



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2020 – 06:10 PM JST

PDB ID : 7CT4  
Title : Crystal structure of D-amino acid oxidase from *Rasamsonia emersonii* strain YA  
Authors : Shimekake, Y.; Hirato, Y.; Okazaki, S.; Funabashi, R.; Goto, M.; Furuichi, T.; Suzuki, H.; Takahashi, S.  
Deposited on : 2020-08-18  
Resolution : 2.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

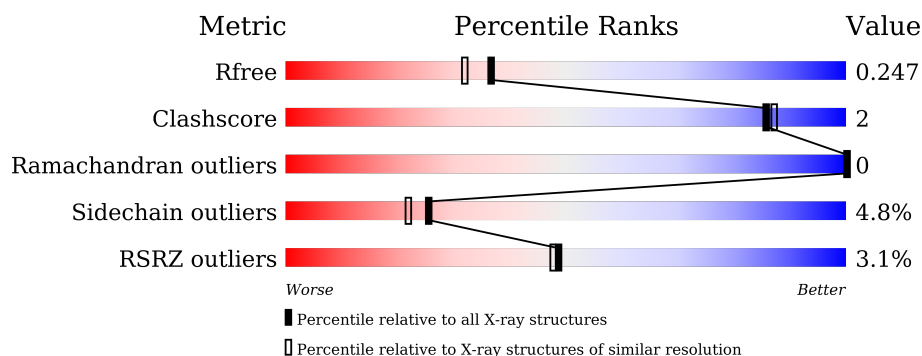
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	388	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>12%</div> </div> </div>
1	B	388	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>11%</div> </div> </div>
1	C	388	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>11%</div> </div> </div>
1	D	388	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>12%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10965 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 D-amino acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2569	1616	465	475	13			
1	B	346	Total	C	N	O	S	0	0	0
			2600	1631	465	491	13			
1	C	347	Total	C	N	O	S	0	1	0
			2623	1649	478	483	13			
1	D	342	Total	C	N	O	S	0	0	0
			2594	1630	468	483	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A499UB99
A	-18	GLY	-	expression tag	UNP A0A499UB99
A	-17	SER	-	expression tag	UNP A0A499UB99
A	-16	SER	-	expression tag	UNP A0A499UB99
A	-15	HIS	-	expression tag	UNP A0A499UB99
A	-14	HIS	-	expression tag	UNP A0A499UB99
A	-13	HIS	-	expression tag	UNP A0A499UB99
A	-12	HIS	-	expression tag	UNP A0A499UB99
A	-11	HIS	-	expression tag	UNP A0A499UB99
A	-10	HIS	-	expression tag	UNP A0A499UB99
A	-9	SER	-	expression tag	UNP A0A499UB99
A	-8	SER	-	expression tag	UNP A0A499UB99
A	-7	GLY	-	expression tag	UNP A0A499UB99
A	-6	LEU	-	expression tag	UNP A0A499UB99
A	-5	VAL	-	expression tag	UNP A0A499UB99
A	-4	PRO	-	expression tag	UNP A0A499UB99
A	-3	ARG	-	expression tag	UNP A0A499UB99
A	-2	GLY	-	expression tag	UNP A0A499UB99
A	-1	SER	-	expression tag	UNP A0A499UB99
A	0	HIS	-	expression tag	UNP A0A499UB99
B	-19	MET	-	initiating methionine	UNP A0A499UB99

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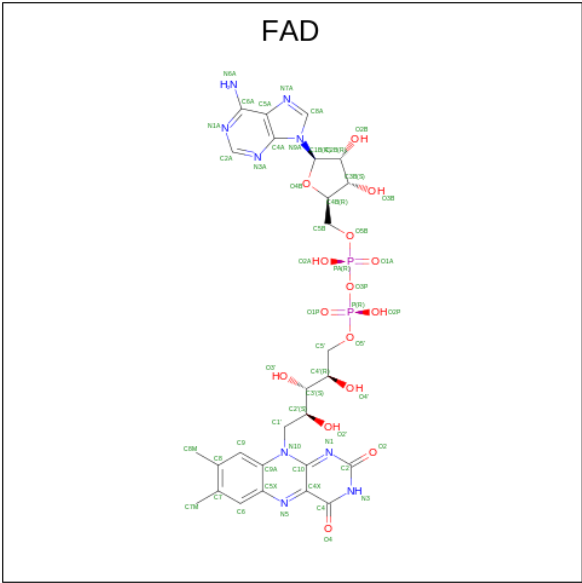
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A499UB99
B	-17	SER	-	expression tag	UNP A0A499UB99
B	-16	SER	-	expression tag	UNP A0A499UB99
B	-15	HIS	-	expression tag	UNP A0A499UB99
B	-14	HIS	-	expression tag	UNP A0A499UB99
B	-13	HIS	-	expression tag	UNP A0A499UB99
B	-12	HIS	-	expression tag	UNP A0A499UB99
B	-11	HIS	-	expression tag	UNP A0A499UB99
B	-10	HIS	-	expression tag	UNP A0A499UB99
B	-9	SER	-	expression tag	UNP A0A499UB99
B	-8	SER	-	expression tag	UNP A0A499UB99
B	-7	GLY	-	expression tag	UNP A0A499UB99
B	-6	LEU	-	expression tag	UNP A0A499UB99
B	-5	VAL	-	expression tag	UNP A0A499UB99
B	-4	PRO	-	expression tag	UNP A0A499UB99
B	-3	ARG	-	expression tag	UNP A0A499UB99
B	-2	GLY	-	expression tag	UNP A0A499UB99
B	-1	SER	-	expression tag	UNP A0A499UB99
B	0	HIS	-	expression tag	UNP A0A499UB99
C	-19	MET	-	initiating methionine	UNP A0A499UB99
C	-18	GLY	-	expression tag	UNP A0A499UB99
C	-17	SER	-	expression tag	UNP A0A499UB99
C	-16	SER	-	expression tag	UNP A0A499UB99
C	-15	HIS	-	expression tag	UNP A0A499UB99
C	-14	HIS	-	expression tag	UNP A0A499UB99
C	-13	HIS	-	expression tag	UNP A0A499UB99
C	-12	HIS	-	expression tag	UNP A0A499UB99
C	-11	HIS	-	expression tag	UNP A0A499UB99
C	-10	HIS	-	expression tag	UNP A0A499UB99
C	-9	SER	-	expression tag	UNP A0A499UB99
C	-8	SER	-	expression tag	UNP A0A499UB99
C	-7	GLY	-	expression tag	UNP A0A499UB99
C	-6	LEU	-	expression tag	UNP A0A499UB99
C	-5	VAL	-	expression tag	UNP A0A499UB99
C	-4	PRO	-	expression tag	UNP A0A499UB99
C	-3	ARG	-	expression tag	UNP A0A499UB99
C	-2	GLY	-	expression tag	UNP A0A499UB99
C	-1	SER	-	expression tag	UNP A0A499UB99
C	0	HIS	-	expression tag	UNP A0A499UB99
D	-19	MET	-	initiating methionine	UNP A0A499UB99
D	-18	GLY	-	expression tag	UNP A0A499UB99
D	-17	SER	-	expression tag	UNP A0A499UB99

