wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 10:46 am GMT

PDB ID	:	4BBY
Title	:	MAMMALIAN ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE: WILD-TYPE
Authors	:	Nenci, S.; Piano, V.; Rosati, S.; Aliverti, A.; Pandini, V.; Fraaije, M.W.; Heck, A.J.R.; Edmondson, D.E.; Mattevi, A.
Deposited on	:	2012-09-28
Resolution	:	1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

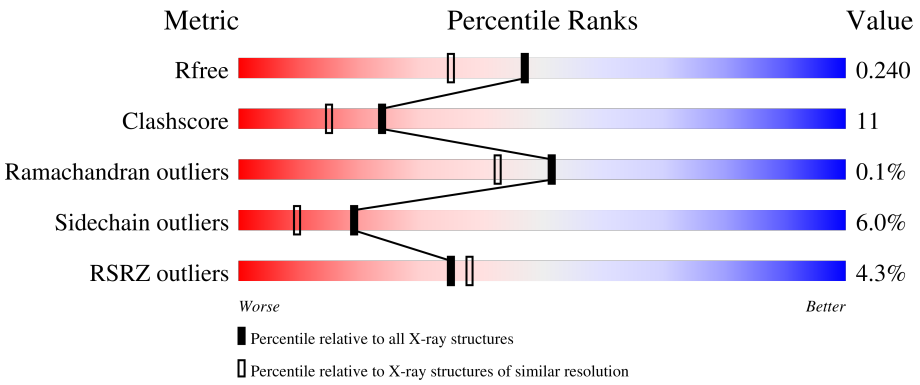
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	658	4% 65% 16% • 16%
1	B	658	4% 62% 17% • • 17%
1	C	658	3% 65% 17% • 15%
1	D	658	3% 65% 15% • • 16%

2 Entry composition (i)

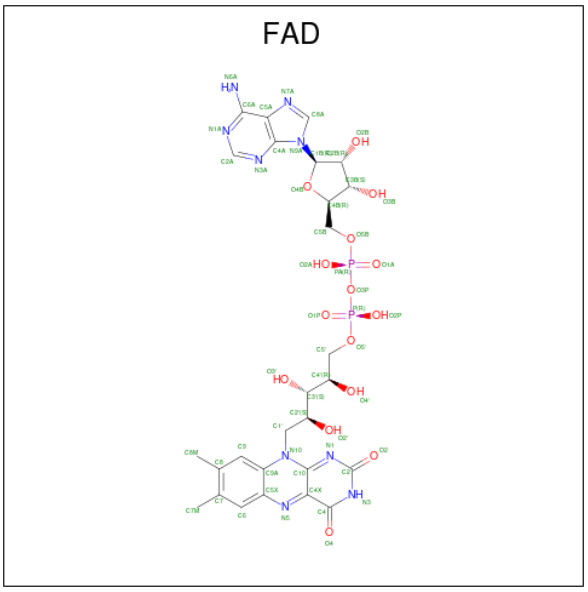
There are 4 unique types of molecules in this entry. The entry contains 18517 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	555	4413	2803	763	821	26	0	4	0
1	B	543	4301	2732	747	798	24	0	0	0
1	C	557	4418	2803	766	823	26	0	3	0
1	D	550	4363	2766	760	812	25	0	2	0

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



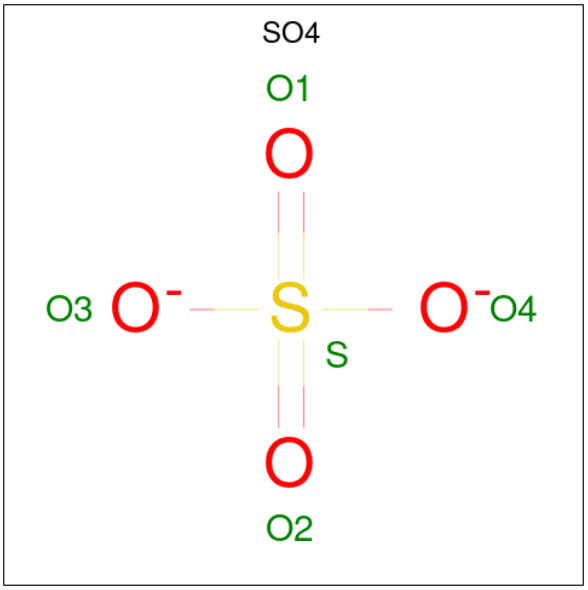
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	227	227	227	0	0
			Total	O		
4	B	175	175	175	0	0

Continued on next page...

Continued from previous page...

