wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 01:07 PM EDT

PDB ID	:	4E0V
Title	:	Structure of L-amino acid oxidase from the B. jararacussu venom
Authors	:	Ullah, A.; Souza, T.A.C.B.; Betzel, C.; Murakami, M.T.; Arni, R.K.
Deposited on	:	2012-03-05
Resolution	:	3.10 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:

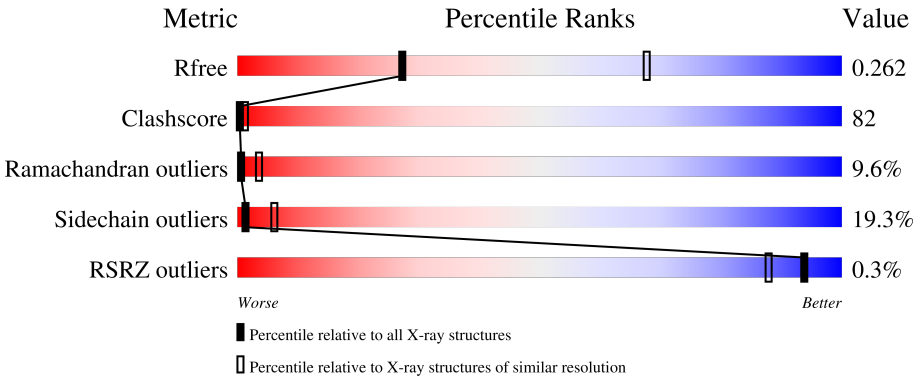
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	497	22% 53% 19% • 5%
1	B	497	21% 57% 16% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	501	-	-	X	-

2 Entry composition (i)

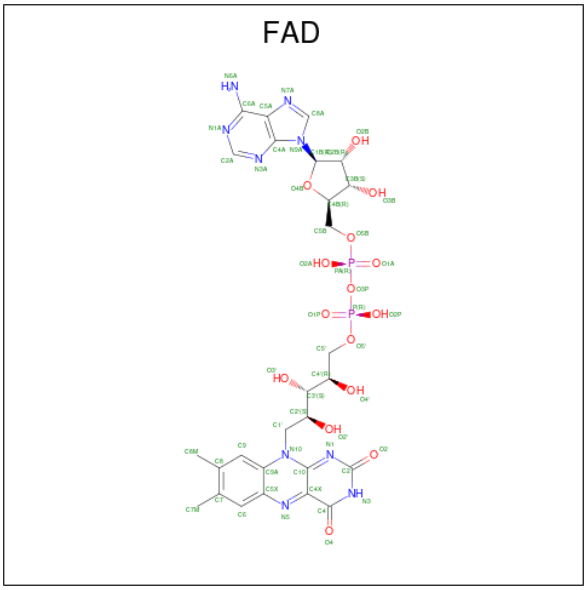
There are 3 unique types of molecules in this entry. The entry contains 7726 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3771	2398	637	722	14			
1	B	480	Total	C	N	O	S	0	0	0
			3833	2432	653	734	14			

- 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.

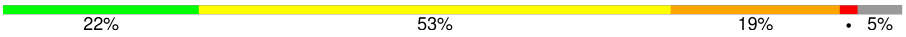
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	9	Total O 9 9	0	0

