD11	1.49	0.92
1:B:549:LYS:HD3	1:B:549:LYS:N	1.90	0.84
1:A:103:HIS:HD2	1:A:134:GLY:H	1.27	0.82
1:B:298:THR:HG23	1:B:607:VAL:HG13	1.65	0.79
1:B:115:ALA:HB3	1:B:120:GLN:HG3	1.66	0.78
1:B:103:HIS:HD2	1:B:134:GLY:H	1.32	0.78
1:A:298:THR:HG23	1:A:607:VAL:HG13	1.65	0.77
1:B:379:ALA:HB3	1:B:428:MET:CE	2.16	0.76
1:A:276:GLY:O	1:A:279:VAL:HG22	1.85	0.75
1:B:379:ALA:HB3	1:B:428:MET:HE3	1.70	0.72
1:A:591:ARG:HG2	1:A:591:ARG:HH11	1.54	0.71
1:A:175:TRP:O	1:A:176:TRP:HB2	1.90	0.71
1:A:19:ILE:O	1:A:23:LEU:HD22	1.92	0.70
1:B:108:LEU:HB2	1:B:109:PRO:HD3	1.74	0.69
1:A:433:ARG:HH11	1:A:433:ARG:HG3	1.58	0.69
1:A:182:LYS:O	1:A:215:HIS:HE1	1.76	0.68
1:B:494:LEU:HD12	1:B:529:ALA:HB2	1.76	0.68
1:B:175:TRP:O	1:B:176:TRP:HB2	1.92	0.67
1:A:442:VAL:HG13	3:A:1419:HOH:O	1.93	0.67
1:A:160:THR:OG1	1:A:162:GLU:HG2	1.94	0.66
1:B:556:ARG:NH1	1:B:560:LEU:HD21	2.09	0.66
1:B:140:GLU:HG2	1:B:174:LYS:HD3	1.78	0.66
1:A:597:THR:HG22	3:A:1385:HOH:O	1.97	0.64
1:A:117:ALA:O	1:A:121:GLU:HG3	1.98	0.64
1:B:636:ALA:O	1:B:639:SER:HB3	1.97	0.64
1:B:477:ILE:HD11	1:B:580:ILE:CD1	2.27	0.63
1:B:230:PHE:O	1:B:412:VAL:HG21	1.99	0.63
1:A:5:LEU:HD22	1:A:626:GLY:HA3	1.81	0.62
1:A:313:LYS:HE2	1:A:315:SER:OG	2.00	0.62
1:A:591:ARG:NH1	1:A:591:ARG:HG2	2.14	0.62
1:B:355:ILE:O	1:B:359:ILE:HG12	2.00	0.61
1:B:72:LYS:O	1:B:76:GLU:HG3	2.01	0.61
1:A:162:GLU:HB2	1:A:247:ILE:O	2.03	0.59
1:A:278:MET:O	1:A:281:VAL:HG22	2.03	0.59
1:A:480:LEU:HD11	1:A:543:LEU:HD23	1.85	0.58
1:B:279:VAL:HG22	1:B:374:THR:HG21	1.85	0.58
1:A:198:GLU:HB2	1:A:200:TYR:CE1	2.39	0.58
1:B:371:HIS:O	1:B:374:THR:HG22	2.04	0.58
1:B:437:LYS:HE3	1:B:441:GLN:NE2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1699:FAD:H8A	2:B:1699:FAD:O1A	2.04	0.58
1:B:147:LEU:HD12	1:B:147:LEU:H	1.68	0.57
1:B:556:ARG:HH11	1:B:560:LEU:HD21	1.68	0.57
1:A:215:HIS:HB2	1:B:650:TYR:CE2	2.39	0.57
1:B:234:GLU:H	1:B:234:GLU:CD	2.08	0.57