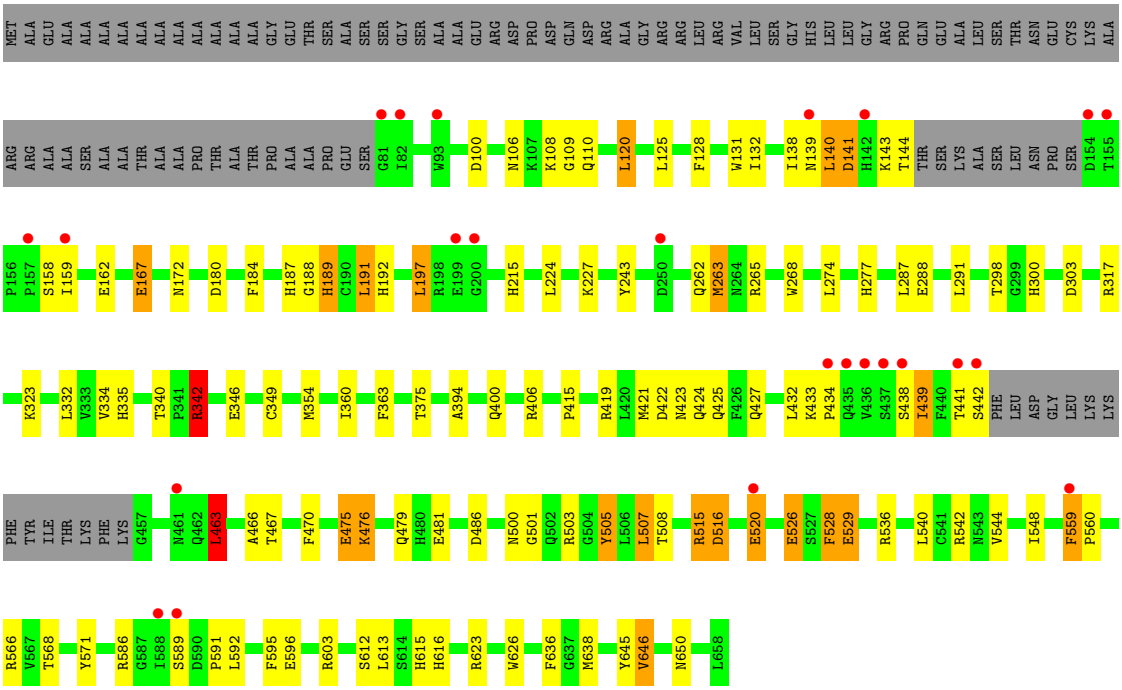
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	215	215	215	0	0
			Total	O		
4	D	173	173	173	0	0

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.

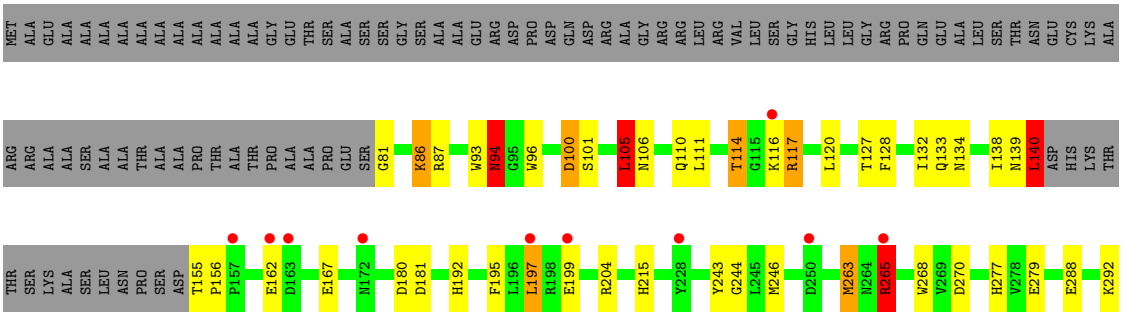
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

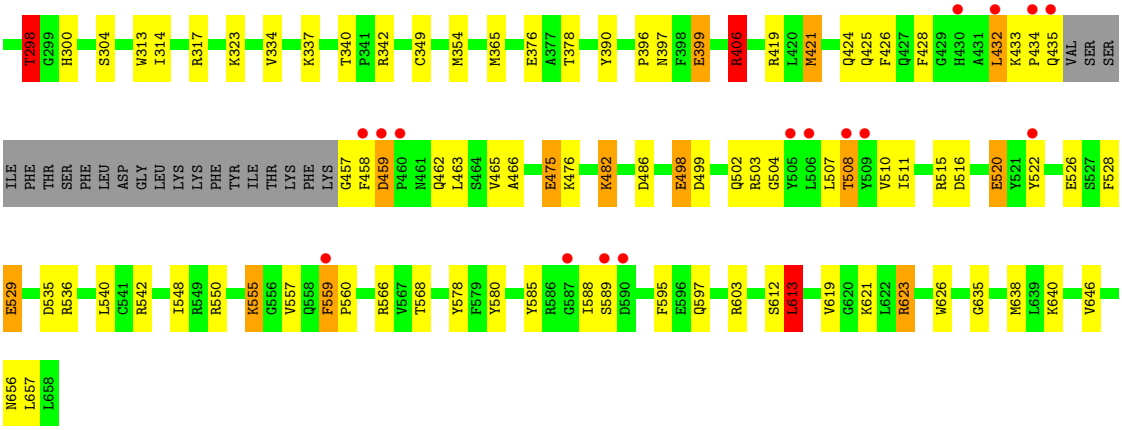
Chain A:



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

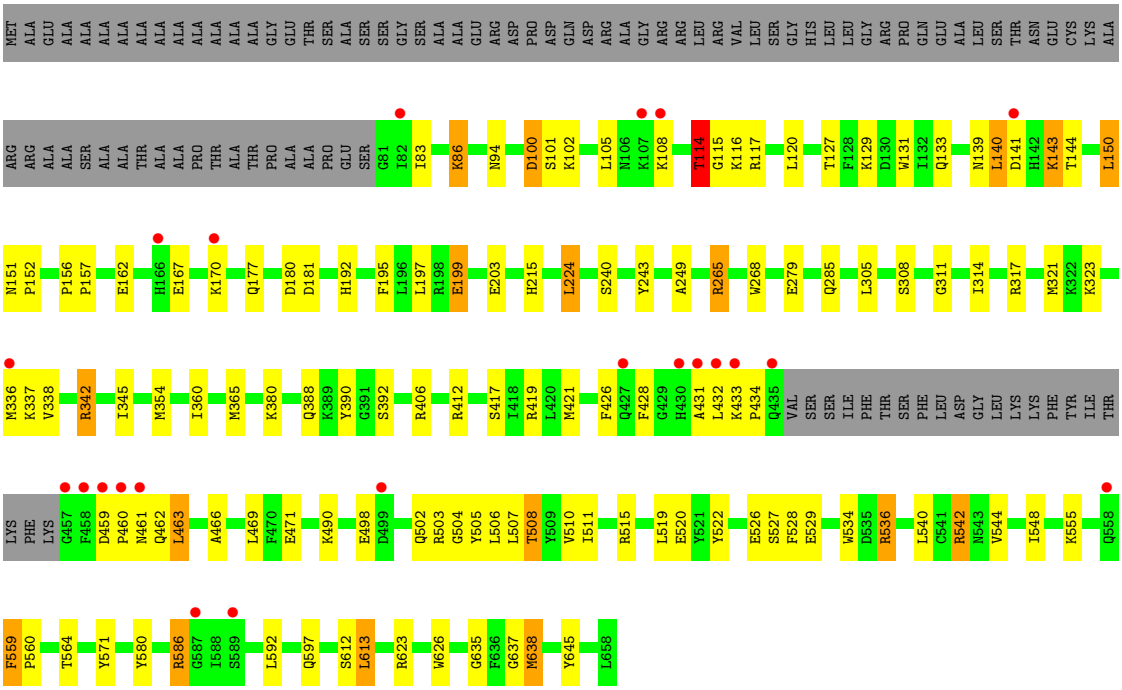
Chain B:





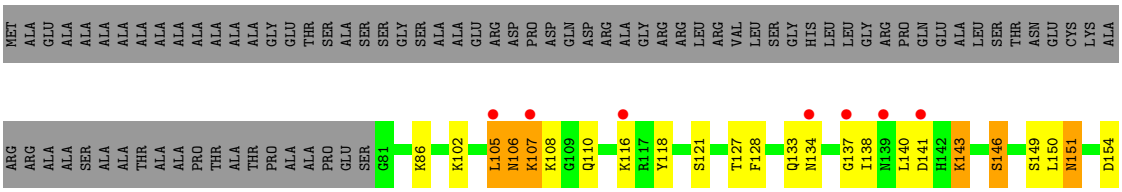
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

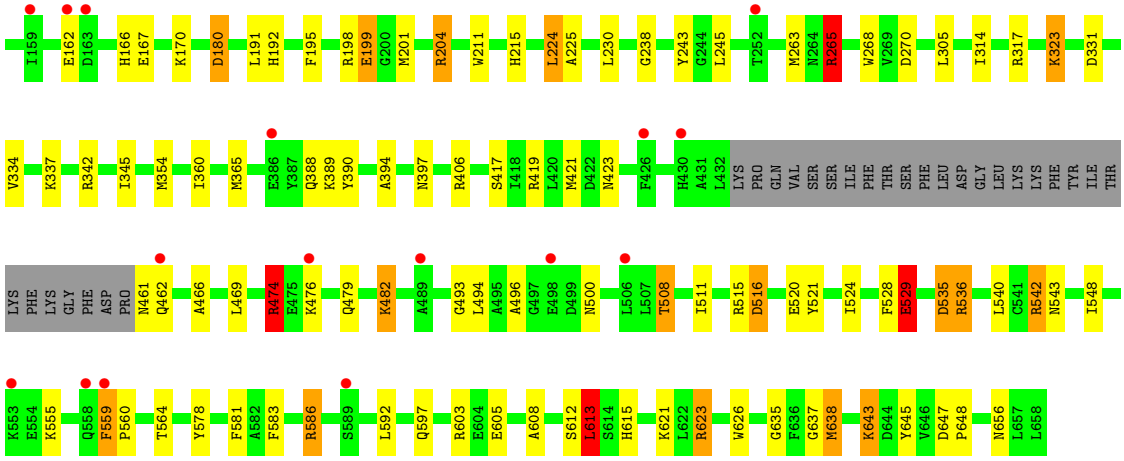
Chain C:



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

Chain D:




I159
E162
D163
H166
E167
K170
D180
L191
H192
F195
R198
E199
G200
M201
R204
W211
H215
L224
A225
L230
G238
Y243
G244
L245
T252
M263
N264
R265
W268
V269
D270
L305
I314
R317
K323
D331
V334
K337
R342
I345
M354
I360
M365
E386
Y387
Q388
K389
Y390
A394
N397
R406
S417
I418
R419
L420
M421
D422
N423
F426
H430
A431
L432
LYS
PRO
GLN
VAL
SER
SER
ILE
PHE
THR
SER
PHE
LEU
ASP
GLY
LEU
LYS
LYS
PHE
TYR
ILE
THR
LYS
PHE
LYS
GLY
PHE
ASP
PRO
N461
Q462
A466
L469
R474
E475
K476
Q479
K482
A489
G493
L494
A495
A496
G497
E498
D499
N500
L506
L507
T508
I511
R515
D516
E520
Y521
I524
F528
E529
D535
R536
L540
C541
R542
N543
I548
K553
E554
K555
Q558
F559
P560
T564
Y578
F581
A582
F583
R586
S589
L592
Q597
R603
E604
E605
A608
S612
L613
S614
H615
K621
L622
R623
W626
G635
F636
G637
M638
K643
D644
Y645
V646
D647
P648
N656
L657
L658

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.30Å 99.17Å 107.83Å 90.43° 92.18° 94.92°	Depositor
Resolution (Å)	19.98 – 1.90 19.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (19.98-1.90) 92.3 (19.96-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.191 , 0.240 0.192 , 0.240	Depositor DCC
R_{free} test set	2004 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.040 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18517	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	1.35	34/4524 (0.8%)	1.34	51/6114 (0.8%)
1	B	1.15	14/4398 (0.3%)	1.19	32/5944 (0.5%)
1	C	1.15	13/4527 (0.3%)	1.19	31/6119 (0.5%)
1	D	1.14	9/4466 (0.2%)	1.27	40/6036 (0.7%)
All	All	1.20	70/17915 (0.4%)	1.25	154/24213 (0.6%)