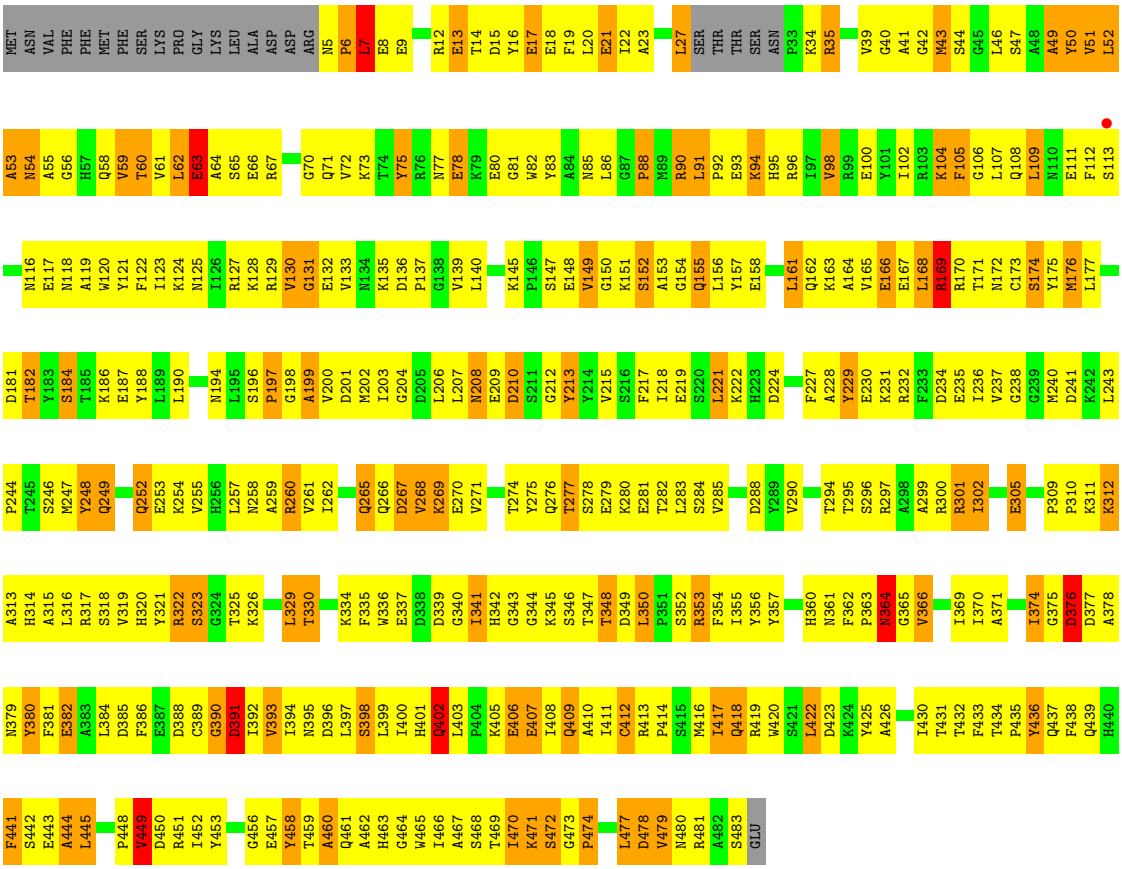
3 Residue-property plots (i)

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: L-amino-acid oxidase

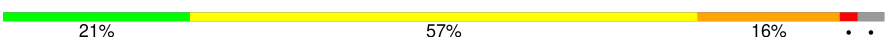
Chain A:

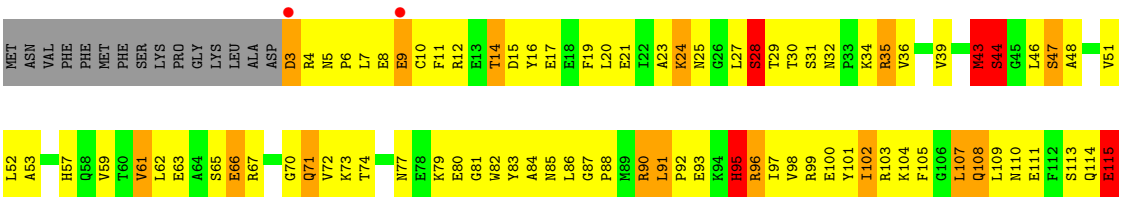


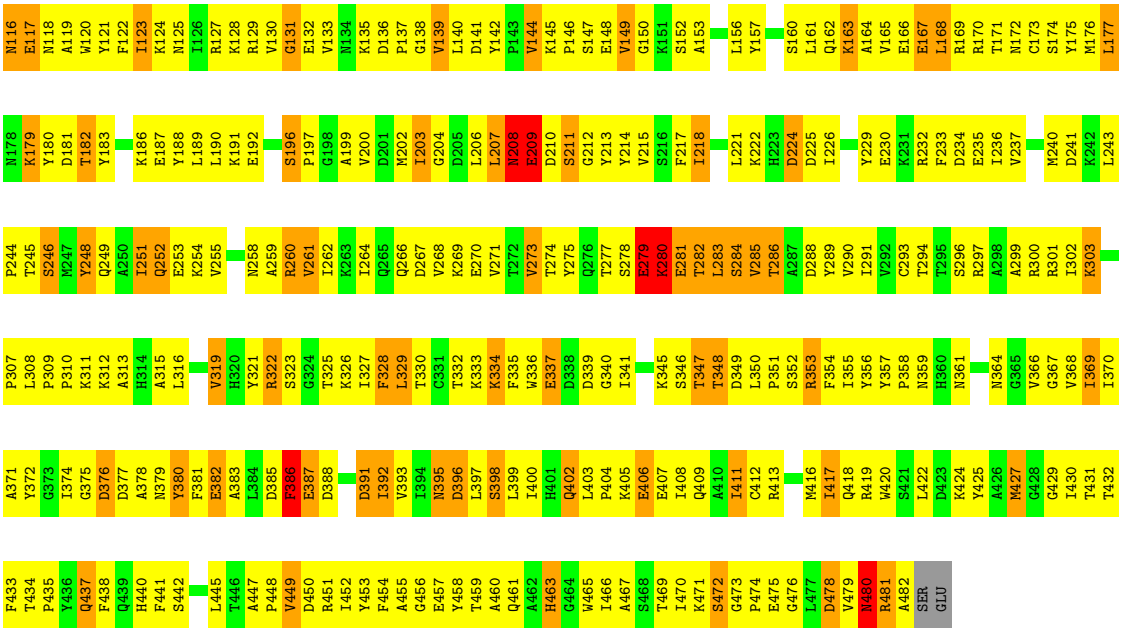


- Molecule 1: L-amino-acid oxidase

Chain B:






N116 E117 N118 A119 W120 Y121 F122 I123 K124 N125 I126 R127 K128 R129 V130 G131 E132 V133 N134 K135 D136 P137 G138 V139 L140 D141 Y142 P143 V144 K145 P146 S147 E148 V149 G150 K151 S152 A153 L156 Y157 S160 L161 Q162 K163 A164 V165 E166 E167 L168 R169 R170 T171 N172 C173 S174 Y175 M176 L177
N178 K179 Y180 D181 T182 Y183 K186 E187 Y188 L189 L190 K191 E192 S196 P197 G198 A199 V200 D201 M202 I203 G204 D205 L206 L207 N208 E209 D210 S211 G212 Y213 Y214 V215 S216 F217 I218 L221 K222 H223 D224 D225 I226 Y229 E230 K231 R232 F233 D234 E235 I236 V237 M240 D241 K242 L243
P244 T245 S246 M247 Y248 Q249 A250 I251 Q252 E253 K254 V255 N258 A259 R260 V261 I262 K263 I264 Q265 Q266 D267 V268 K269 E270 V271 T272 V273 T274 Y275 Q276 T277 S278 E279 K280 E281 T282 L283 S284 V285 T286 A287 D288 Y289 V290 I291 V292 C293 T294 T295 S296 R297 A298 A299 R300 R301 I302 K303
P307 L308 P309 P310 K311 K312 A313 H314 A315 L316 V319 H320 Y321 R322 S323 G324 T325 K326 I327 F328 L329 T330 C331 T332 K333 K334 F335 W336 E337 D338 D339 G340 I341 K345 S346 T347 T348 D349 L350 P351 S352 R353 F354 I355 Y356 Y357 P358 N359 H360 N361 N364 G365 V366 G367 V368 I369 I370
A371 Y372 G373 I374 G375 D376 D377 A378 N379 Y380 F381 E382 A383 L384 D385 F386 E387 D388 D391 I392 V393 I394 N395 D396 L397 S398 L399 I400 H401 Q402 L403 P404 K405 E406 E407 I408 Q409 A410 I411 C412 R413 M416 I417 Q418 R419 W420 S421 L422 D423 K424 Y425 A426 M427 G428 G429 I430 T431 T432
F433 T434 P435 Y436 Q437 F438 Q439 H440 F441 S442 L445 T446 A447 P448 V449 D450 R451 I452 Y453 F454 A455 G456 E457 Y458 T459 A460 Q461 A462 H463 G464 W465 I466 A467 S468 T469 I470 K471 S472 G473 P474 E475 G476 L477 D478 V479 N480 R481 A482 SER GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.39Å 72.19Å 101.53Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	29.02 – 3.10 28.79 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.02-3.10) 94.7 (28.79-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.181 , 0.259 0.188 , 0.262	Depositor DCC
R_{free} test set	852 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 73.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7726	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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