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A499UB99
D	-15	HIS	-	expression tag	UNP A0A499UB99
D	-14	HIS	-	expression tag	UNP A0A499UB99
D	-13	HIS	-	expression tag	UNP A0A499UB99
D	-12	HIS	-	expression tag	UNP A0A499UB99
D	-11	HIS	-	expression tag	UNP A0A499UB99
D	-10	HIS	-	expression tag	UNP A0A499UB99
D	-9	SER	-	expression tag	UNP A0A499UB99
D	-8	SER	-	expression tag	UNP A0A499UB99
D	-7	GLY	-	expression tag	UNP A0A499UB99
D	-6	LEU	-	expression tag	UNP A0A499UB99
D	-5	VAL	-	expression tag	UNP A0A499UB99
D	-4	PRO	-	expression tag	UNP A0A499UB99
D	-3	ARG	-	expression tag	UNP A0A499UB99
D	-2	GLY	-	expression tag	UNP A0A499UB99
D	-1	SER	-	expression tag	UNP A0A499UB99
D	0	HIS	-	expression tag	UNP A0A499UB99

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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

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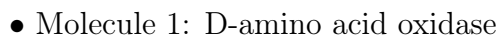
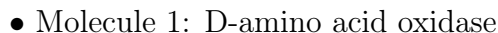
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

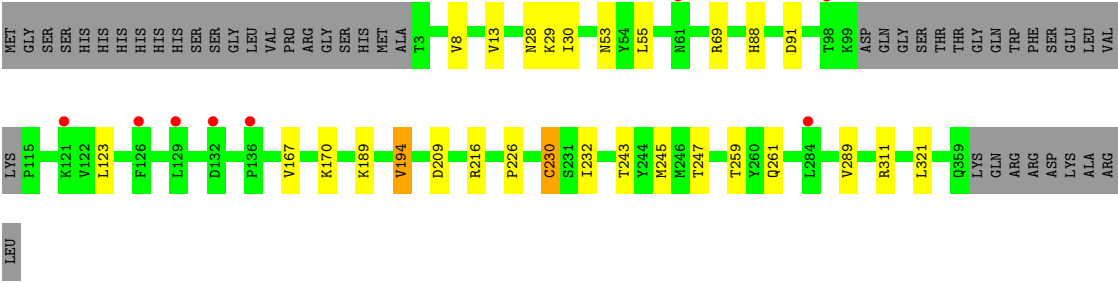
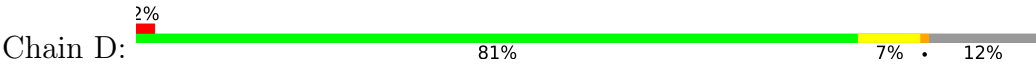
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		
3	B	84	Total	O	0	0
			84	84		
3	C	93	Total	O	0	0
			93	93		
3	D	99	Total	O	0	0
			99	99		



- Molecule 1: D-amino acid oxidase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.13Å 79.13Å 366.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.62 – 2.00 41.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.62-2.00) 100.0 (41.62-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	220.34 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.206 , 0.246 0.204 , 0.247	Depositor DCC
$R_{free}$ test set	4229 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10965	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: 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	0.42	0/2631	0.66	0/3590
1	B	0.44	0/2663	0.63	0/3637
1	C	0.43	0/2688	0.65	0/3666
1	D	0.43	0/2656	0.63	0/3620
All	All	0.43	0/10638	0.64	0/14513

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 [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	2569	0	2486	11	0
1	B	2600	0	2484	10	0
1	C	2623	0	2541	17	0
1	D	2594	0	2518	8	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	91	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	84	0	0	0	0
3	C	93	0	0	0	0
3	D	99	0	0	0	0
All	All	10965	0	10153	46	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 2.

All (46) 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:221:VAL:HG12	1:B:301:ILE:HD12	1.73	0.69
1:C:278:MET:HE2	1:C:298:LEU:HD12	1.75	0.68
1:D:230:CYS:SG	1:D:245:MET:HE2	2.33	0.68
1:B:211:THR:HB	1:B:312:GLU:HG2	1.78	0.66
1:A:88:HIS:HB2	1:A:249:ALA:HB2	1.77	0.64
1:A:221:VAL:HG12	1:A:301:ILE:HD12	1.82	0.60
1:C:67:TRP:HE1	1:C:347:THR:HG21	1.65	0.60
1:C:8:VAL:HG22	1:C:194:VAL:HG13	1.86	0.56
1:C:92:THR:HG23	1:C:229:MET:HB2	1.89	0.55
1:C:88:HIS:HE1	1:C:247:THR:O	1.90	0.55
1:D:209:ASP:OD2	1:D:311:ARG:NH1	2.38	0.54
1:B:217:GLY:HA2	1:B:259:THR:HG22	1.91	0.53
1:D:232:ILE:HG22	1:D:243:THR:HB	1.91	0.53
1:D:28:ASN:HB3	1:D:30:ILE:HD11	1.91	0.51
1:C:215:ALA:HB3	1:C:308:ARG:HB2	1.92	0.51
1:C:278:MET:HE1	1:C:300:ILE:HD11	1.93	0.51
1:C:98:THR:HA	1:C:139:ASP:HB2	1.93	0.51
1:D:30:ILE:HB	1:D:167:VAL:HG22	1.95	0.49
1:C:93:VAL:HG22	1:C:143:ARG:HE	1.78	0.49
1:A:155:LEU:HB2	1:A:156:PRO:HD3	1.94	0.48
1:C:131:LYS:HA	1:C:134:LEU:HD22	1.96	0.48
1:A:270:ASP:HB3	1:A:273:LEU:HD12	1.94	0.48
1:B:223:ARG:HB2	1:B:299:ASP:HB3	1.96	0.47
1:B:97:ARG:HA	1:B:138:ILE:HA	1.98	0.46
1:C:311:ARG:CZ	1:C:316:ARG:HB2	2.45	0.46
1:B:87:ILE:HG23	1:B:147:VAL:HG13	1.99	0.45
1:A:232:ILE:HG22	1:A:243:THR:HB	1.98	0.45
1:B:155:LEU:HB2	1:B:156:PRO:HD3	1.98	0.44
1:A:176:HIS:HD2	1:A:178:ALA:H	1.65	0.44
1:C:92:THR:O	1:C:143:ARG:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ARG:HB3	1:D:261:GLN:HB2	1.99	0.44
1:C:221:VAL:HG12	1:C:301:ILE:HD12	2.00	0.43
1:D:8:VAL:HG22	1:D:194:VAL:HG13	2.00	0.43
1:C:278:MET:HE2	1:C:298:LEU:CD1	2.46	0.43
1:C:67:TRP:HE1	1:C:347:THR:CG2	2.32	0.43
1:B:134:LEU:HA	1:B:135:PRO:HD3	1.91	0.43
1:B:43:ILE:HG13	1:B:43:ILE:H	1.70	0.42
1:A:29:LYS:HD2	1:A:184:HIS:HE1	1.84	0.42
1:B:33:ALA:HA	1:B:170:LYS:O	2.20	0.42
1:A:134:LEU:HA	1:A:135:PRO:HD3	1.94	0.41
1:A:244:TYR:CZ	1:A:257:GLY:HA3	2.55	0.41
1:C:9:LEU:HD22	1:C:180:ALA:HB2	2.01	0.41
1:C:114:LYS:HA	1:C:115:PRO:HD3	1.96	0.41
1:A:279:LYS:HB2	1:A:295:ILE:HD11	2.03	0.41
1:A:79:ALA:HB2	1:A:87:ILE:HG22	2.02	0.41
1:D:226:PRO:HD2	1:D:247:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