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	1	1
1	D	0	1
All	All	1	2

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	ARG	CZ-NH1	-13.52	1.15	1.33
1	A	528	PHE	CG-CD2	-11.33	1.21	1.38
1	A	167	GLU	CD-OE1	-11.31	1.13	1.25
1	A	528	PHE	CG-CD1	-10.40	1.23	1.38
1	A	526	GLU	CD-OE1	-10.37	1.14	1.25

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	603	ARG	NE-CZ-NH1	26.51	133.56	120.30
1	B	265	ARG	NE-CZ-NH2	26.51	133.55	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	265	ARG	NE-CZ-NH2	-25.99	107.31	120.30
1	A	542	ARG	NE-CZ-NH2	25.05	132.83	120.30
1	C	623	ARG	NE-CZ-NH1	19.60	130.10	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	298	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	406	ARG	Sidechain
1	D	265	ARG	Sidechain

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	4413	0	4359	98	0
1	B	4301	0	4242	117	7
1	C	4418	0	4365	106	6
1	D	4363	0	4313	95	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
4	A	227	0	0	14	0
4	B	175	0	0	22	0
4	C	215	0	0	14	1
4	D	173	0	0	14	0
All	All	18517	0	17403	392	7

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 11.

The worst 5 of 392 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:THR:HG22	4:D:2095:HOH:O	1.37	1.23
1:A:192:HIS:HB3	1:A:243:TYR:OH	1.43	1.15
1:C:192:HIS:HB3	1:C:243:TYR:OH	1.46	1.14
1:D:192:HIS:HB3	1:D:243:TYR:OH	1.44	1.14
1:A:559:PHE:HE2	1:D:608:ALA:CB	1.58	1.14

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ARG:NE	1:C:151:ASN:OD1[1_556]	1.55	0.65
1:B:265:ARG:NH2	1:C:152:PRO:CD[1_556]	1.67	0.53
1:B:134:ASN:OD1	4:C:2180:HOH:O[1_546]	1.85	0.35
1:B:265:ARG:NH2	1:C:151:ASN:CA[1_556]	1.98	0.22
1:B:265:ARG:NH2	1:C:150:LEU:O[1_556]	2.14	0.06

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	553/658 (84%)	542 (98%)	10 (2%)	1 (0%)	47	38
1	B	537/658 (82%)	516 (96%)	21 (4%)	0	100	100
1	C	556/658 (84%)	536 (96%)	18 (3%)	2 (0%)	34	24
1	D	548/658 (83%)	534 (97%)	14 (3%)	0	100	100
All	All	2194/2632 (83%)	2128 (97%)	63 (3%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	506	LEU
1	C	508	THR
1	A	140	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	480/545 (88%)	456 (95%)	24 (5%)	24 15
1	B	464/545 (85%)	430 (93%)	34 (7%)	14 6
1	C	480/545 (88%)	458 (95%)	22 (5%)	27 17
1	D	473/545 (87%)	439 (93%)	34 (7%)	14 6
All	All	1897/2180 (87%)	1783 (94%)	114 (6%)	19 9

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	613	LEU
1	D	564	THR
1	C	406	ARG
1	D	559	PHE
1	D	388	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	597	GLN
1	D	177	GLN
1	C	650	ASN
1	D	110	GLN
1	D	650	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	SO4	A	1660	-	4,4,4	0.69	0	6,6,6	0.50	0
3	SO4	A	1659	-	4,4,4	0.66	0	6,6,6	0.62	0
2	FAD	A	999	-	53,58,58	2.00	14 (26%)	68,89,89	1.99	19 (27%)
2	FAD	D	999	-	53,58,58	1.33	5 (9%)	68,89,89	1.68	15 (22%)
2	FAD	C	999	-	53,58,58	1.87	13 (24%)	68,89,89	1.97	22 (32%)
2	FAD	B	999	-	53,58,58	2.08	16 (30%)	68,89,89	1.91	20 (29%)
3	SO4	B	1659	-	4,4,4	0.39	0	6,6,6	0.50	0
3	SO4	D	1659	-	4,4,4	0.51	0	6,6,6	0.91	0

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	C	999	-	-	3/30/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	999	-	-	6/30/50/50	0/6/6/6
2	FAD	D	999	-	-	3/30/50/50	0/6/6/6
2	FAD	B	999	-	-	3/30/50/50	0/6/6/6

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	FAD	C1'-C2'	6.00	1.61	1.52
2	A	999	FAD	O4B-C1B	5.90	1.49	1.41
2	B	999	FAD	C5'-C4'	5.69	1.59	1.51
2	B	999	FAD	C4A-N3A	-5.49	1.28	1.35
2	A	999	FAD	C9A-C5X	5.28	1.50	1.41

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	999	FAD	N3A-C2A-N1A	-7.25	117.34	128.68
2	A	999	FAD	C4-C4X-N5	5.23	125.67	118.23
2	C	999	FAD	C4-C4X-N5	4.84	125.11	118.23
2	B	999	FAD	C4A-C5A-N7A	-4.83	104.37	109.40
2	C	999	FAD	C10-N1-C2	4.64	126.19	116.90

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	FAD	N10-C1'-C2'-O2'
2	A	999	FAD	N10-C1'-C2'-C3'
2	B	999	FAD	N10-C1'-C2'-O2'
2	B	999	FAD	N10-C1'-C2'-C3'
2	C	999	FAD	N10-C1'-C2'-O2'

There are no ring outliers.