1:B:51:TYR:OH	1:B:66:LYS:NZ	2.38	0.56
1:A:231:GLY:HA3	1:A:412:VAL:HG13	1.86	0.56
1:A:550:ALA:O	1:A:554:VAL:HG23	2.06	0.56
1:B:556:ARG:NE	3:B:1294:HOH:O	2.39	0.56
1:A:335:LEU:HD23	1:A:335:LEU:O	2.05	0.56
1:A:86:MET:HE1	1:A:90:ASN:HD21	1.70	0.56
1:A:103:HIS:CD2	1:A:134:GLY:H	2.15	0.56
1:B:115:ALA:CB	1:B:120:GLN:HG3	2.33	0.56
1:B:40:ILE:CD1	1:B:91:SER:HB2	2.36	0.56
1:B:379:ALA:HB3	1:B:428:MET:HE2	1.87	0.56
1:B:520:SER:O	1:B:524:VAL:HG23	2.05	0.55
1:A:223:VAL:HG12	1:A:240:LEU:HD13	1.88	0.55
1:B:147:LEU:O	1:B:150:LEU:HG	2.06	0.55
1:A:234:GLU:H	1:A:234:GLU:CD	2.09	0.55
1:A:312:ILE:O	1:B:513:GLU:HG2	2.07	0.55
1:A:513:GLU:OE1	1:B:314:GLN:HG2	2.07	0.54
1:B:56:ARG:NH1	3:B:1249:HOH:O	2.40	0.54
1:B:67:SER:O	1:B:70:MET:HB3	2.07	0.54
1:B:298:THR:HG23	1:B:607:VAL:CG1	2.36	0.54
1:B:364:LEU:HD12	1:B:364:LEU:N	2.23	0.54
1:A:273:LEU:HD11	1:A:278:MET:HE3	1.89	0.53
1:B:108:LEU:HD21	1:B:127:ALA:CB	2.38	0.53
1:A:513:GLU:HG2	1:B:312:ILE:O	2.09	0.53
1:A:641:LEU:HB2	3:B:1050:HOH:O	2.08	0.53
1:A:174:LYS:O	1:A:239:TYR:HA	2.09	0.52
1:A:278:MET:HA	1:A:278:MET:HE2	1.91	0.52
1:A:67:SER:HB3	1:A:100:LEU:HD12	1.91	0.52
1:B:355:ILE:HD12	1:B:366:GLU:HB2	1.90	0.52
1:A:40:ILE:HD12	1:A:40:ILE:N	2.25	0.52
1:B:126:PRO:O	1:B:131:GLU:HB3	2.10	0.52
1:B:15:ASN:C	1:B:15:ASN:HD22	2.12	0.52
1:B:48:HIS:CE1	1:B:66:LYS:HZ2	2.28	0.51
1:B:385:ALA:O	1:B:389:ILE:HG12	2.09	0.51
1:B:3:PRO:HA	1:B:6:ARG:HG2	1.91	0.51
1:B:600:ARG:HB3	1:B:601:PRO:HD3	1.93	0.51
1:A:134:GLY:HA2	1:A:186:HIS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:SER:HB3	3:A:1247:HOH:O	2.11	0.51
1:A:610:PHE:HB3	1:A:612:PHE:CE1	2.46	0.51
1:A:108:LEU:HB2	1:A:109:PRO:HD3	1.92	0.51
1:A:393:ARG:HB2	1:A:407:ILE:HG21	1.93	0.51
1:A:185:ASN:HA	1:A:210:ARG:HB2	1.93	0.51
1:A:294:SER:OG	1:A:342:HIS:HE1	1.94	0.51
1:A:433:ARG:CG	1:A:433:ARG:HH11	2.23	0.50
1:A:335:LEU:HD23	1:A:335:LEU:C	2.32	0.50