## 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	337/388 (87%)	328 (97%)	9 (3%)	0	100	100
1	B	342/388 (88%)	328 (96%)	14 (4%)	0	100	100
1	C	344/388 (89%)	336 (98%)	8 (2%)	0	100	100
1	D	338/388 (87%)	334 (99%)	4 (1%)	0	100	100
All	All	1361/1552 (88%)	1326 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	267/318 (84%)	255 (96%)	12 (4%)	27	24
1	B	270/318 (85%)	254 (94%)	16 (6%)	19	15
1	C	271/318 (85%)	262 (97%)	9 (3%)	38	37
1	D	272/318 (86%)	257 (94%)	15 (6%)	21	17
All	All	1080/1272 (85%)	1028 (95%)	52 (5%)	25	22

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	53	ASN
1	A	123	LEU
1	A	127	ARG
1	A	147	VAL
1	A	177	VAL
1	A	201	SER
1	A	210	ASN
1	A	213	LEU
1	A	224	ASN
1	A	313	ASP
1	A	356	LEU
1	B	3	THR
1	B	13	VAL
1	B	53	ASN
1	B	75	LEU
1	B	80	GLN
1	B	88	HIS
1	B	97	ARG
1	B	123	LEU
1	B	147	VAL
1	B	177	VAL
1	B	210	ASN
1	B	213	LEU

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Mol	Chain	Res	Type
1	B	259	THR
1	B	268	LEU
1	B	354	GLU
1	B	356	LEU
1	C	53	ASN
1	C	88	HIS
1	C	123	LEU
1	C	134	LEU
1	C	142	ASN
1	C	194	VAL
1	C	228	LEU
1	C	259	THR
1	C	360	LYS
1	D	13	VAL
1	D	29	LYS
1	D	53	ASN
1	D	55	LEU
1	D	69	ARG
1	D	88	HIS
1	D	91	ASP
1	D	123	LEU
1	D	170	LYS
1	D	189	LYS
1	D	194	VAL
1	D	230	CYS
1	D	259	THR
1	D	289	VAL
1	D	321	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	176	HIS
1	A	195	ASN
1	B	53	ASN
1	B	88	HIS
1	B	195	ASN
1	B	210	ASN
1	B	333	HIS
1	C	53	ASN
1	C	88	HIS

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Mol	Chain	Res	Type
1	C	303	HIS
1	C	359	GLN
1	D	53	ASN
1	D	303	HIS

### 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](#)

4 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	-	51,58,58	1.73	7 (13%)	60,89,89	1.81	12 (20%)
2	FAD	D	501	-	51,58,58	1.86	9 (17%)	60,89,89	1.86	10 (16%)
2	FAD	B	501	-	51,58,58	1.83	9 (17%)	60,89,89	1.78	11 (18%)
2	FAD	C	501	-	51,58,58	1.75	9 (17%)	60,89,89	1.85	11 (18%)

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	-	-	1/30/50/50	0/6/6/6
2	FAD	D	501	-	-	1/30/50/50	0/6/6/6
2	FAD	B	501	-	-	1/30/50/50	0/6/6/6
2	FAD	C	501	-	-	1/30/50/50	0/6/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C10-N1	7.08	1.42	1.33
2	B	501	FAD	C10-N1	6.42	1.41	1.33
2	A	501	FAD	C10-N1	6.33	1.41	1.33
2	C	501	FAD	C10-N1	5.98	1.40	1.33
2	D	501	FAD	C2A-N3A	5.36	1.40	1.32
2	A	501	FAD	C2A-N3A	5.30	1.40	1.32
2	B	501	FAD	C2A-N3A	5.25	1.40	1.32
2	C	501	FAD	C2A-N3A	5.24	1.40	1.32
2	B	501	FAD	C4-N3	5.14	1.42	1.33
2	D	501	FAD	C4-N3	4.67	1.41	1.33
2	A	501	FAD	C4-N3	4.32	1.40	1.33
2	C	501	FAD	C4-N3	4.28	1.40	1.33
2	C	501	FAD	O4B-C1B	3.78	1.46	1.41
2	B	501	FAD	C2A-N1A	3.76	1.40	1.33
2	D	501	FAD	C2A-N1A	3.61	1.40	1.33
2	A	501	FAD	C2A-N1A	3.49	1.40	1.33
2	C	501	FAD	C2A-N1A	3.47	1.40	1.33
2	D	501	FAD	O4B-C1B	3.45	1.45	1.41
2	D	501	FAD	C1'-N10	2.91	1.51	1.48
2	B	501	FAD	O4B-C1B	2.71	1.44	1.41
2	C	501	FAD	C1'-N10	2.51	1.50	1.48
2	B	501	FAD	C2B-C1B	-2.43	1.50	1.53
2	C	501	FAD	C4X-C10	2.39	1.41	1.38
2	D	501	FAD	C4X-C10	2.33	1.41	1.38
2	A	501	FAD	C5A-C4A	-2.31	1.34	1.40
2	C	501	FAD	C6A-C5A	-2.24	1.35	1.43
2	B	501	FAD	C5A-C4A	-2.22	1.35	1.40
2	B	501	FAD	C4X-N5	2.22	1.36	1.33
2	A	501	FAD	C6A-C5A	-2.21	1.35	1.43
2	B	501	FAD	C6A-C5A	-2.14	1.35	1.43
2	D	501	FAD	C6A-C5A	-2.11	1.35	1.43
2	A	501	FAD	C4X-C10	2.05	1.40	1.38
2	D	501	FAD	C5A-C4A	-2.05	1.35	1.40
2	C	501	FAD	C5A-C4A	-2.04	1.35	1.40