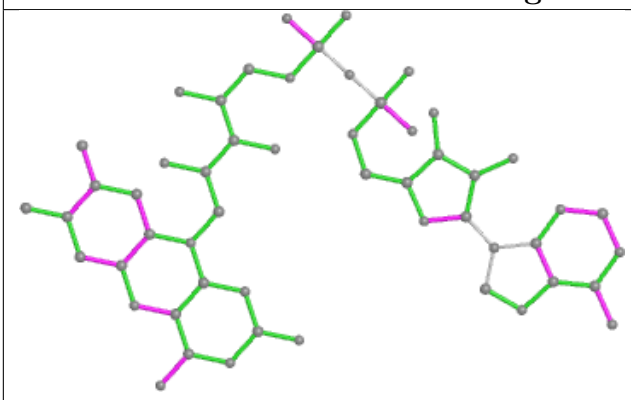
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	999	FAD	1	0

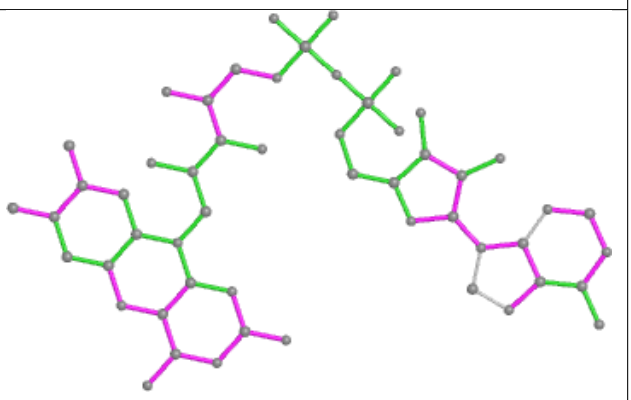
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