1:A:438:ILE:HG23	1:A:448:VAL:HG21	1.94	0.50
1:A:325:GLN:NE2	1:A:593:LEU:HD22	2.27	0.50
1:B:328:GLN:HG2	1:B:332:PHE:CE1	2.46	0.50
1:B:376:GLY:O	1:B:428:MET:HE1	2.11	0.50
1:B:417:ALA:HA	1:B:420:PHE:CE1	2.47	0.50
1:A:103:HIS:HD2	1:A:134:GLY:N	2.04	0.50
1:A:490:ARG:O	1:A:494:LEU:HD23	2.12	0.50
1:B:126:PRO:C	1:B:128:TRP:H	2.14	0.50
1:B:376:GLY:HA2	1:B:428:MET:CE	2.42	0.50
1:B:182:LYS:O	1:B:215:HIS:HE1	1.94	0.50
1:A:620:VAL:O	1:A:623:ARG:HG3	2.11	0.49
1:B:298:THR:O	1:B:302:ARG:HB2	2.12	0.49
1:B:38:ASN:HD21	1:B:613:LYS:HZ1	1.59	0.49
1:B:439:TYR:O	1:B:442:VAL:HG22	2.12	0.49
1:B:38:ASN:HD21	1:B:613:LYS:NZ	2.10	0.49
1:A:298:THR:HG23	1:A:607:VAL:CG1	2.38	0.49
1:A:72:LYS:O	1:A:76:GLU:HG3	2.13	0.49
1:A:193:LEU:HD23	1:A:193:LEU:C	2.33	0.48
1:A:301:ILE:CD1	1:A:335:LEU:HD12	2.43	0.48
1:A:223:VAL:CG1	1:A:240:LEU:HD13	2.42	0.48
1:A:443:ARG:HH11	1:A:443:ARG:HG2	1.77	0.48
1:A:258:GLN:NE2	1:A:267:LYS:HE2	2.28	0.48
1:A:282:ARG:HG3	1:A:282:ARG:NH1	2.27	0.48
1:A:58:GLN:O	1:A:62:VAL:HG23	2.12	0.48
1:B:32:ARG:NH1	1:B:35:GLU:OE2	2.46	0.48
1:A:14:PHE:CD2	1:A:554:VAL:HG21	2.48	0.48
1:B:40:ILE:HD13	1:B:91:SER:HB2	1.96	0.48
1:B:289:ALA:HA	1:B:414:PHE:CE2	2.48	0.48
1:B:437:LYS:HE3	1:B:441:GLN:HE22	1.76	0.48
1:B:509:ARG:NH1	1:B:518:LEU:HD11	2.29	0.48
1:A:282:ARG:HH11	1:A:282:ARG:HG3	1.79	0.47
1:A:273:LEU:HD11	1:A:278:MET:CE	2.44	0.47
1:A:93:HIS:CD2	1:A:98:GLU:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:LEU:HB2	1:B:544:PRO:HD3	1.95	0.47
1:A:643:LYS:HG3	1:A:644:THR:HG23	1.95	0.47
1:B:103:HIS:CD2	1:B:134:GLY:H	2.20	0.47
1:A:289:ALA:HA	1:A:414:PHE:CE2	2.49	0.47
1:A:12:ALA:HA	1:A:602:ASN:OD1	2.15	0.47
1:A:19:ILE:HG22	1:A:23:LEU:CD2	2.44	0.47
1:A:40:ILE:HG23	1:A:46:PHE:CD1	2.48	0.47
1:A:480:LEU:HD11	1:A:543:LEU:CD2	2.44	0.47
1:B:112:LEU:O	1:B:112:LEU:HD13	2.15	0.47
1:B:15:ASN:HD22	1:B:16:PRO:N	2.13	0.47
1:B:187:ALA:O	1:B:207:VAL:HG13	2.15	0.47
