



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 10:11 AM EDT

PDB ID : 5VQB  
Title : Crystal structure of rifampin monoxygenase from *Streptomyces venezuelae*, complex with FAD  
Authors : Cox, G.; Kelso, J.; Stogios, P.J.; Savchenko, A.; Anderson, W.F.; Wright, G.D.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2017-05-08  
Resolution : 3.39 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

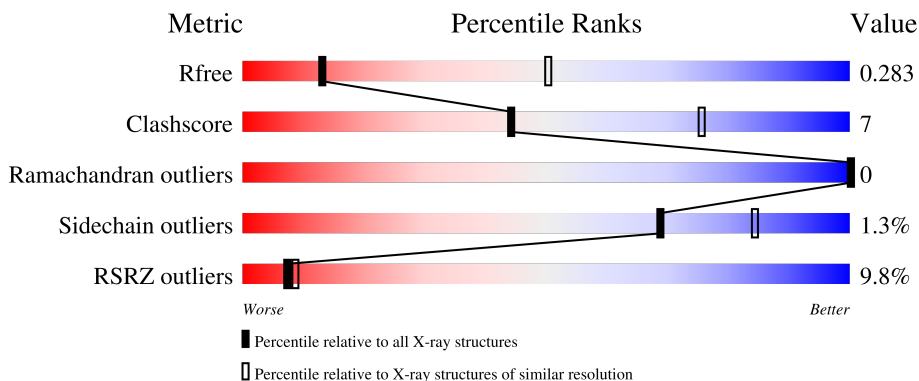
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.39 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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  $\geq 3$ , 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	476	 5% 82% 17%
1	B	476	 11% 82% 14% ..
1	C	476	 12% 79% 18% .

## 2 Entry composition [i](#)

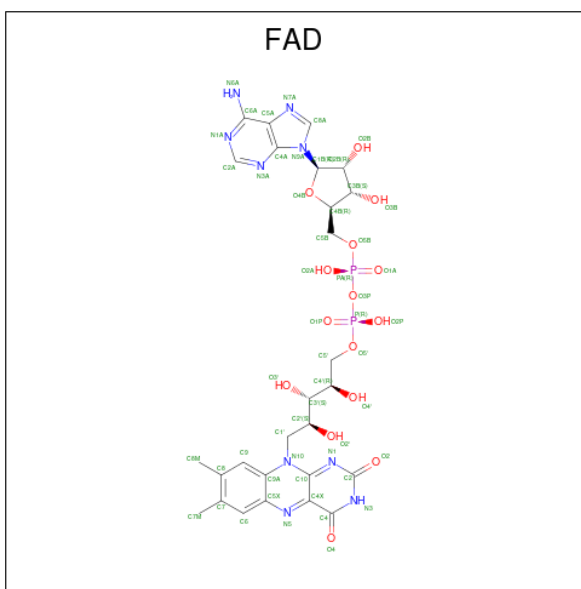
There are 5 unique types of molecules in this entry. The entry contains 10862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Rifampin monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	474	Total 3605	C 2262	N 669	O 661	S 13	0	1	0
1	B	460	Total 3502	C 2195	N 648	O 649	S 10	0	0	0
1	C	464	Total 3522	C 2208	N 654	O 647	S 13	0	0	0

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

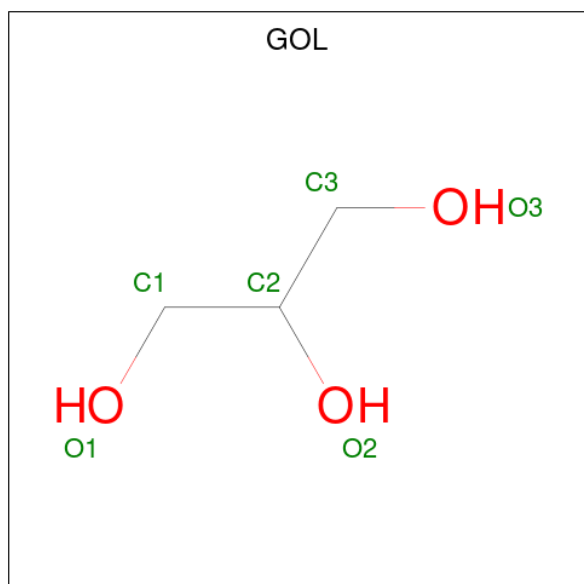


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	B	4	Total Cl 4 4	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0