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	0.67	1/3856 (0.0%)	0.80	0/5218
1	B	0.61	0/3920	0.76	0/5305
All	All	0.64	1/7776 (0.0%)	0.78	0/10523

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	PRO	N-CD	11.01	1.63	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	LEU	Peptide
1	A	63	GLU	Peptide
1	B	449	VAL	Peptide

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	3771	0	3678	591	1
1	B	3833	0	3747	655	1
2	A	53	0	31	29	0
2	B	53	0	31	18	0
3	A	7	0	0	0	0
3	B	9	0	0	1	0
All	All	7726	0	7487	1242	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 82.

The worst 5 of 1242 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:15:ASP:HB3	1:A:19:PHE:CE2	1.54	1.42
1:B:315:ALA:O	1:B:319:VAL:HG23	1.24	1.35
1:A:92:PRO:HG2	1:A:95:HIS:ND1	1.39	1.34
1:B:473:GLY:HA2	1:B:475:GLU:OE1	1.18	1.30
1:A:269:LYS:HE3	1:A:269:LYS:C	1.56	1.26

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:O	1:B:387:GLU:OE2[2_545]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone

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	470/497 (95%)	326 (69%)	96 (20%)	48 (10%)	0 3
1	B	478/497 (96%)	357 (75%)	78 (16%)	43 (9%)	1 4
All	All	948/994 (95%)	683 (72%)	174 (18%)	91 (10%)	0 3

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	51	VAL
1	A	53	ALA
1	A	96	ARG
1	A	278	SER

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	403/427 (94%)	322 (80%)	81 (20%)	1 5
1	B	412/427 (96%)	336 (82%)	76 (18%)	1 7
All	All	815/854 (95%)	658 (81%)	157 (19%)	1 6

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	218	ILE
1	B	391	ASP
1	B	246	SER
1	B	286	THR
1	B	427	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	379	ASN
1	B	402	GLN
1	B	437	GLN
1	A	401	HIS
1	A	379	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)

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	501	-	54,58,58	1.34	7 (12%)	71,89,89	2.61	20 (28%)
2	FAD	B	501	-	54,58,58	1.22	6 (11%)	71,89,89	1.57	10 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	501	-	-	15/30/50/50	0/6/6/6
2	FAD	B	501	-	-	14/30/50/50	0/6/6/6

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C2A-N3A	4.10	1.38	1.32
2	A	501	FAD	PA-O3P	3.98	1.63	1.59
2	A	501	FAD	C4X-N5	3.51	1.38	1.30
2	A	501	FAD	C2A-N3A	3.18	1.37	1.32
2	B	501	FAD	C10-N1	2.98	1.39	1.33

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FAD	C4B-O4B-C1B	-13.92	97.18	109.92
2	A	501	FAD	N3A-C2A-N1A	-7.29	118.78	128.67
2	B	501	FAD	N3A-C2A-N1A	-6.49	119.87	128.67
2	A	501	FAD	O4B-C1B-N9A	5.41	115.91	108.75
2	A	501	FAD	C1B-N9A-C4A	-4.15	119.36	126.64

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O2A
2	A	501	FAD	C5B-O5B-PA-O3P
2	A	501	FAD	N10-C1'-C2'-O2'
2	A	501	FAD	N10-C1'-C2'-C3'
2	A	501	FAD	C2'-C3'-C4'-O4'

There are no ring outliers.

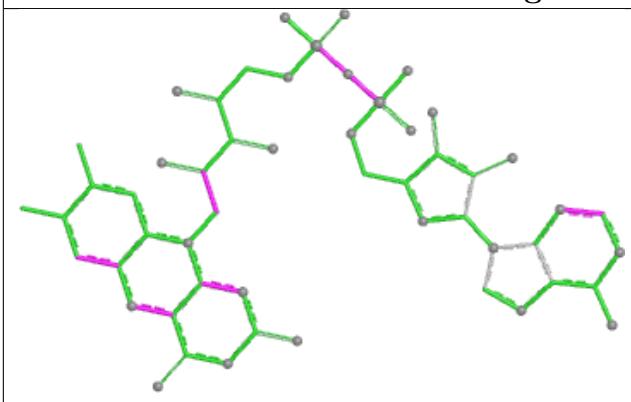
2 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	29	0
2	B	501	FAD	18	0