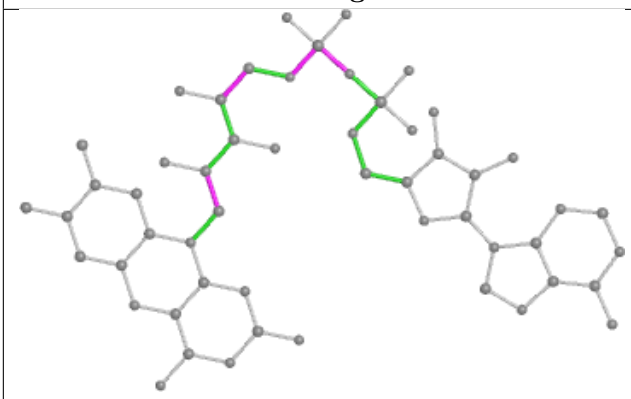
Ligand FAD A 999



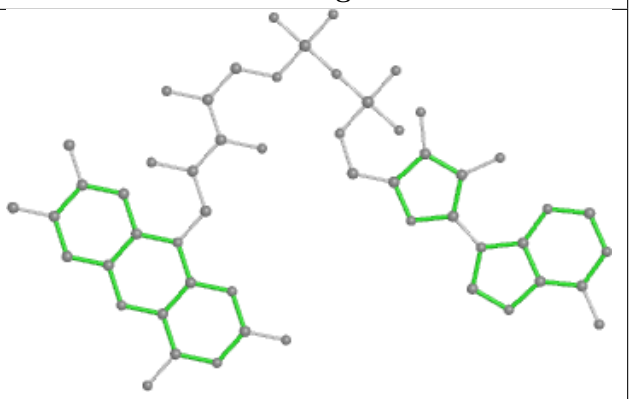
Bond lengths



Bond angles

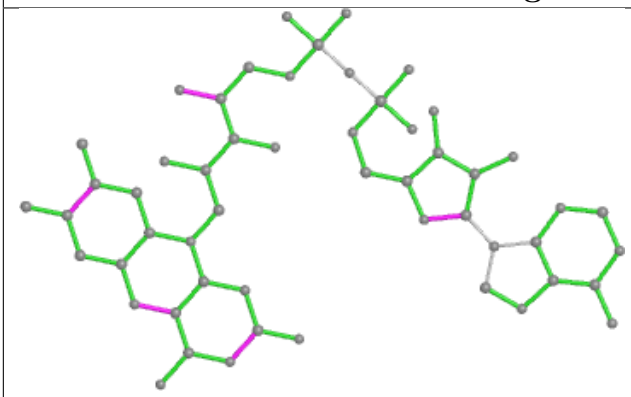


Torsions

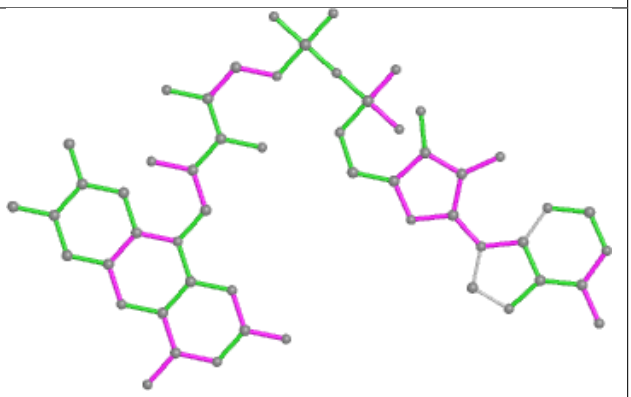


Rings

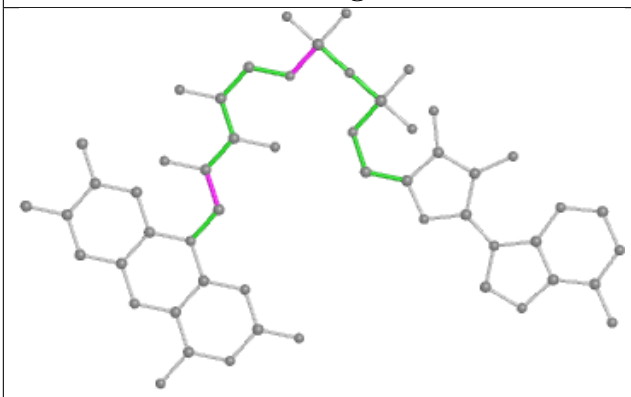
Ligand FAD D 999



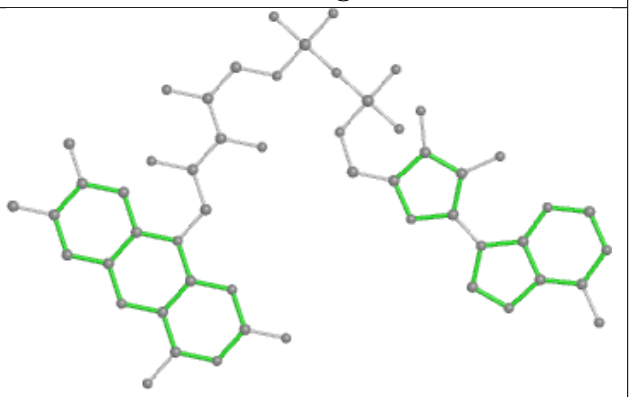
Bond lengths



Bond angles

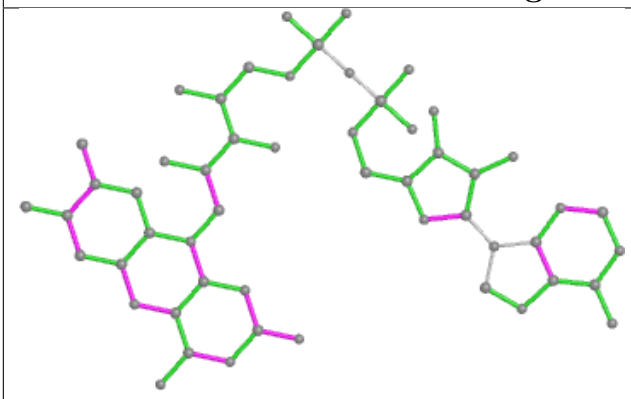


Torsions

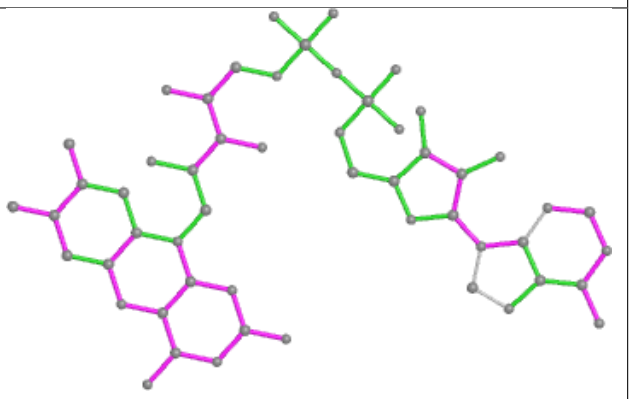


Rings

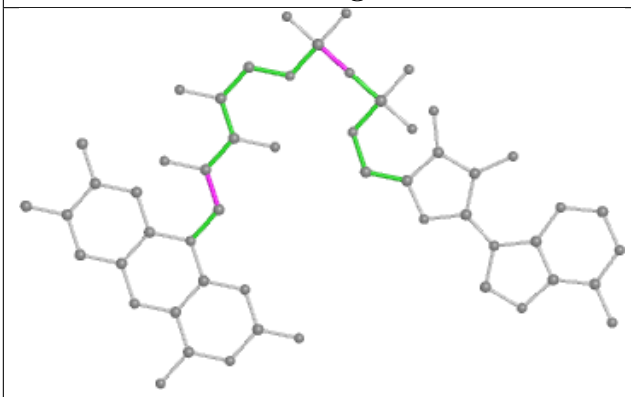
Ligand FAD C 999



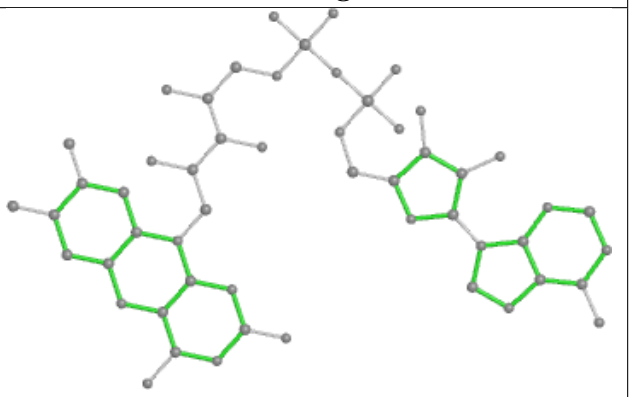
Bond lengths



Bond angles

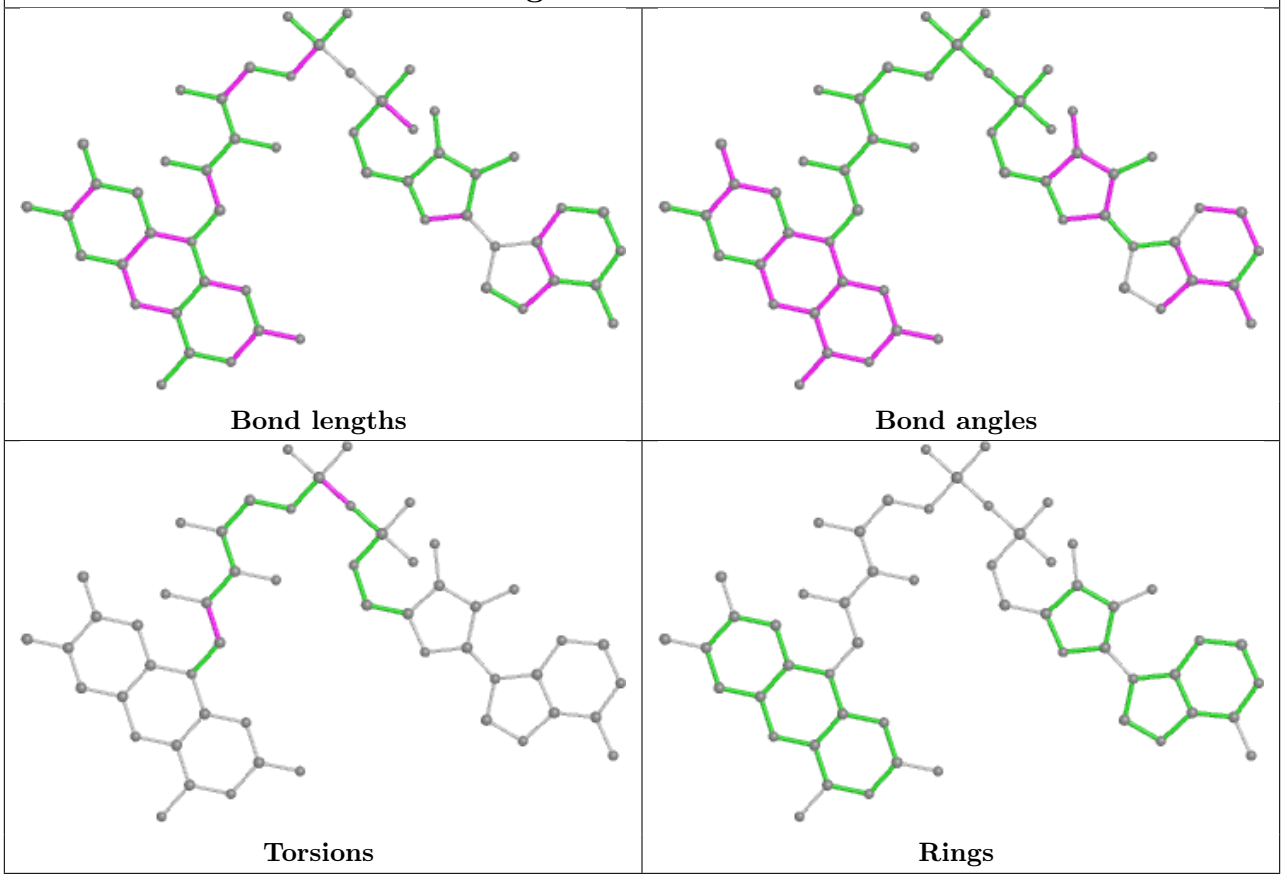


Torsions



Rings

Ligand FAD B 999



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	555/658 (84%)	0.01	24 (4%)	35	38	11, 26, 55, 88	0