All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FAD	N3A-C2A-N1A	-7.19	117.44	128.68
2	D	501	FAD	C4-N3-C2	6.96	121.02	115.14
2	D	501	FAD	N3A-C2A-N1A	-6.85	117.97	128.68
2	B	501	FAD	N3A-C2A-N1A	-6.84	117.98	128.68
2	A	501	FAD	N3A-C2A-N1A	-6.77	118.09	128.68
2	C	501	FAD	C4-N3-C2	6.60	120.72	115.14
2	A	501	FAD	C4-N3-C2	6.17	120.36	115.14
2	B	501	FAD	C4-N3-C2	5.32	119.63	115.14
2	B	501	FAD	P-O3P-PA	-4.16	118.56	132.83
2	A	501	FAD	C4X-N5-C5X	3.91	120.67	116.77
2	A	501	FAD	P-O3P-PA	-3.89	119.49	132.83
2	C	501	FAD	C1'-N10-C9A	3.83	121.31	118.29
2	D	501	FAD	C4X-N5-C5X	3.80	120.56	116.77
2	C	501	FAD	C4X-N5-C5X	3.66	120.43	116.77
2	B	501	FAD	C4X-N5-C5X	3.66	120.43	116.77
2	D	501	FAD	P-O3P-PA	-3.59	120.52	132.83
2	D	501	FAD	C1'-N10-C9A	3.47	121.02	118.29
2	C	501	FAD	C10-C4X-N5	-3.42	118.89	121.26
2	B	501	FAD	C10-C4X-N5	-3.26	119.00	121.26
2	C	501	FAD	P-O3P-PA	-3.26	121.64	132.83
2	D	501	FAD	C5X-C9A-N10	3.18	120.02	117.72
2	A	501	FAD	C10-C4X-N5	-3.12	119.10	121.26
2	B	501	FAD	C1'-N10-C9A	3.11	120.74	118.29
2	C	501	FAD	C4X-C4-N3	-2.91	119.45	123.43
2	A	501	FAD	C1'-N10-C9A	2.89	120.57	118.29
2	A	501	FAD	C5X-C9A-N10	2.75	119.71	117.72
2	D	501	FAD	C4X-C4-N3	-2.72	119.72	123.43
2	B	501	FAD	C5X-C9A-N10	2.69	119.66	117.72
2	A	501	FAD	O4B-C1B-C2B	-2.67	103.02	106.93
2	D	501	FAD	O4B-C1B-C2B	-2.61	103.11	106.93
2	A	501	FAD	C4-C4X-N5	2.56	121.52	118.60
2	B	501	FAD	C4-C4X-N5	2.53	121.49	118.60
2	D	501	FAD	C10-C4X-N5	-2.44	119.57	121.26
2	B	501	FAD	C4X-C4-N3	-2.41	120.14	123.43
2	A	501	FAD	C4X-C4-N3	-2.29	120.30	123.43
2	B	501	FAD	C4'-C3'-C2'	-2.24	108.69	113.36
2	C	501	FAD	C5X-C9A-N10	2.23	119.33	117.72
2	C	501	FAD	C4-C4X-N5	2.21	121.12	118.60
2	D	501	FAD	C4A-C5A-N7A	-2.19	107.12	109.40
2	B	501	FAD	C4A-C5A-N7A	-2.17	107.14	109.40
2	A	501	FAD	C5A-C6A-N6A	-2.08	117.19	120.35
2	A	501	FAD	C4A-C5A-N7A	-2.06	107.25	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FAD	C1B-N9A-C4A	-2.05	123.05	126.64
2	C	501	FAD	C4A-C5A-N7A	-2.00	107.31	109.40

There are no chirality outliers.

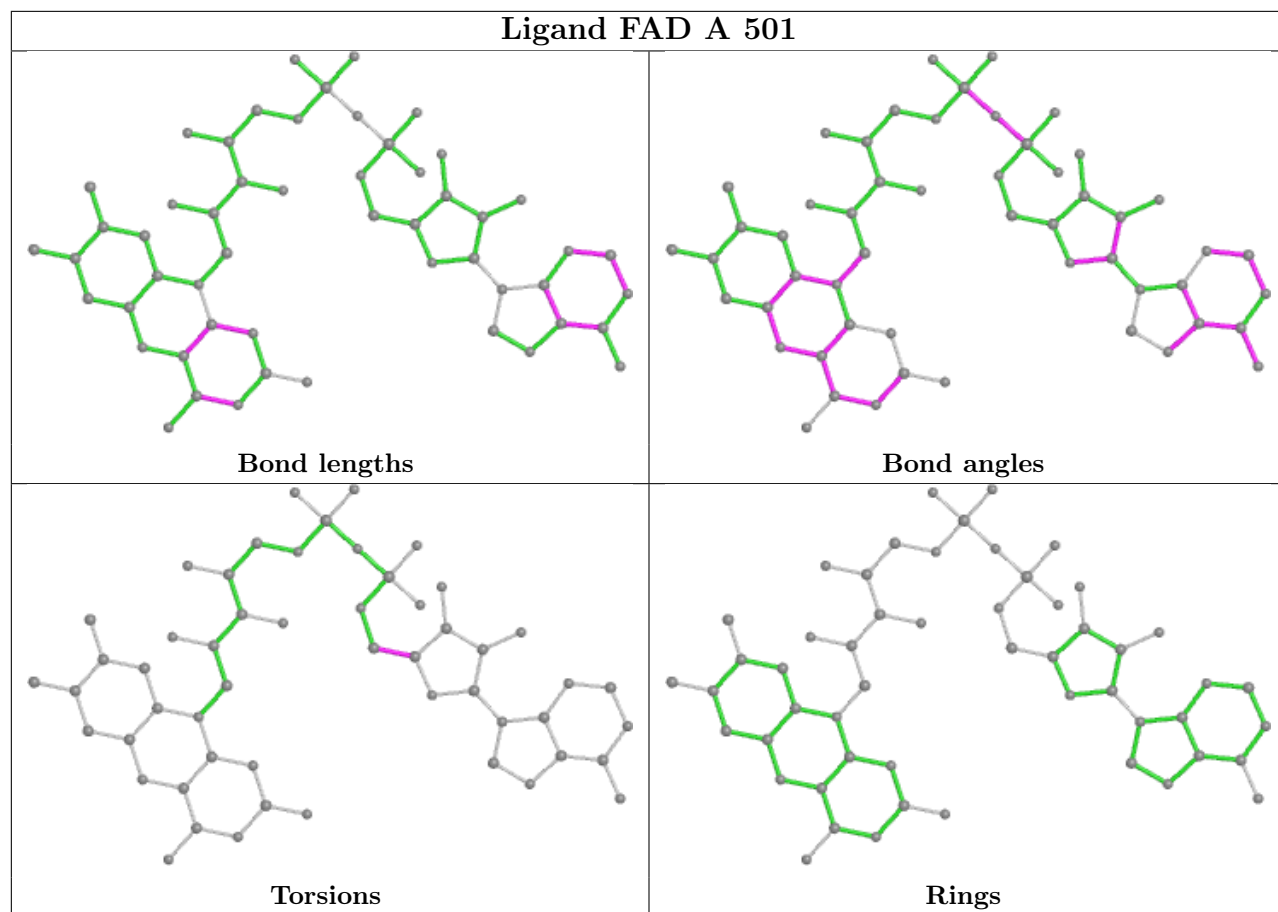
All (4) torsion outliers are listed below:

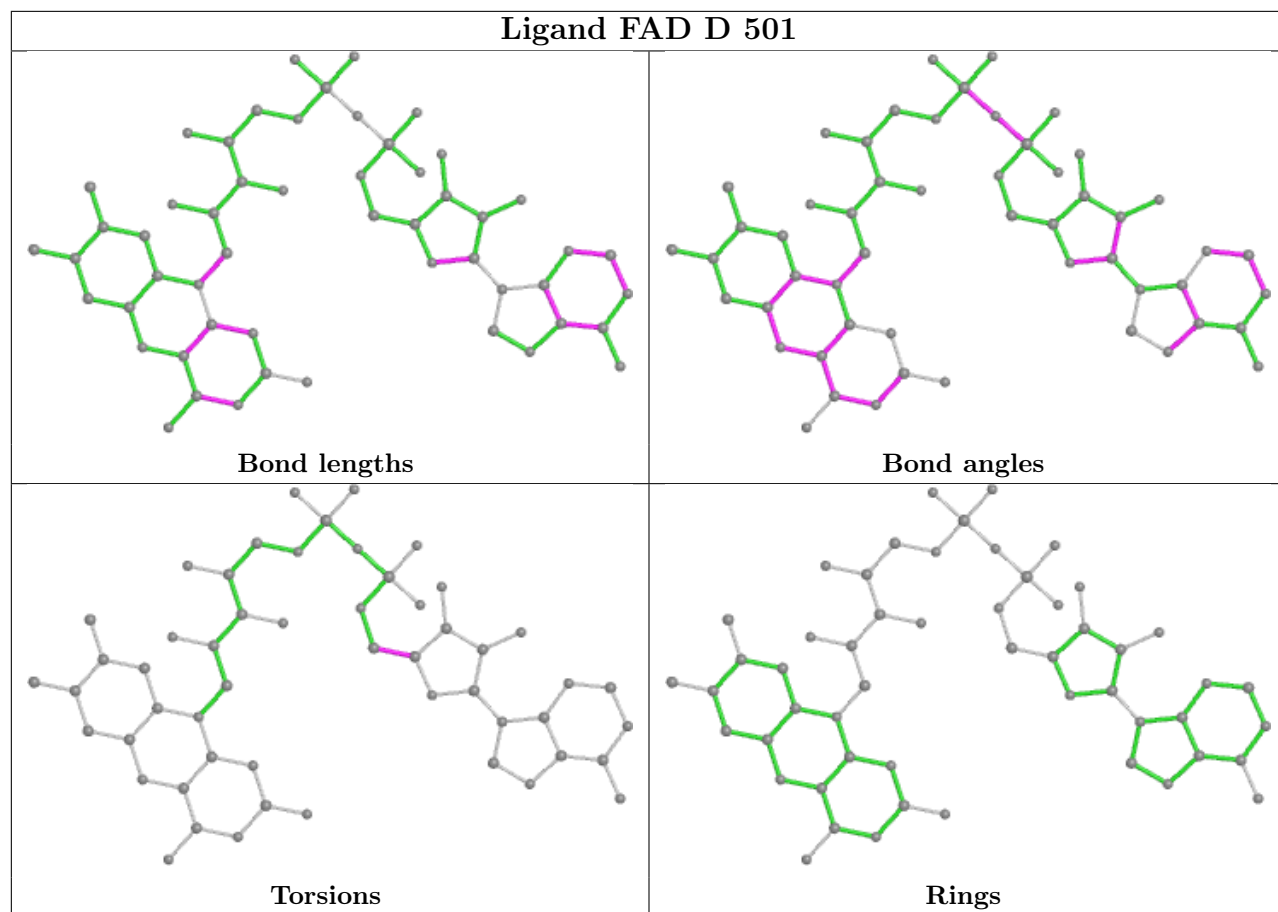
Mol	Chain	Res	Type	Atoms
2	A	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	O4B-C4B-C5B-O5B
2	C	501	FAD	O4B-C4B-C5B-O5B