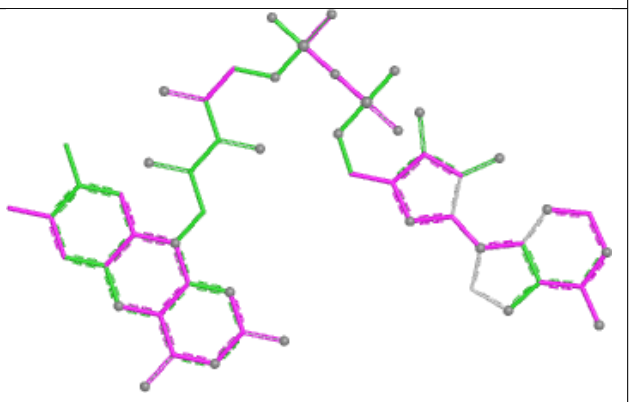
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

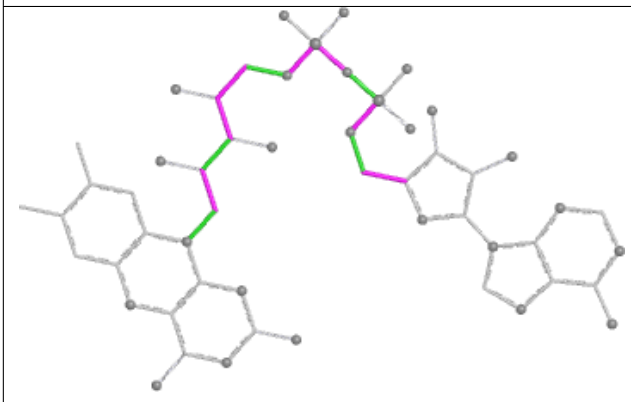
Ligand FAD A 501



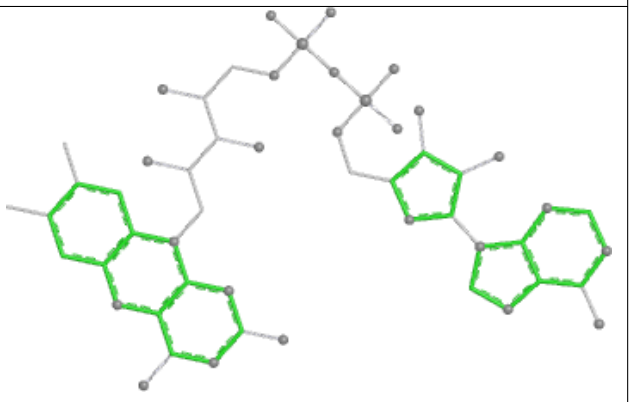
Bond lengths



Bond angles

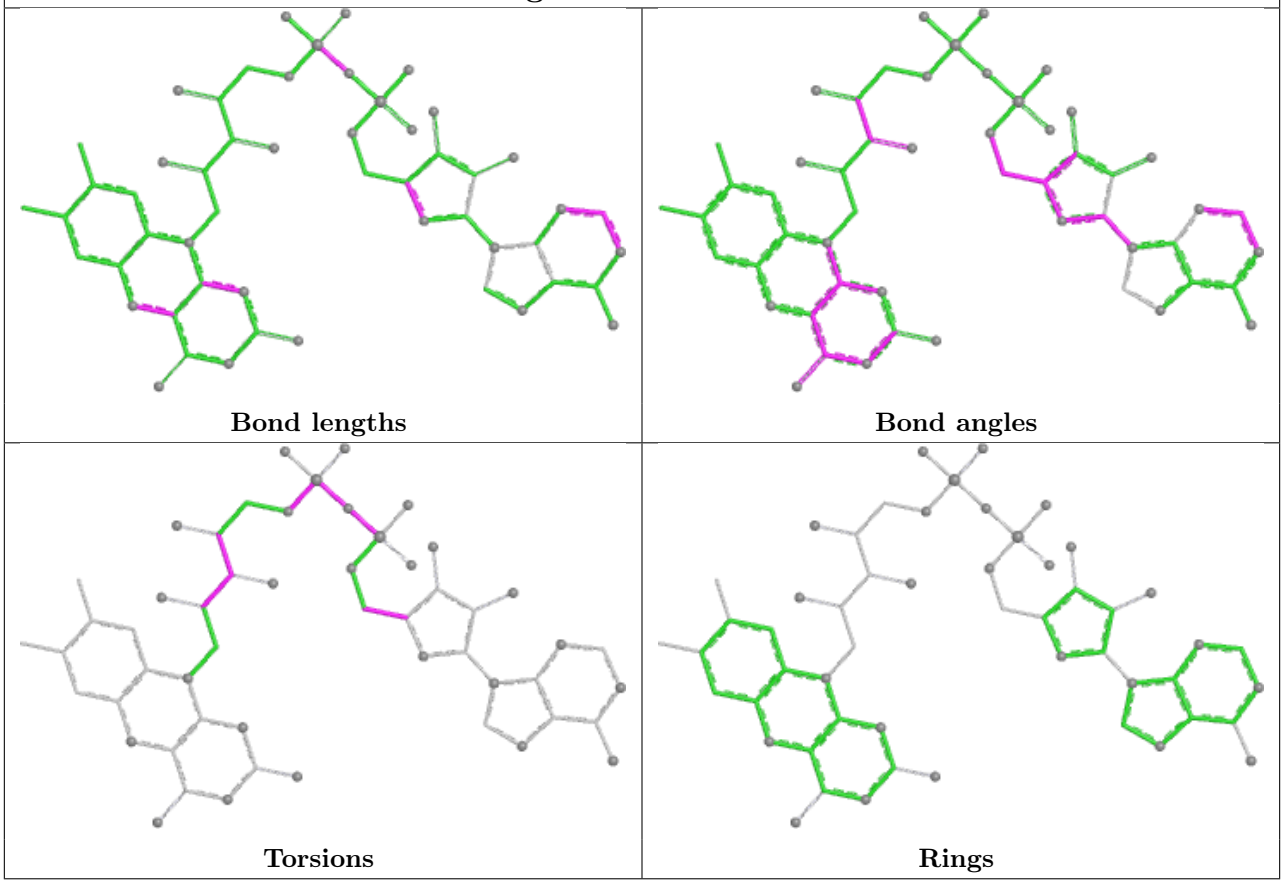


Torsions



Rings

Ligand FAD B 501



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	474/497 (95%)	-0.53	1 (0%)	95	90	18, 30, 44, 53	11 (2%)
1	B	480/497 (96%)	-0.49	2 (0%)	92	84	14, 31, 49, 63	16 (3%)