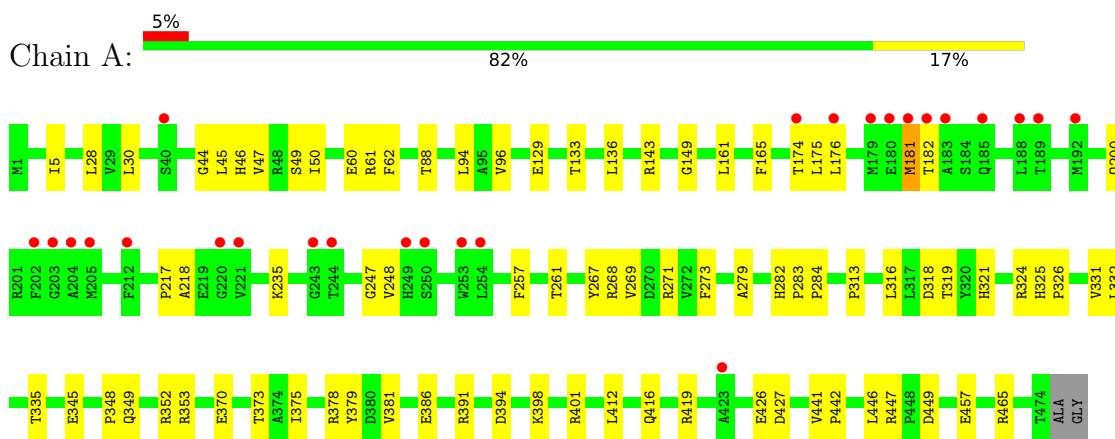
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	37	Total O 37 37	0	0
5	B	12	Total O 12 12	0	0
5	C	11	Total O 11 11	0	0

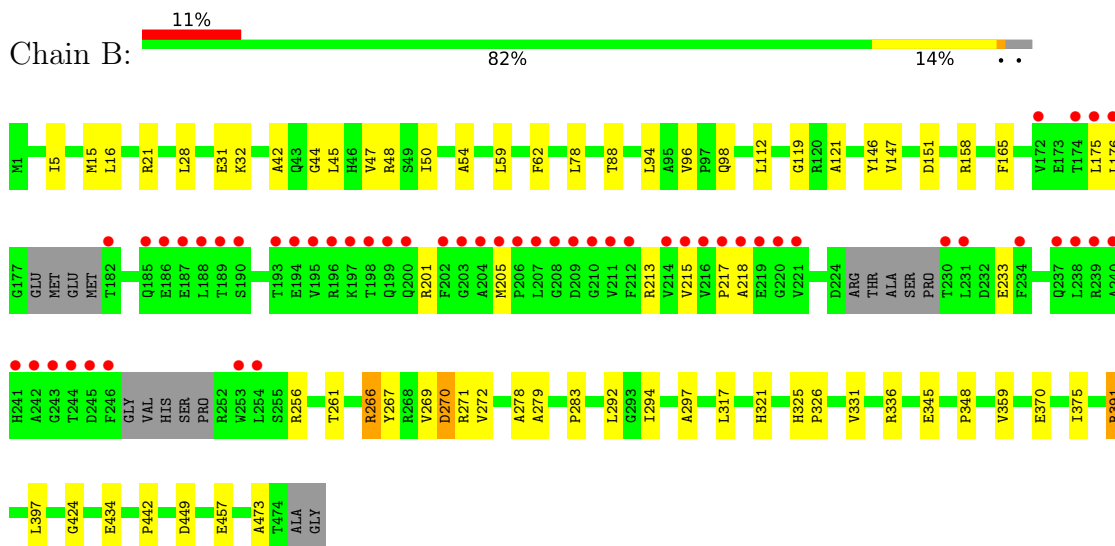
### 3 Residue-property plots [i](#)

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.