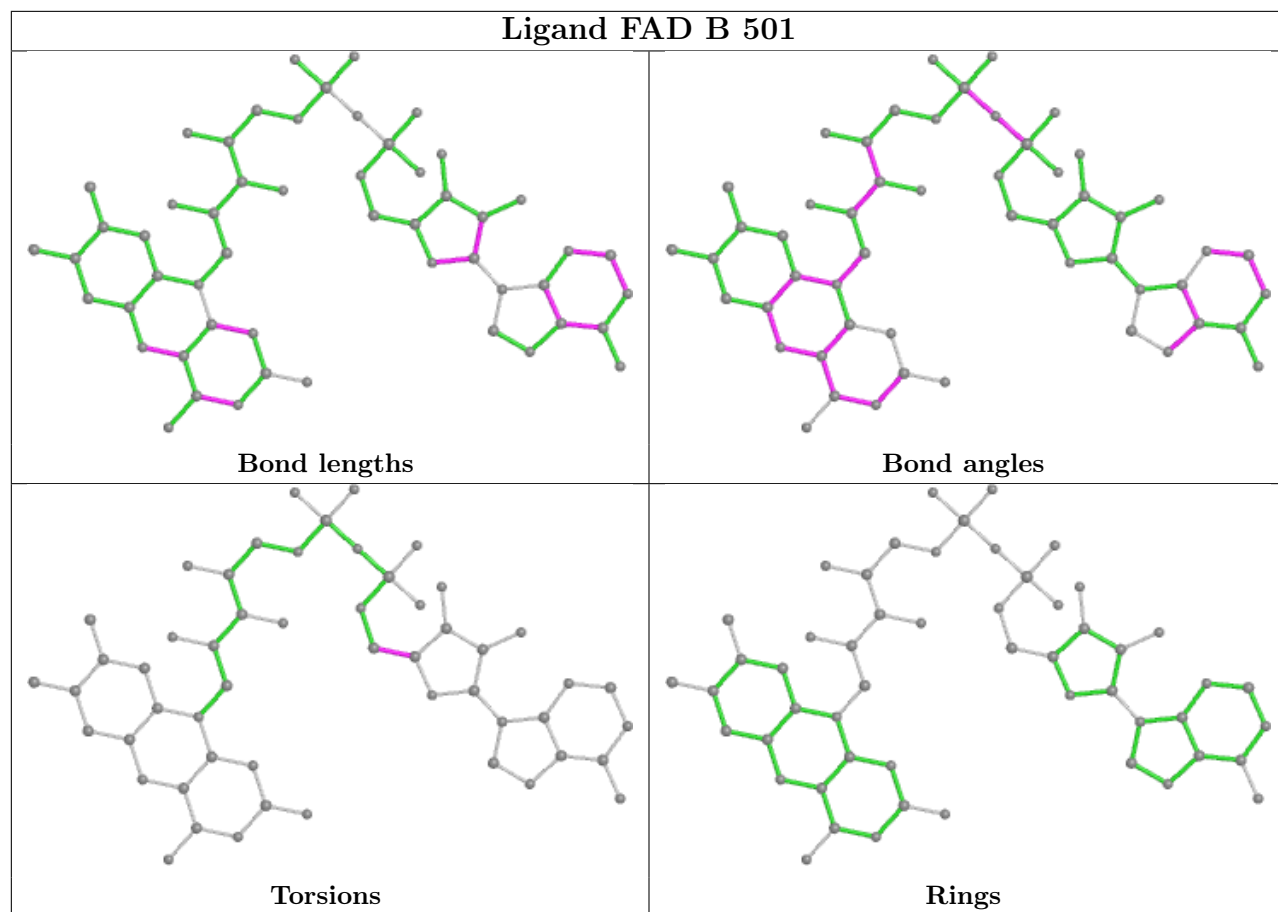
There are no ring outliers.

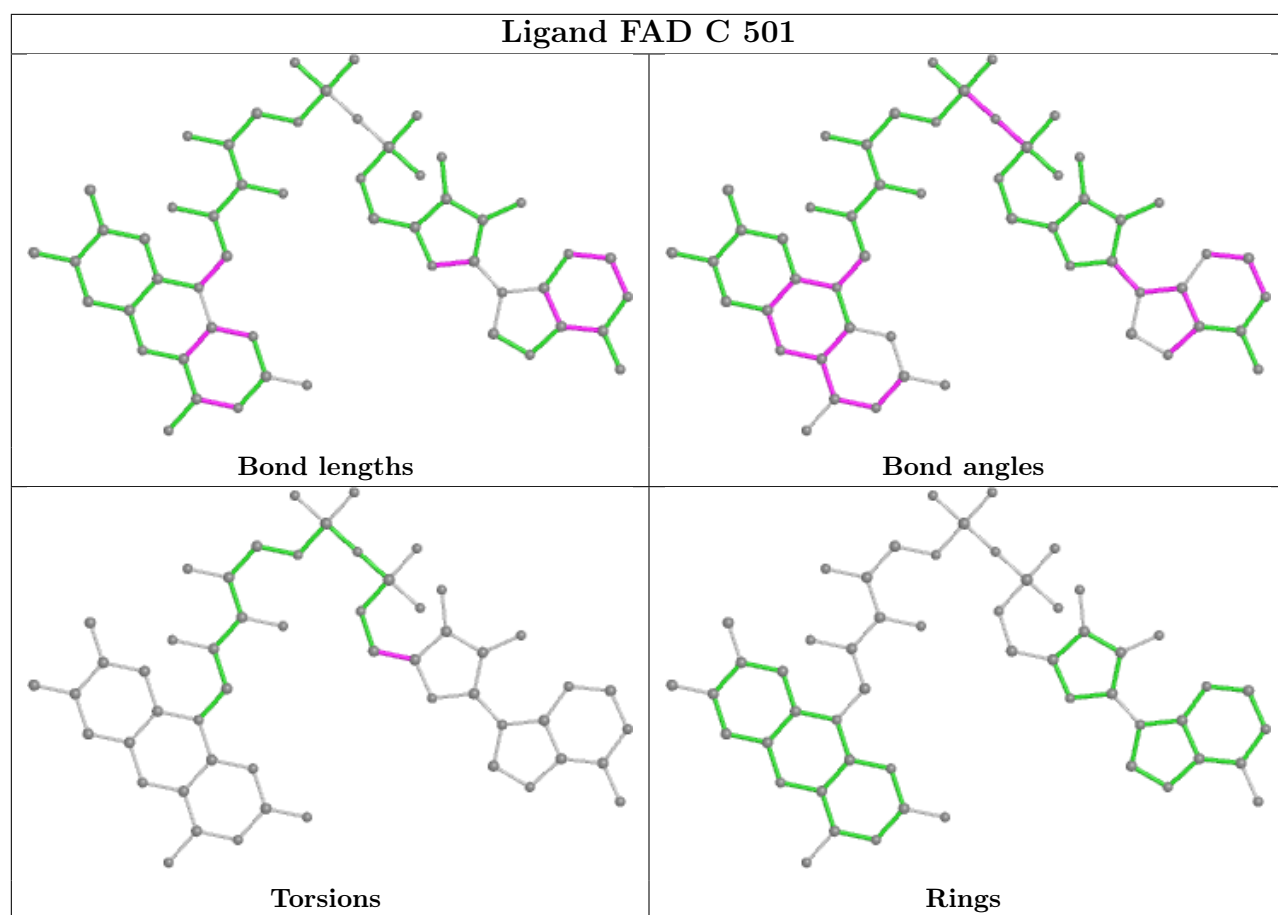
No monomer is involved in short contacts.