1:A:86:MET:CE	1:A:90:ASN:HD21	2.27	0.47
1:B:31:ARG:C	1:B:31:ARG:HD3	2.36	0.47
1:B:376:GLY:O	1:B:428:MET:CE	2.63	0.47
1:B:451:MET:SD	1:B:537:LYS:HD3	2.55	0.46
1:B:51:TYR:HB3	1:B:59:ARG:HD3	1.95	0.46
1:A:103:HIS:HE1	3:A:1093:HOH:O	1.97	0.46
1:A:126:PRO:HB3	1:A:131:GLU:OE1	2.15	0.46
1:A:635:TRP:CH2	1:B:228:PRO:HD2	2.51	0.46
1:B:344:VAL:O	1:B:348:MET:HG3	2.15	0.46
1:B:414:PHE:C	1:B:416:PRO:HD2	2.35	0.46
1:A:252:MET:CE	1:A:254:MET:HG2	2.45	0.46
1:B:376:GLY:HA2	1:B:428:MET:HE2	1.97	0.46
1:A:5:LEU:HD22	1:A:626:GLY:CA	2.45	0.46
1:A:48:HIS:HE1	1:A:66:LYS:HZ3	1.63	0.46
1:A:438:ILE:CG2	1:A:448:VAL:HG21	2.46	0.46
1:B:185:ASN:HA	1:B:210:ARG:HB2	1.98	0.46
1:B:198:GLU:HB3	1:B:200:TYR:CE1	2.51	0.46
1:B:546:ILE:HD13	1:B:555:LEU:HD12	1.97	0.46
1:A:298:THR:HA	1:A:607:VAL:CG1	2.46	0.45
1:A:650:TYR:CE2	1:B:215:HIS:HB2	2.51	0.45
1:B:174:LYS:O	1:B:239:TYR:HA	2.16	0.45
1:A:222:THR:HB	1:A:241:LYS:HB3	1.97	0.45
1:A:175:TRP:O	1:A:176:TRP:CB	2.61	0.45
1:A:126:PRO:O	1:A:131:GLU:HB3	2.15	0.45
1:A:278:MET:HE2	1:A:281:VAL:HG11	1.99	0.45
1:A:286:VAL:HG23	3:A:1421:HOH:O	2.16	0.45
1:B:112:LEU:HB2	1:B:124:PHE:CE1	2.52	0.45
1:B:302:ARG:NH2	3:B:1005:HOH:O	2.41	0.45
1:B:40:ILE:HD12	1:B:91:SER:HB2	1.98	0.45
1:B:15:ASN:HD22	1:B:16:PRO:CD	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:SER:HB2	1:A:640:PRO:HD2	1.99	0.45
1:A:344:VAL:HG21	1:A:535:VAL:HG22	1.98	0.45
1:B:115:ALA:HB3	1:B:120:GLN:CG	2.43	0.45
1:B:15:ASN:ND2	1:B:17:GLU:H	2.14	0.45
1:A:653:HIS:CE1	1:B:65:LYS:HD2	2.52	0.44
1:B:407:ILE:N	1:B:408:PRO:CD	2.81	0.44
1:B:180:LEU:HD12	1:B:238:GLY:C	2.37	0.44
1:B:58:GLN:O	1:B:62:VAL:HG23	2.17	0.44
1:B:451:MET:HG2	1:B:534:VAL:HG22	1.98	0.44
1:B:67:SER:HB3	1:B:100:LEU:HD22	1.98	0.44
1:A:113:HIS:O	1:A:255:LYS:HE3	2.17	0.44
1:B:477:ILE:HD13	1:B:477:ILE:HA	1.80	0.44
1:B:640:PRO:O	1:B:643:LYS:HG2	2.17	0.44
1:B:243:ASP:O	1:B:244:ASN:C	2.56	0.44
1:A:448:VAL:HG22	1:A:449:GLY:N	2.33	0.43