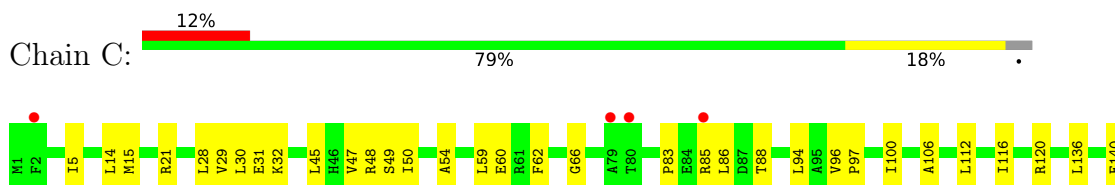
- Molecule 1: Rifampin monooxygenase

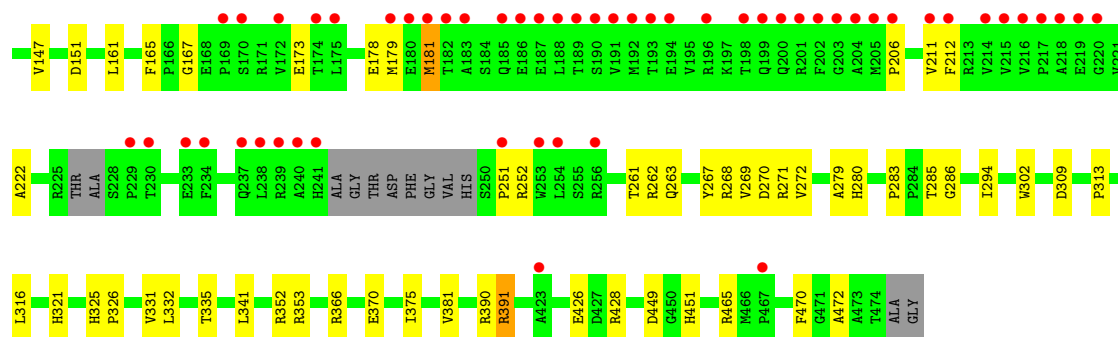


- Molecule 1: Rifampin monooxygenase



- Molecule 1: Rifampin monooxygenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.09Å 129.28Å 75.31Å 90.00° 105.52° 90.00°	Depositor
Resolution (Å)	48.92 – 3.39 48.92 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.92-3.39) 89.8 (48.92-3.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.29	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 3.40Å)	Xtrriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, $R_{free}$	0.226 , 0.284 0.226 , 0.283	Depositor DCC
$R_{free}$ test set	1296 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	10862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: GOL, CL, 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	0.23	0/3677	0.42	0/4992
1	B	0.23	0/3565	0.42	1/4837 (0.0%)
1	C	0.23	0/3587	0.41	0/4868
All	All	0.23	0/10829	0.42	1/14697 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	ASP	N-CA-C	5.19	125.00	111.00

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	3605	0	3532	47	0
1	B	3502	0	3416	42	0
1	C	3522	0	3443	52	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
3	A	3	0	0	0	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	1	0	0	0	0
4	B	6	0	8	0	0
5	A	37	0	0	1	0
5	B	12	0	0	0	0
5	C	11	0	0	1	0
All	All	10862	0	10492	141	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 7.

All (141) 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:201:ARG:HG3	1:B:217:PRO:HG3	1.76	0.66
1:C:370:GLU:HG2	1:C:375:ILE:HD11	1.78	0.64
1:A:50:ILE:HD11	1:A:94:LEU:H	1.64	0.63
1:A:331:VAL:O	1:A:335:THR:HG23	1.98	0.63
1:A:378:ARG:NH2	1:A:386:GLU:O	2.33	0.62
1:B:292:LEU:HD22	1:B:331:VAL:HG11	1.80	0.62
1:B:261:THR:HG22	1:B:283:PRO:HD3	1.83	0.61
1:A:261:THR:HG22	1:A:283:PRO:HD3	1.83	0.60
1:B:370:GLU:HG2	1:B:375:ILE:HD11	1.83	0.60
1:A:370:GLU:HG2	1:A:375:ILE:HD11	1.82	0.59
1:A:416:GLN:NE2	1:A:441:VAL:O	2.35	0.59
1:A:133:THR:OG1	1:A:143:ARG:NH1	2.35	0.59
1:B:42:ALA:HB3	1:B:98:GLN:HB2	1.85	0.59
1:C:66:GLY:HA3	1:C:96:VAL:HG22	1.84	0.59
1:A:381:VAL:HG12	1:A:465:ARG:HH22	1.69	0.58
1:B:62:PHE:HB3	1:B:94:LEU:HD21	1.86	0.57
1:A:419:ARG:NH1	1:A:457:GLU:O	2.37	0.57
1:B:5:ILE:HG12	1:B:28:LEU:HB3	1.85	0.57
1:A:442:PRO:HG2	1:A:457:GLU:HB3	1.87	0.57
1:B:424:GLY:HA3	1:B:473:ALA:HB1	1.87	0.56
1:C:178:GLU:OE1	1:C:252:ARG:NH1	2.37	0.56
1:C:120:ARG:NH1	1:C:140:GLU:OE2	2.36	0.56
1:B:270:ASP:CG	1:B:270:ASP:O	2.41	0.56
1:A:175:LEU:HD13	1:A:218:ALA:HB2	1.89	0.54
1:B:50:ILE:HD11	1:B:94:LEU:H	1.70	0.54
1:B:442:PRO:HG2	1:B:457:GLU:HB3	1.88	0.54
1:B:45:LEU:HD12	1:B:94:LEU:HD23	1.88	0.54