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 than 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.









## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	341/388 (87%)	0.11	6 (1%) 68 66	30, 41, 60, 82	0
1	B	346/388 (89%)	0.25	16 (4%) 32 31	31, 41, 67, 82	0
1	C	347/388 (89%)	0.17	13 (3%) 41 41	29, 39, 62, 78	0
1	D	342/388 (88%)	0.18	8 (2%) 60 59	31, 40, 59, 83	0
All	All	1376/1552 (88%)	0.18	43 (3%) 49 48	29, 40, 62, 83	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	THR	5.8
1	B	-1	SER	5.1
1	B	292	GLY	4.4
1	B	98	THR	4.1
1	B	130	SER	3.9
1	B	239	ASP	3.9
1	D	132	ASP	3.9
1	B	129	LEU	3.8
1	D	121	LYS	3.5
1	C	136	PRO	3.5
1	B	290	ALA	3.5
1	C	321	LEU	3.3
1	C	236	ASP	3.2
1	A	239	ASP	3.2
1	C	135	PRO	3.1
1	B	140	ASN	3.1
1	C	115	PRO	2.9
1	B	132	ASP	2.9
1	C	134	LEU	2.9
1	A	98	THR	2.9
1	D	98	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	126	PHE	2.8
1	C	139	ASP	2.7
1	B	139	ASP	2.5
1	C	232	ILE	2.5
1	C	292	GLY	2.5
1	D	284	LEU	2.4
1	C	291	PRO	2.4
1	B	236	ASP	2.4
1	A	126	PHE	2.4
1	B	100	ASP	2.4
1	C	61	ASN	2.3
1	A	61	ASN	2.3
1	B	135	PRO	2.3
1	B	291	PRO	2.2
1	A	115	PRO	2.2
1	D	129	LEU	2.2
1	A	323	ASP	2.1
1	D	136	PRO	2.1
1	B	282	ILE	2.0
1	D	61	ASN	2.0
1	C	326	TRP	2.0
1	B	356	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	FAD	D	501	53/53	0.95	0.11	29,34,36,36	0

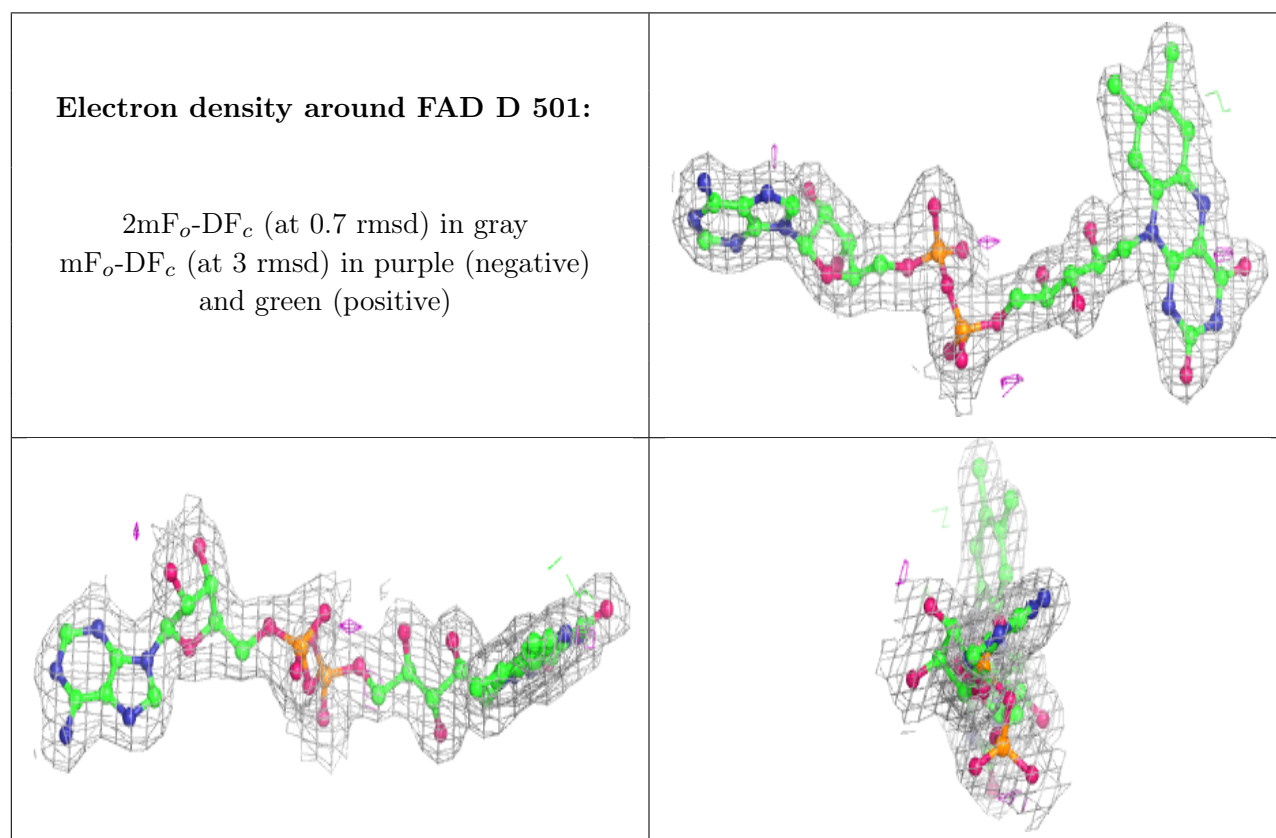
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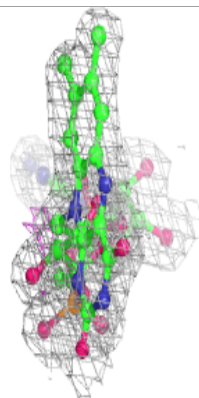
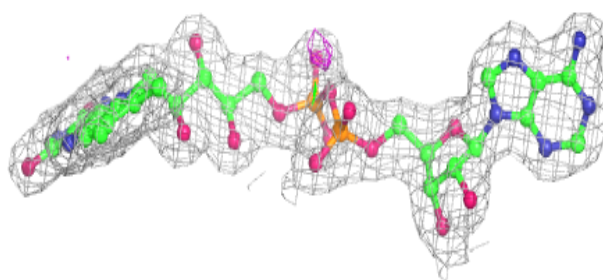
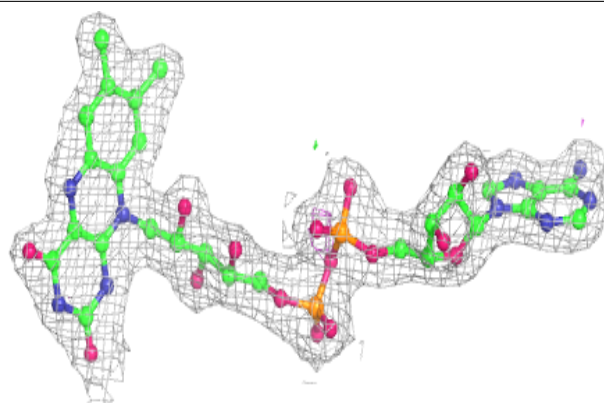
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	B	501	53/53	0.95	0.12	31,35,38,40	0
2	FAD	C	501	53/53	0.95	0.12	29,33,36,37	0
2	FAD	A	501	53/53	0.96	0.10	34,37,39,40	0