1:B:147:LEU:C	1:B:149:GLY:H	2.20	0.43
1:B:254:MET:HB3	1:B:258:GLN:HG3	2.00	0.43
1:B:38:ASN:ND2	1:B:613:LYS:NZ	2.67	0.43
1:A:408:PRO:O	1:A:412:VAL:HB	2.18	0.43
1:A:439:TYR:CE2	1:A:499:ALA:HB1	2.53	0.43
1:B:249:ARG:NH1	1:B:250:GLU:OE2	2.52	0.43
1:A:278:MET:HA	1:A:278:MET:CE	2.48	0.43
1:A:27:PRO:HD2	3:A:1354:HOH:O	2.18	0.43
1:A:481:GLU:OE2	1:A:481:GLU:N	2.52	0.43
1:B:202:LEU:HD22	1:B:202:LEU:N	2.34	0.43
1:B:15:ASN:ND2	1:B:15:ASN:C	2.71	0.43
1:B:5:LEU:HD12	1:B:626:GLY:HA3	2.01	0.43
1:B:620:VAL:O	1:B:623:ARG:HG3	2.19	0.43
1:B:102:LEU:HD12	1:B:178:GLY:O	2.19	0.42
1:B:108:LEU:HD21	1:B:127:ALA:HB3	2.00	0.42
1:B:112:LEU:HD13	1:B:112:LEU:C	2.39	0.42
1:B:542:LYS:O	1:B:542:LYS:HD3	2.19	0.42
1:B:641:LEU:HD12	1:B:641:LEU:HA	1.87	0.42
1:A:42:ASN:O	1:A:44:PRO:HD3	2.18	0.42
1:B:161:GLN:NE2	1:B:261:PRO:HB3	2.33	0.42
1:B:4:ASP:O	1:B:8:GLU:HG2	2.20	0.42
1:A:282:ARG:HD2	1:A:284:PHE:CZ	2.54	0.42
1:A:480:LEU:CD1	1:A:543:LEU:HD23	2.48	0.42
1:B:151:GLU:HB2	1:B:172:SER:CB	2.49	0.42
1:B:282:ARG:HH11	1:B:374:THR:HG23	1.84	0.42
1:A:258:GLN:HB2	1:A:266:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ASN:C	1:B:131:GLU:N	2.72	0.42
1:B:282:ARG:NE	1:B:427:MET:CE	2.82	0.42
1:B:175:TRP:O	1:B:177:PRO:HD3	2.19	0.42
1:B:652:LYS:HG3	1:B:653:HIS:CD2	2.54	0.42
1:B:481:GLU:H	1:B:481:GLU:CD	2.23	0.42
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.86	0.42
1:A:177:PRO:HB2	1:A:180:LEU:HB2	2.02	0.42
1:A:452:VAL:HG22	1:A:455:LEU:HD12	2.01	0.42
1:B:170:VAL:HG13	1:B:171:THR:N	2.35	0.42
1:A:243:ASP:O	1:A:244:ASN:C	2.58	0.42
1:A:7:LYS:HZ3	1:A:320:GLN:HE22	1.67	0.42
1:B:176:TRP:O	1:B:177:PRO:C	2.58	0.42
1:A:258:GLN:HB2	1:A:266:VAL:HG22	2.02	0.41
1:B:82:PRO:HA	1:B:85:ILE:HD12	2.01	0.41
1:A:67:SER:O	1:A:70:MET:HB3	2.19	0.41
1:A:184:SER:O	1:A:210:ARG:HD2	2.20	0.41
1:A:40:ILE:HD12	1:A:40:ILE:H	1.85	0.41
1:B:298:THR:HA	1:B:607:VAL:CG1	2.50	0.41