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:LEU:HB3	1:C:352:ARG:HG3	1.88	0.54
1:B:233:GLU:OE2	1:B:256:ARG:NH1	2.27	0.53
1:B:151:ASP:N	1:B:151:ASP:OD1	2.41	0.53
1:A:353:ARG:NH1	5:A:602:HOH:O	2.41	0.53
1:C:179:MET:HB3	1:C:251:PRO:HB3	1.91	0.53
1:B:44:GLY:HA2	1:B:96:VAL:H	1.74	0.52
1:A:345:GLU:HB2	1:A:348:PRO:HD2	1.92	0.52
1:B:269:VAL:HG23	1:B:272:VAL:HB	1.92	0.52
1:A:419:ARG:HH22	1:A:457:GLU:HB2	1.75	0.52
1:B:158:ARG:NH1	1:B:278:ALA:O	2.42	0.52
1:C:83:PRO:HB3	1:C:366:ARG:HB3	1.90	0.51
1:B:175:LEU:HG	1:B:218:ALA:HB2	1.92	0.51
1:C:267:TYR:H	1:C:321:HIS:CD2	2.29	0.51
1:C:50:ILE:HD11	1:C:94:LEU:H	1.75	0.50
1:A:129:GLU:O	1:A:271:ARG:NH2	2.44	0.50
1:A:268:ARG:NH1	1:A:318:ASP:OD1	2.44	0.50
1:C:206:PRO:HA	1:C:212:PHE:HD1	1.76	0.50
1:C:5:ILE:HG12	1:C:28:LEU:HB3	1.92	0.50
1:A:5:ILE:HG12	1:A:28:LEU:HB3	1.93	0.50
1:A:313:PRO:HD2	1:A:316:LEU:HD22	1.93	0.50
1:B:146:TYR:HD1	1:B:271:ARG:HA	1.76	0.50
1:A:412:LEU:HD23	1:A:446:LEU:HD12	1.94	0.50
1:A:394:ASP:OD2	1:A:401:ARG:NH2	2.37	0.50
1:A:324:ARG:NH1	1:A:379:TYR:OH	2.36	0.49
1:A:47:VAL:HG11	1:A:88:THR:HG21	1.94	0.49
1:A:60:GLU:HG2	1:C:60:GLU:HG2	1.93	0.49
1:B:261:THR:OG1	1:B:336:ARG:NH1	2.46	0.49
1:C:261:THR:HG22	1:C:283:PRO:HD3	1.94	0.49
1:A:30:LEU:HD13	1:A:136:LEU:HD21	1.94	0.49
1:C:30:LEU:HD13	1:C:136:LEU:HD21	1.93	0.48
1:A:182:THR:N	1:A:247:GLY:O	2.40	0.48
1:C:167:GLY:HA3	1:C:262:ARG:HA	1.95	0.48
1:B:54:ALA:HB2	1:B:59:LEU:HD22	1.95	0.48
1:B:175:LEU:HD23	1:B:256:ARG:HG3	1.96	0.48
1:B:15:MET:HG2	1:B:294:ILE:HG23	1.95	0.48
1:C:97:PRO:HD2	1:C:100:ILE:HD12	1.96	0.48
1:A:181:MET:HA	1:A:248:VAL:HA	1.96	0.47
1:C:31:GLU:OE1	1:C:32:LYS:N	2.47	0.47
1:C:331:VAL:O	1:C:335:THR:HG23	2.14	0.47
1:B:176:LEU:HD12	1:B:215:VAL:HB	1.95	0.47
1:C:391:ARG:HA	1:C:451:HIS:HA	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:HE3	1:A:248:VAL:HG22	1.95	0.47
1:B:31:GLU:OE1	1:B:32:LYS:N	2.47	0.47
1:C:181:MET:SD	1:C:181:MET:N	2.88	0.47
1:A:267:TYR:CE1	1:A:279:ALA:HB1	2.50	0.47
1:B:78:LEU:HD13	1:B:359:VAL:HG11	1.96	0.47
1:B:449:ASP:OD1	1:B:449:ASP:N	2.48	0.47
1:C:285:THR:OG1	1:C:286:GLY:N	2.48	0.46
1:A:426:GLU:N	1:A:426:GLU:OE1	2.48	0.46
1:B:21:ARG:NE	1:B:112:LEU:O	2.44	0.46
1:B:397:LEU:HB3	1:B:434:GLU:HB3	1.97	0.46
1:A:62:PHE:HB3	1:A:94:LEU:HD21	1.97	0.46
1:C:94:LEU:HG	1:C:96:VAL:HG23	1.98	0.46
1:C:428:ARG:NH1	1:C:472:ALA:O	2.48	0.46
1:C:62:PHE:HB3	1:C:94:LEU:HD21	1.98	0.46
1:C:270:ASP:O	1:C:271:ARG:HB2	2.16	0.46
1:C:428:ARG:NH1	1:C:470:PHE:O	2.48	0.46
1:A:44:GLY:HA2	1:A:96:VAL:H	1.81	0.45
1:A:282:HIS:HB3	1:A:332:LEU:HG	1.98	0.45
1:C:325:HIS:HB3	1:C:326:PRO:HD3	1.97	0.45
1:A:200:GLN:HG2	1:A:352:ARG:CZ	2.47	0.45
1:C:313:PRO:HD2	1:C:316:LEU:HB2	1.97	0.45
1:C:286:GLY:O	1:C:335:THR:HG22	2.17	0.45
1:C:173:GLU:HG3	1:C:222:ALA:H	1.81	0.45
1:C:268:ARG:HG2	1:C:270:ASP:H	1.82	0.45
1:C:302:TRP:NE1	1:C:449:ASP:OD2	2.47	0.44
1:B:16:LEU:HB2	1:B:297:ALA:HB1	1.98	0.44