All	All	954/994 (95%)	-0.51	3 (0%)	94	88	14, 30, 45, 63	27 (2%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	SER	2.3
1	B	3	ASP	2.0
1	B	9	GLU	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

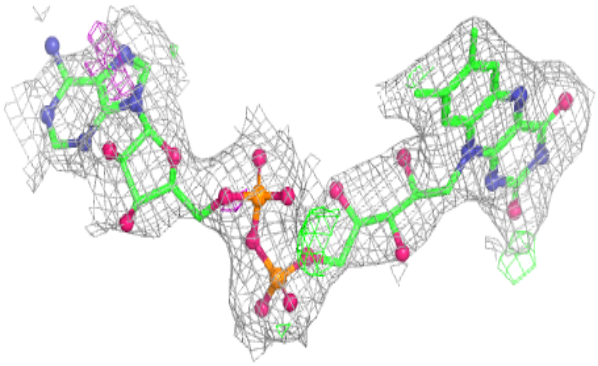
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

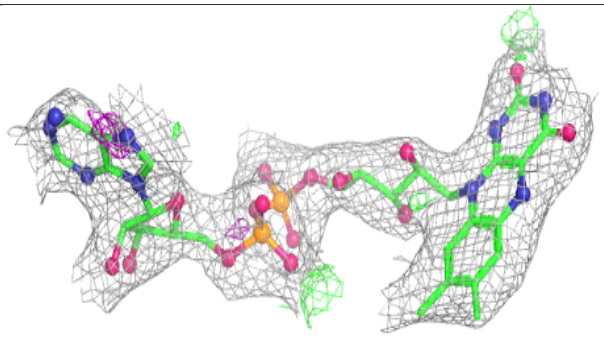
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	A	501	53/53	0.94	0.18	8,19,39,40	0
2	FAD	B	501	53/53	0.95	0.16	13,25,28,32	0