1:B:41:LEU:HD13	1:B:41:LEU:C	2.40	0.41
1:B:81:ASP:HA	1:B:82:PRO:HD2	1.91	0.41
1:A:451:MET:HA	1:A:451:MET:HE2	2.01	0.41
1:B:19:ILE:O	1:B:23:LEU:HG	2.21	0.41
2:A:699:FAD:H51A	1:B:397:GLY:HA3	2.03	0.41
1:B:66:LYS:HE3	1:B:92:VAL:O	2.21	0.41
1:B:282:ARG:NE	1:B:427:MET:HE3	2.36	0.41
1:B:175:TRP:O	1:B:176:TRP:CB	2.64	0.41
1:B:503:GLN:HA	1:B:506:VAL:HG22	2.01	0.41
1:A:452:VAL:HG22	1:A:455:LEU:CD1	2.51	0.40
1:B:188:ILE:HA	1:B:205:PHE:O	2.21	0.40
1:B:254:MET:HA	1:B:257:ALA:O	2.20	0.40
1:A:378:LYS:CE	1:A:420:PHE:O	2.69	0.40
1:B:128:TRP:C	1:B:130:LEU:H	2.24	0.40
1:B:415:THR:N	1:B:416:PRO:HD2	2.36	0.40
1:B:41:LEU:HD12	1:B:42:ASN:OD1	2.22	0.40
1:B:116:THR:OG1	1:B:119:GLN:HG3	2.21	0.40
1:B:639:SER:HA	1:B:640:PRO:HD3	1.92	0.40
1:B:250:GLU:H	1:B:250:GLU:CD	2.24	0.40
1:B:326:THR:O	1:B:330:LYS:HG3	2.22	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	631/661 (96%)	615 (98%)	15 (2%)	1 (0%)	47	55
1	B	623/661 (94%)	597 (96%)	22 (4%)	4 (1%)	25	26
All	All	1254/1322 (95%)	1212 (97%)	37 (3%)	5 (0%)	34	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	TRP
1	B	176	TRP
1	B	114	GLN
1	B	82	PRO
1	B	144	GLY

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	539/571 (94%)	517 (96%)	22 (4%)	30	39
1	B	519/571 (91%)	491 (95%)	28 (5%)	22	26
All	All	1058/1142 (93%)	1008 (95%)	50 (5%)	26	33

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU

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Mol	Chain	Res	Type
1	A	23	LEU
1	A	56	ARG
1	A	59	ARG
1	A	112	LEU
1	A	125	MET
1	A	147	LEU
1	A	180	LEU
1	A	207	VAL
1	A	215	HIS
1	A	218	LEU
1	A	282	ARG
1	A	293	LEU
1	A	412	VAL
1	A	429	LEU
1	A	443	ARG
1	A	539	PHE
1	A	543	LEU
1	A	575	LEU
1	A	607	VAL
1	A	615	MET
1	A	617	LEU
1	B	6	ARG
1	B	15	ASN
1	B	100	LEU
1	B	130	LEU
1	B	207	VAL
1	B	215	HIS
1	B	218	LEU
1	B	223	VAL
1	B	249	ARG
1	B	293	LEU
1	B	335	LEU
1	B	344	VAL
1	B	352	TYR
1	B	412	VAL
1	B	419	THR
1	B	420	PHE