1:C:280:HIS:ND1	1:C:280:HIS:O	2.51	0.44
1:C:426:GLU:OE1	1:C:426:GLU:N	2.51	0.44
1:B:31:GLU:O	1:B:119:GLY:N	2.48	0.44
1:C:161:LEU:HD22	1:C:269:VAL:HG21	2.00	0.44
1:B:32:LYS:HG3	1:B:121:ALA:HB2	2.00	0.43
1:C:267:TYR:CE1	1:C:279:ALA:HB1	2.53	0.43
1:B:325:HIS:HB3	1:B:326:PRO:HD3	2.00	0.43
1:A:174:THR:HG23	1:A:217:PRO:HA	2.00	0.43
1:A:316:LEU:O	1:A:319:THR:OG1	2.27	0.43
1:A:427:ASP:OD1	1:A:427:ASP:N	2.47	0.43
1:C:29:VAL:HB	1:C:116:ILE:HA	2.01	0.43
1:C:151:ASP:OD1	1:C:151:ASP:N	2.36	0.43
1:B:48:ARG:NH1	1:B:391:ARG:HD3	2.34	0.43
1:B:267:TYR:CE1	1:B:279:ALA:HB1	2.54	0.42
1:B:151:ASP:HA	2:B:501:FAD:H52A	1.99	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ARG:HB3	1:C:112:LEU:HB3	2.02	0.42
1:C:178:GLU:HB3	1:C:211:VAL:HG21	2.02	0.42
1:C:381:VAL:HG12	1:C:465:ARG:HH22	1.84	0.42
1:A:176:LEU:HB2	1:A:257:PHE:HE1	1.83	0.42
1:A:267:TYR:HB2	1:A:321:HIS:HB2	2.02	0.42
1:A:447:ARG:NH2	1:A:449:ASP:OD2	2.51	0.42
1:C:47:VAL:HG11	1:C:88:THR:HG21	2.01	0.42
1:A:149:GLY:N	1:A:273:PHE:O	2.40	0.42
1:B:205:MET:HB2	1:B:213:ARG:HB3	2.01	0.42
1:A:283:PRO:HA	1:A:284:PRO:HD3	1.95	0.42
1:B:266:ARG:HA	1:B:321:HIS:CE1	2.55	0.41
1:A:325:HIS:HB3	1:A:326:PRO:HD3	2.03	0.41
1:C:31:GLU:OE2	2:C:501:FAD:O3B	2.27	0.41
1:B:317:LEU:HD12	1:B:317:LEU:HA	1.95	0.41
1:C:45:LEU:HB3	1:C:49:SER:HB2	2.02	0.41
1:C:263:GLN:HB2	1:C:332:LEU:HD22	2.02	0.41
1:C:353:ARG:NH2	5:C:601:HOH:O	2.54	0.41
1:C:14:LEU:HD22	1:C:106:ALA:HA	2.01	0.41
1:A:161:LEU:HD13	1:A:269:VAL:HG21	2.02	0.41
1:B:47:VAL:HG11	1:B:88:THR:HG21	2.02	0.41
1:C:15:MET:HG2	1:C:294:ILE:HG23	2.01	0.41
1:C:86:LEU:O	1:C:88:THR:N	2.52	0.41
1:C:147:VAL:O	1:C:272:VAL:HA	2.21	0.41
1:A:200:GLN:NE2	1:A:349:GLN:OE1	2.49	0.41
1:C:48:ARG:NH1	1:C:391:ARG:HD3	2.36	0.40
2:A:501:FAD:H9	2:A:501:FAD:H1'1	1.90	0.40
1:A:419:ARG:HH12	1:A:457:GLU:HB2	1.85	0.40
1:B:345:GLU:HB2	1:B:348:PRO:HD2	2.03	0.40
1:A:45:LEU:HB3	1:A:49:SER:HB2	2.02	0.40
1:A:46:HIS:CD2	1:A:373:THR:HG22	2.57	0.40
1:B:147:VAL:O	1:B:272:VAL:HA	2.21	0.40
1:C:54:ALA:HB2	1:C:59:LEU:HD22	2.02	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	473/476 (99%)	432 (91%)	41 (9%)	0	100	100
1	B	452/476 (95%)	422 (93%)	30 (7%)	0	100	100
1	C	458/476 (96%)	421 (92%)	37 (8%)	0	100	100
All	All	1383/1428 (97%)	1275 (92%)	108 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 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	357/379 (94%)	352 (99%)	5 (1%)	67	83
1	B	347/379 (92%)	344 (99%)	3 (1%)	78	90
1	C	349/379 (92%)	343 (98%)	6 (2%)	60	80
All	All	1053/1137 (93%)	1039 (99%)	14 (1%)	69	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	165	PHE
1	A	181	MET
1	A	391	ARG
1	A	398	LYS
1	B	165	PHE
1	B	266	ARG
1	B	391	ARG
1	C	85	ARG
1	C	165	PHE
1	C	181	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	309	ASP
1	C	390	ARG
1	C	391	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	B	340	GLN