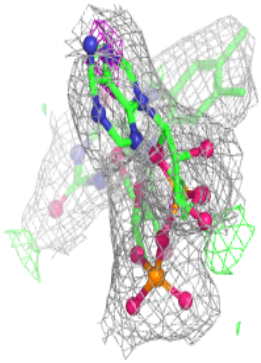
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 501:

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

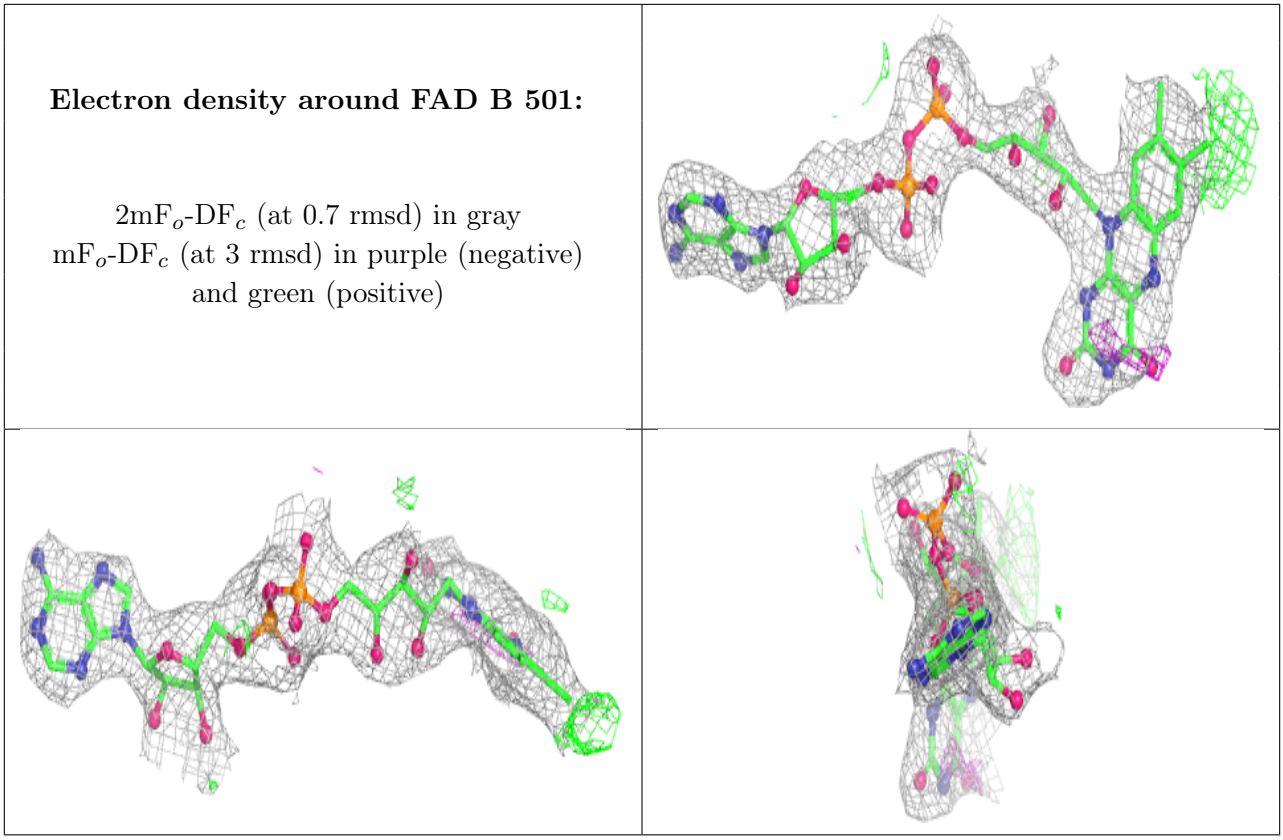






Electron density around FAD B 501:

$2mF_o$-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.