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.

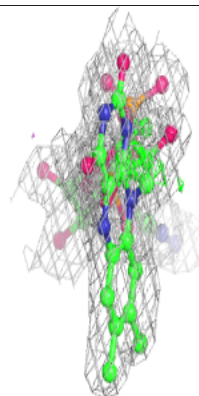
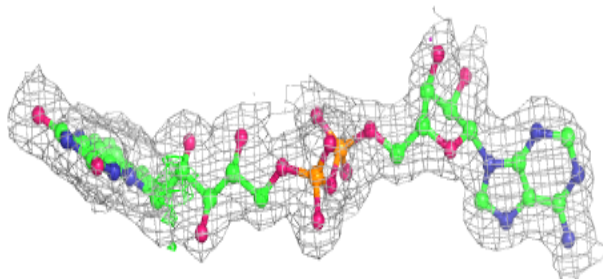
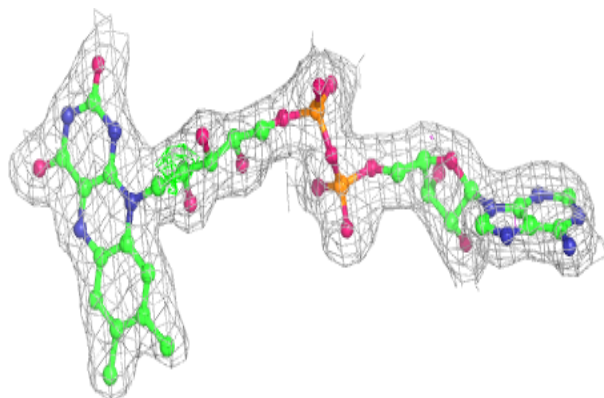


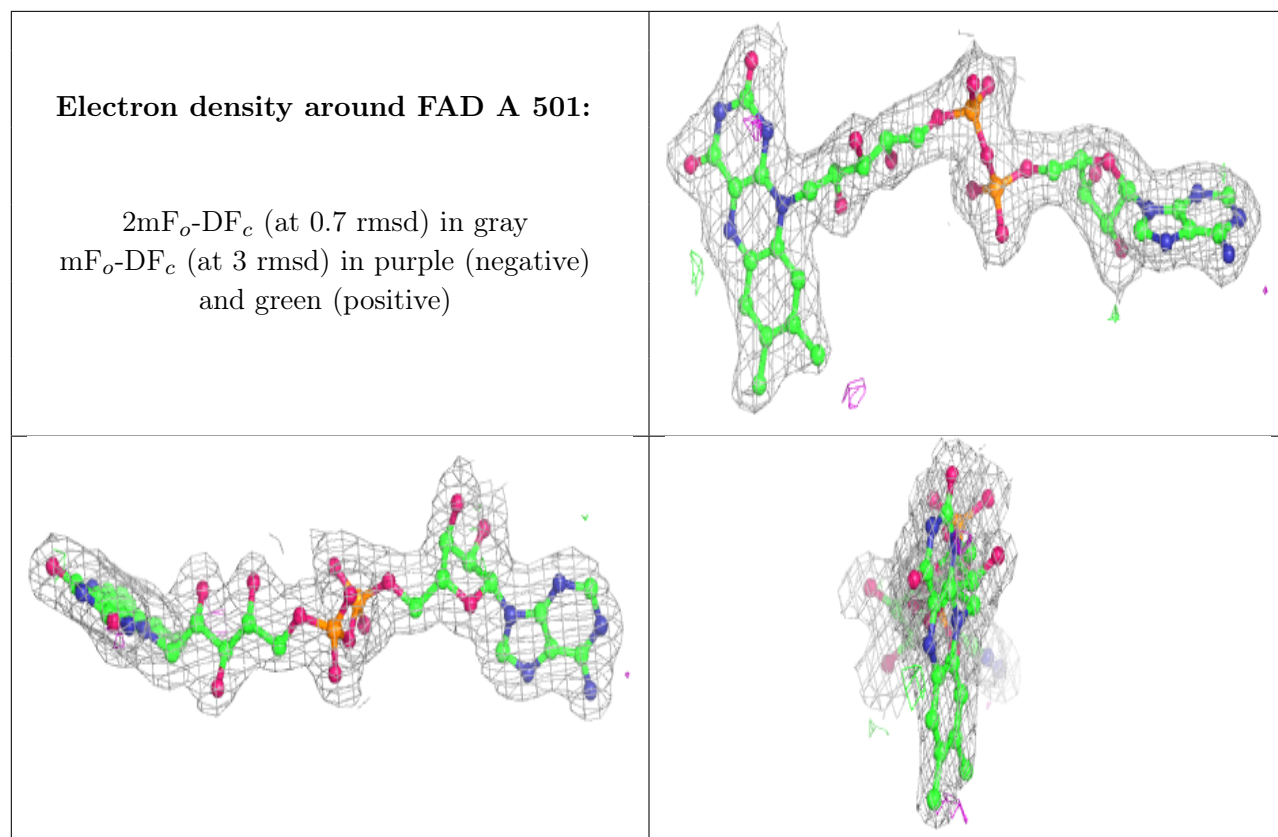
**Electron density around FAD B 501:**

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

**Electron density around FAD C 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.