### 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](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
4	GOL	B	502	-	5,5,5	0.90	0	5,5,5	1.01	0
2	FAD	B	501	-	53,58,58	0.45	0	68,89,89	0.47	1 (1%)
2	FAD	A	501	-	53,58,58	0.45	0	68,89,89	0.52	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	C	501	-	53,58,58	0.45	0	68,89,89	0.50	2 (2%)

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
4	GOL	B	502	-	-	0/4/4/4	-
2	FAD	B	501	-	-	10/30/50/50	0/6/6/6
2	FAD	A	501	-	-	9/30/50/50	0/6/6/6
2	FAD	C	501	-	-	11/30/50/50	0/6/6/6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	P-O3P-PA	-2.54	124.11	132.83
2	C	501	FAD	P-O3P-PA	-2.38	124.65	132.83
2	A	501	FAD	C5A-C6A-N6A	2.33	123.89	120.35
2	B	501	FAD	C5A-C6A-N6A	2.28	123.82	120.35
2	C	501	FAD	C5A-C6A-N6A	2.27	123.81	120.35

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C5B-O5B-PA-O2A
2	A	501	FAD	C5'-O5'-P-O3P
2	B	501	FAD	C5B-O5B-PA-O3P
2	B	501	FAD	O4'-C4'-C5'-O5'
2	C	501	FAD	C5B-O5B-PA-O3P
2	C	501	FAD	P-O3P-PA-O5B
2	C	501	FAD	O3'-C3'-C4'-C5'
2	C	501	FAD	O3'-C3'-C4'-O4'
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	C3B-C4B-C5B-O5B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	501	FAD	O4B-C4B-C5B-O5B
2	C	501	FAD	C3B-C4B-C5B-O5B
2	C	501	FAD	C2'-C3'-C4'-O4'
2	C	501	FAD	C2'-C3'-C4'-C5'
2	B	501	FAD	P-O3P-PA-O5B
2	B	501	FAD	C4B-C5B-O5B-PA
2	A	501	FAD	C5B-O5B-PA-O3P
2	A	501	FAD	C5'-O5'-P-O1P
2	A	501	FAD	C5'-O5'-P-O2P
2	B	501	FAD	C5B-O5B-PA-O1A
2	C	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	N10-C1'-C2'-O2'
2	C	501	FAD	N10-C1'-C2'-O2'
2	B	501	FAD	C4'-C5'-O5'-P
2	C	501	FAD	C4B-C5B-O5B-PA
2	B	501	FAD	O3'-C3'-C4'-C5'
2	B	501	FAD	P-O3P-PA-O2A

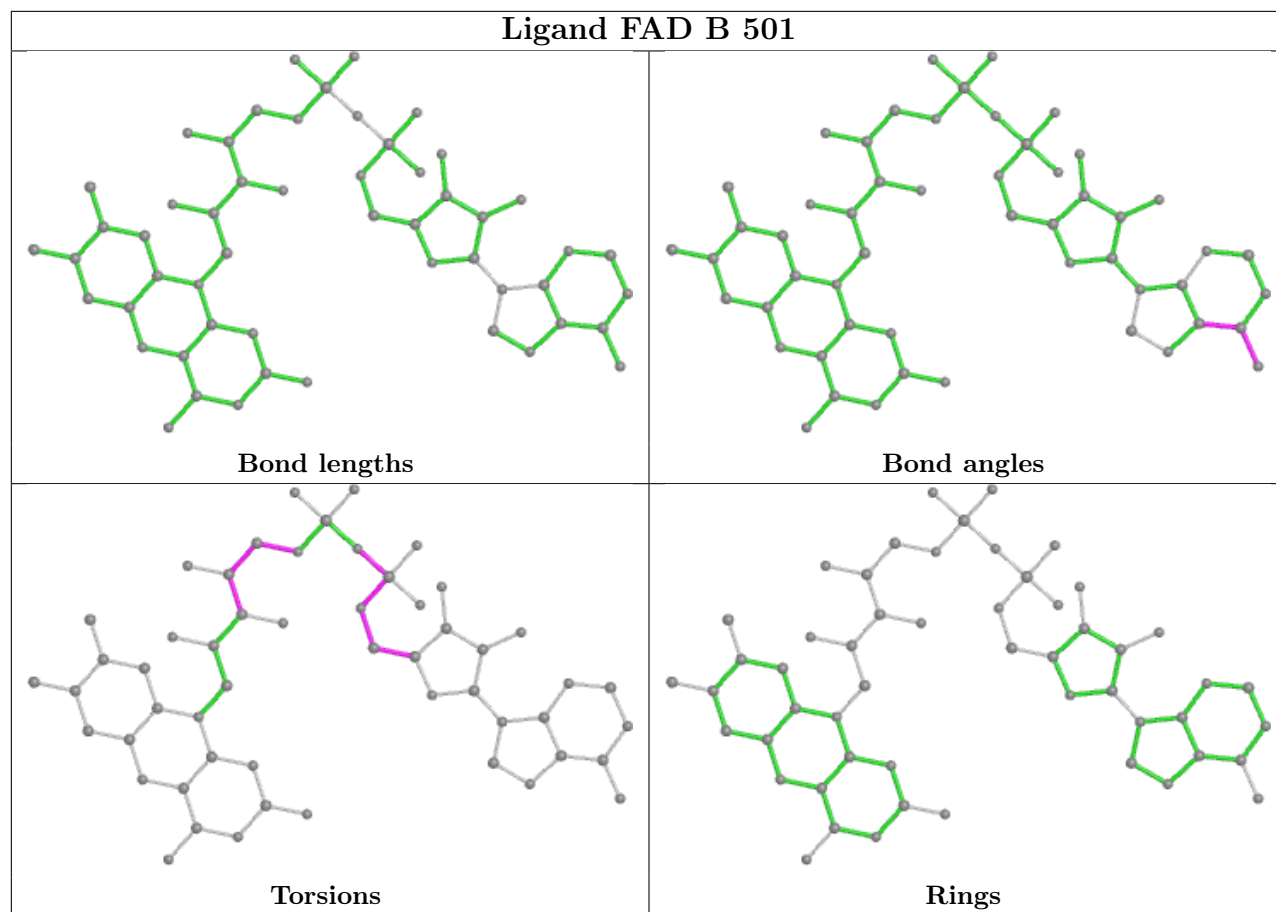
There are no ring outliers.