1	B	429	LEU
1	B	433	ARG
1	B	443	ARG
1	B	480	LEU
1	B	539	PHE

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Mol	Chain	Res	Type
1	B	549	LYS
1	B	554	VAL
1	B	560	LEU
1	B	561	LEU
1	B	580	ILE
1	B	585	LEU
1	B	639	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	38	ASN
1	A	47	GLN
1	A	48	HIS
1	A	52	ASN
1	A	90	ASN
1	A	103	HIS
1	A	114	GLN
1	A	203	HIS
1	A	215	HIS
1	A	258	GLN
1	A	291	GLN
1	A	314	GLN
1	A	320	GLN
1	A	409	ASN
1	A	557	ASN
1	A	587	GLN
1	A	647	HIS
1	A	653	HIS
1	B	15	ASN
1	B	38	ASN
1	B	48	HIS
1	B	103	HIS
1	B	138	GLN
1	B	161	GLN
1	B	203	HIS
1	B	215	HIS
1	B	342	HIS
1	B	361	GLN
1	B	399	HIS
1	B	430	GLN

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Mol	Chain	Res	Type
1	B	441	GLN
1	B	557	ASN
1	B	589	ASN
1	B	627	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

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	699	-	51,58,58	2.45	13 (25%)	60,89,89	1.78	11 (18%)
2	FAD	B	1699	-	51,58,58	2.48	16 (31%)	60,89,89	1.72	10 (16%)

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	699	-	-	4/30/50/50	0/6/6/6
2	FAD	B	1699	-	-	3/30/50/50	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	699	FAD	C4X-C10	9.62	1.48	1.38
2	B	1699	FAD	C4X-C10	9.46	1.48	1.38
2	B	1699	FAD	C9A-N10	6.28	1.47	1.38
2	A	699	FAD	O4B-C1B	5.59	1.48	1.41
2	A	699	FAD	C9A-N10	5.44	1.45	1.38
2	B	1699	FAD	O4B-C1B	5.26	1.48	1.41
2	A	699	FAD	PA-O2A	-4.24	1.35	1.55
2	B	1699	FAD	PA-O2A	-4.20	1.35	1.55
2	A	699	FAD	O5'-C5'	4.10	1.60	1.44
2	B	1699	FAD	O5'-C5'	3.78	1.59	1.44
2	B	1699	FAD	P-O2P	-3.69	1.38	1.55
2	A	699	FAD	P-O2P	-3.64	1.38	1.55
2	B	1699	FAD	C4-C4X	3.40	1.47	1.41
2	A	699	FAD	C4-N3	3.29	1.38	1.33
2	B	1699	FAD	C4-N3	3.27	1.38	1.33
2	B	1699	FAD	C10-N1	3.20	1.37	1.33
2	A	699	FAD	C10-N1	3.10	1.37	1.33
2	B	1699	FAD	C2-N3	2.90	1.43	1.38
2	A	699	FAD	C8-C7	2.90	1.48	1.40
2	A	699	FAD	C4-C4X	2.88	1.46	1.41
2	B	1699	FAD	C8-C7	2.83	1.48	1.40