1	B	543/658 (82%)	0.16	26 (4%)	30	33	14, 30, 59, 84	0
1	C	557/658 (84%)	0.05	22 (3%)	39	42	11, 27, 55, 75	1 (0%)
1	D	550/658 (83%)	0.18	23 (4%)	36	39	12, 32, 60, 78	0
All	All	2205/2632 (83%)	0.10	95 (4%)	35	38	11, 29, 58, 88	1 (0%)

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	PRO	6.0
1	B	458	PHE	6.0
1	A	559	PHE	4.8
1	D	559	PHE	4.7
1	B	435	GLN	4.6

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

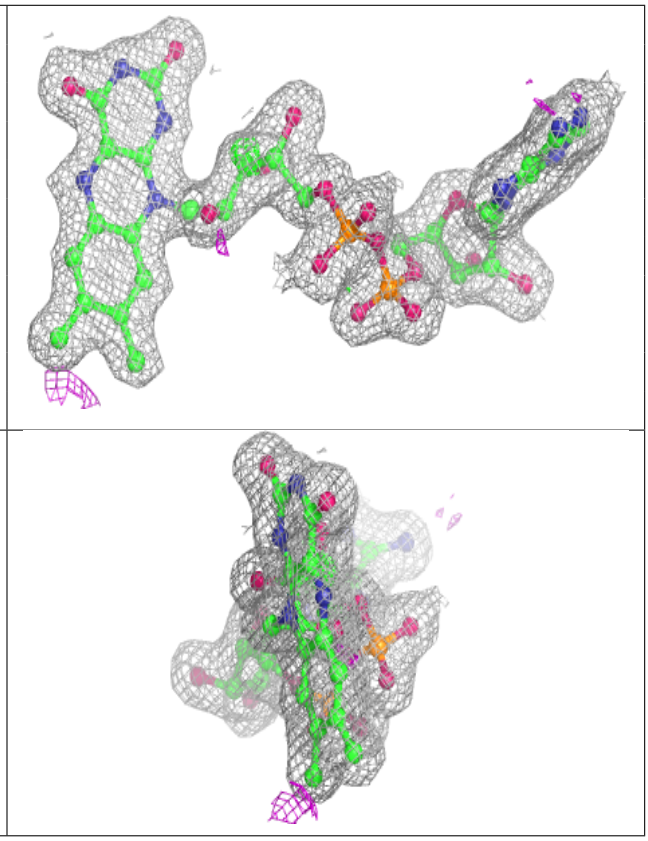
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	1659	5/5	0.94	0.23	41,51,57,66	0
3	SO4	D	1659	5/5	0.95	0.15	39,40,44,58	0
3	SO4	A	1659	5/5	0.96	0.17	34,37,43,59	0
3	SO4	A	1660	5/5	0.96	0.19	47,51,61,62	0
2	FAD	B	999	53/53	0.98	0.08	13,15,19,20	0
2	FAD	D	999	53/53	0.98	0.07	10,13,17,21	0
2	FAD	A	999	53/53	0.98	0.07	10,14,17,18	0
2	FAD	C	999	53/53	0.99	0.07	9,12,16,19	0