2	A	699	FAD	C2-N3	2.74	1.43	1.38
2	B	1699	FAD	O4B-C4B	2.17	1.49	1.45
2	B	1699	FAD	C4A-N3A	2.17	1.38	1.35
2	A	699	FAD	C2-N1	-2.15	1.33	1.38
2	B	1699	FAD	C2B-C1B	-2.13	1.50	1.53
2	B	1699	FAD	C5X-N5	2.11	1.38	1.35
2	B	1699	FAD	C2A-N3A	2.07	1.35	1.32
2	A	699	FAD	O4B-C4B	2.05	1.49	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	699	FAD	C4-N3-C2	7.84	121.76	115.14
2	B	1699	FAD	C4-N3-C2	7.76	121.69	115.14
2	A	699	FAD	C4X-C4-N3	-4.74	116.95	123.43
2	B	1699	FAD	C4X-C4-N3	-4.70	117.00	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	699	FAD	O5B-PA-O1A	-3.09	96.97	109.07
2	A	699	FAD	C5A-C6A-N6A	2.99	124.89	120.35
2	B	1699	FAD	O5B-PA-O1A	-2.84	97.97	109.07
2	A	699	FAD	O3B-C3B-C4B	2.61	118.58	111.05
2	B	1699	FAD	C2A-N1A-C6A	2.58	123.17	118.75
2	B	1699	FAD	C5X-C9A-N10	-2.55	115.86	117.72
2	A	699	FAD	C2A-N1A-C6A	2.54	123.10	118.75
2	B	1699	FAD	C4-C4X-C10	-2.50	118.30	119.95
2	A	699	FAD	C4-C4X-C10	-2.49	118.30	119.95
2	A	699	FAD	C5A-C6A-N1A	-2.46	114.78	120.35
2	B	1699	FAD	C5A-C6A-N6A	2.44	124.07	120.35
2	B	1699	FAD	O4B-C1B-C2B	-2.42	103.39	106.93
2	B	1699	FAD	C5A-C6A-N1A	-2.42	114.87	120.35
2	A	699	FAD	C5X-C9A-N10	-2.32	116.03	117.72
2	A	699	FAD	O4B-C1B-C2B	-2.26	103.62	106.93
2	B	1699	FAD	O3B-C3B-C4B	2.19	117.39	111.05
2	A	699	FAD	C1'-N10-C10	2.07	120.26	118.41

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	699	FAD	P-O3P-PA-O2A
2	A	699	FAD	PA-O3P-P-O2P
2	B	1699	FAD	P-O3P-PA-O2A
2	A	699	FAD	P-O3P-PA-O1A
2	B	1699	FAD	PA-O3P-P-O2P
2	A	699	FAD	PA-O3P-P-O1P
2	B	1699	FAD	PA-O3P-P-O1P

There are no ring outliers.

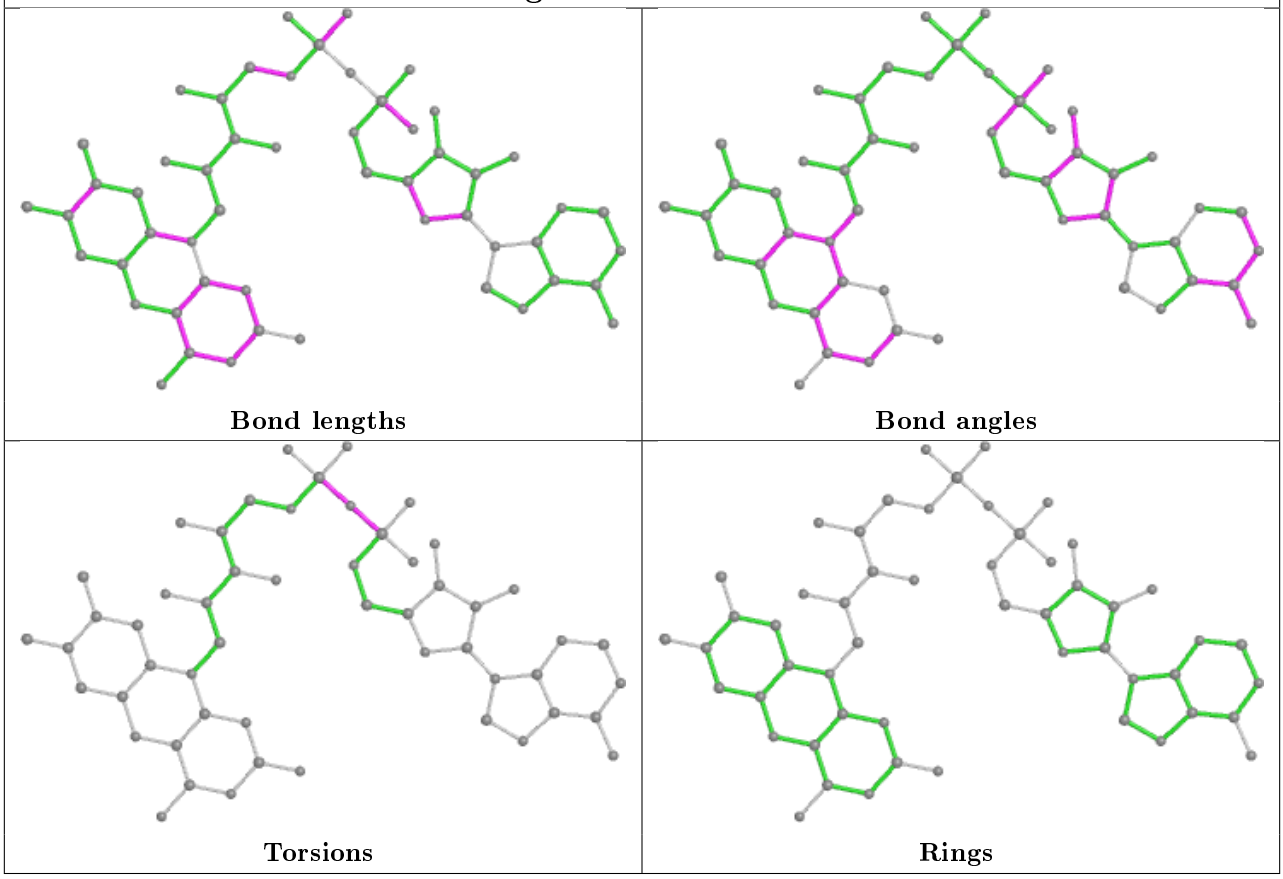
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	699	FAD	1	0
2	B	1699	FAD	1	0

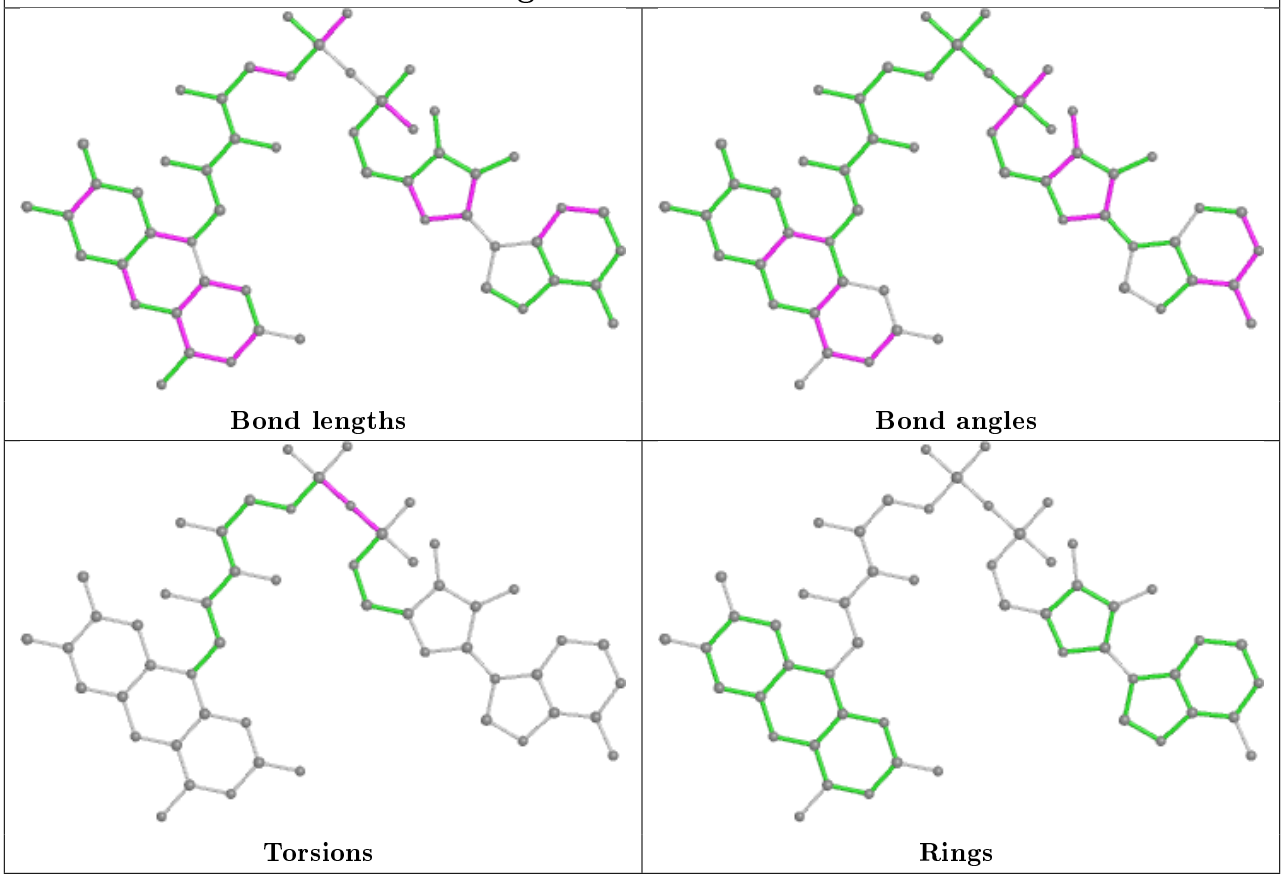
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 699



Ligand FAD B 1699



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.