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

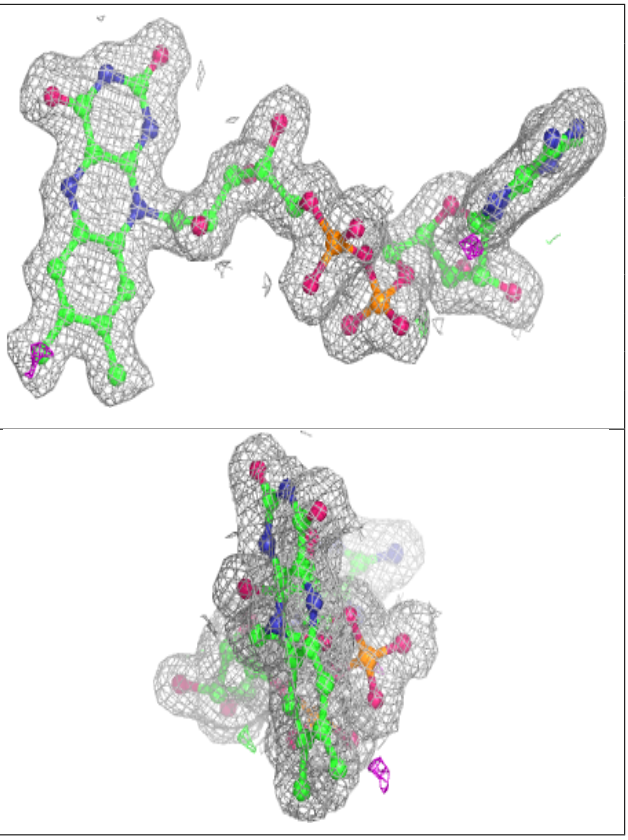
Electron density around FAD B 999:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



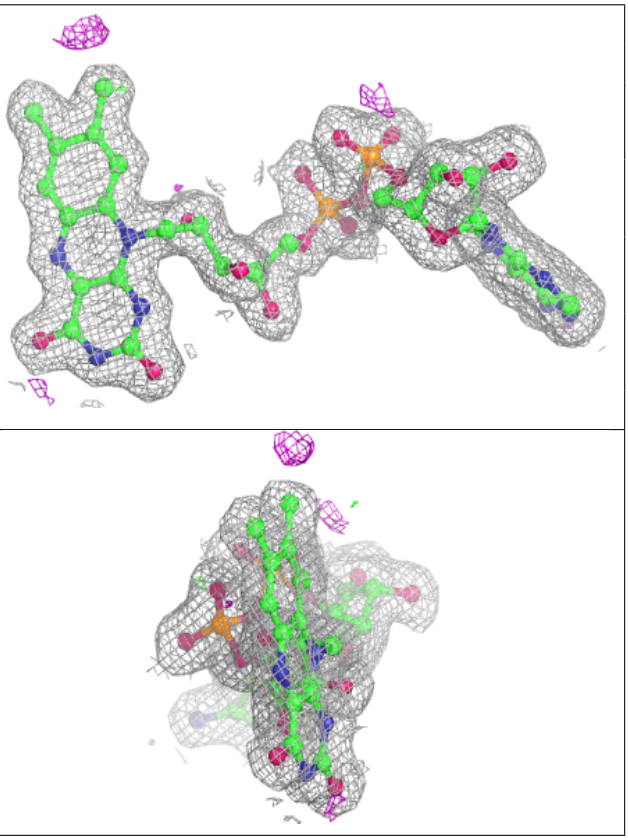
Electron density around FAD D 999:

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



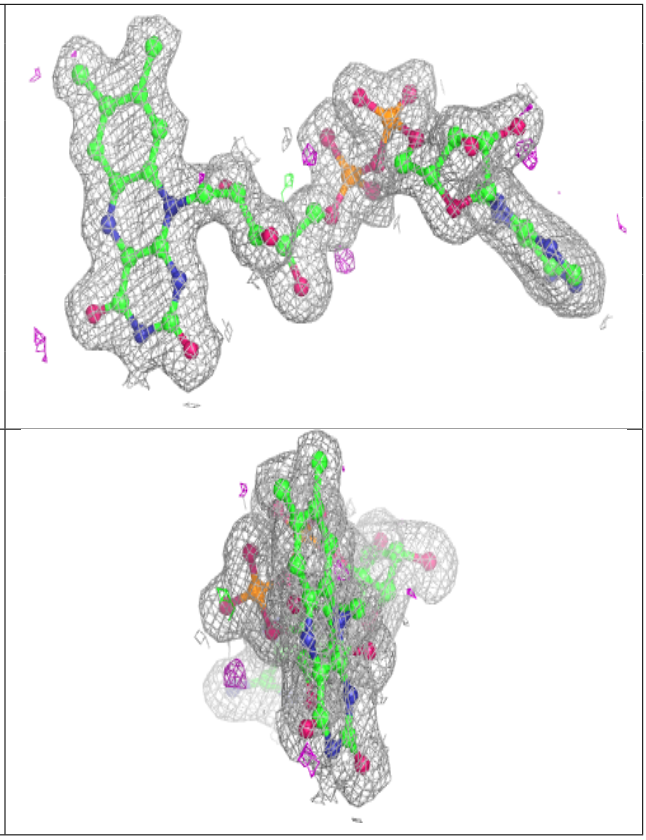
Electron density around FAD A 999:

$2mF_o$-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 999:

$2mF_o$-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.