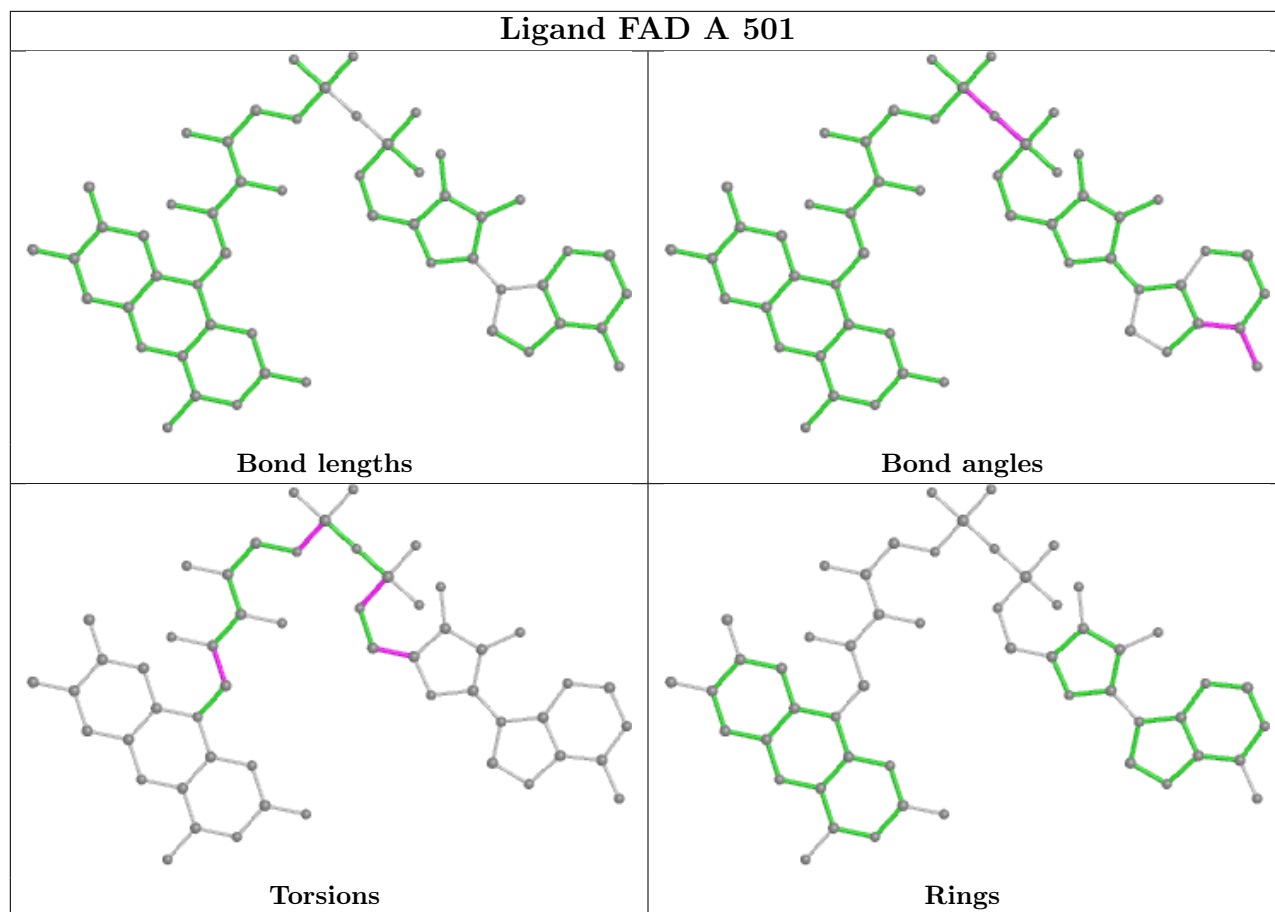
3 monomers are involved in 3 short contacts:

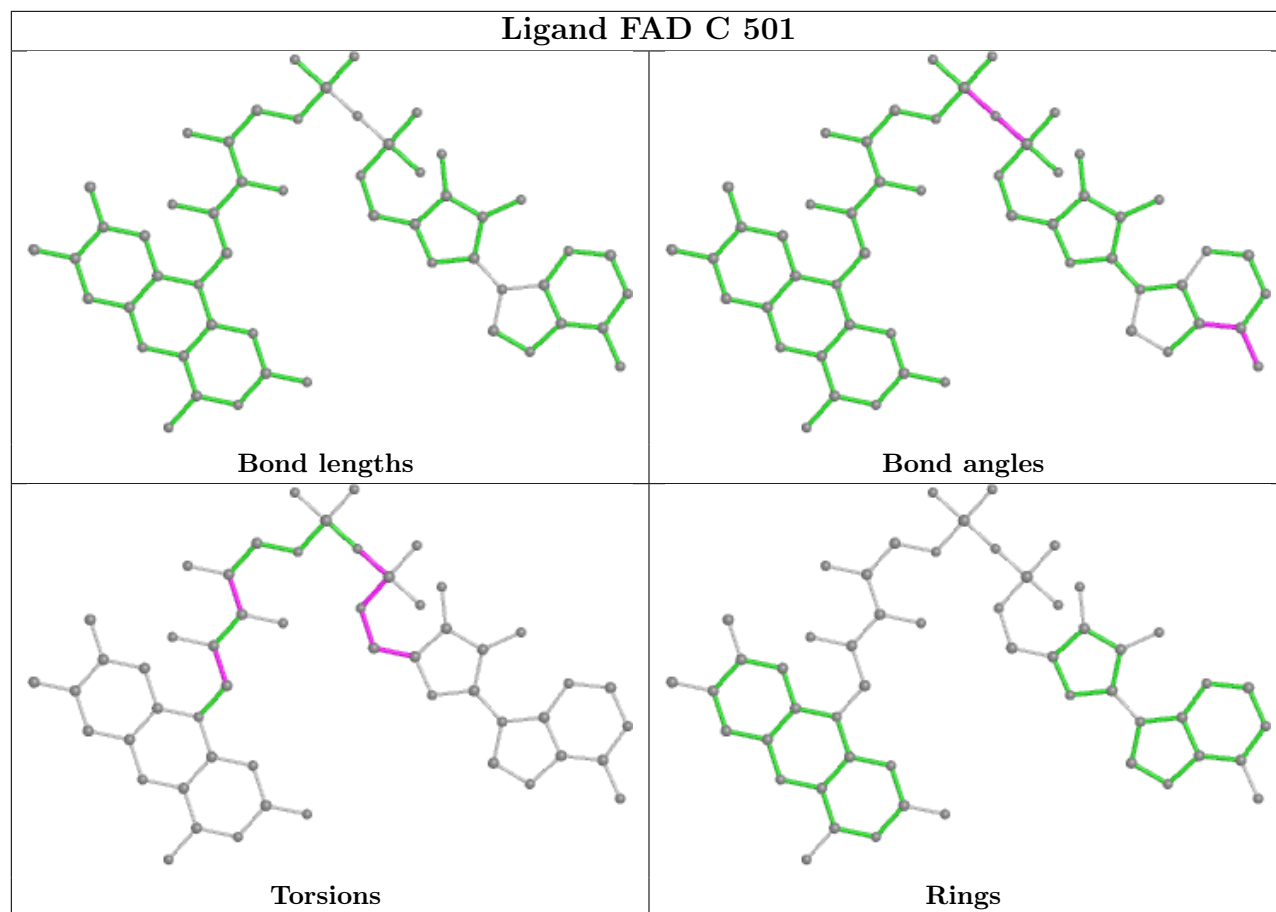
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FAD	1	0
2	A	501	FAD	1	0
2	C	501	FAD	1	0

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 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	474/476 (99%)	0.16	26 (5%) 25 25	20, 54, 145, 190	0
1	B	460/476 (96%)	0.40	53 (11%) 4 5	27, 55, 200, 295	0
1	C	464/476 (97%)	0.55	58 (12%) 3 4	32, 69, 205, 268	0
All	All	1398/1428 (97%)	0.37	137 (9%) 7 9	20, 59, 188, 295	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	GLU	9.6
1	B	194	GLU	8.8
1	C	240	ALA	8.0
1	C	203	GLY	7.6
1	B	206	PRO	7.2
1	B	220	GLY	6.7
1	B	238	LEU	6.7
1	C	241	HIS	6.4
1	C	186	GLU	5.9
1	C	194	GLU	5.8
1	B	205	MET	5.7
1	C	220	GLY	5.7
1	C	238	LEU	5.5
1	B	172	VAL	5.5
1	B	189	THR	5.2
1	C	192	MET	5.1
1	B	243	GLY	5.1
1	C	202	PHE	4.9
1	B	176	LEU	4.9
1	C	181	MET	4.8
1	C	216	VAL	4.8
1	B	240	ALA	4.7
1	B	237	GLN	4.7

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	193	THR	4.7
1	B	245	ASP	4.6
1	B	234	PHE	4.6
1	B	212	PHE	4.5
1	B	185	GLN	4.5
1	C	179	MET	4.5
1	C	229	PRO	4.3
1	C	239	ARG	4.3
1	A	202	PHE	4.2
1	B	188	LEU	4.2
1	A	181	MET	4.2
1	B	204	ALA	4.2
1	C	79	ALA	4.1
1	B	207	LEU	4.1
1	C	188	LEU	4.0
1	C	189	THR	4.0
1	C	214	VAL	4.0
1	B	195	VAL	4.0
1	C	193	THR	4.0
1	A	204	ALA	3.9
1	B	221	VAL	3.9
1	B	174	THR	3.9
1	B	175	LEU	3.9
1	C	200	GLN	3.9
1	C	215	VAL	3.9
1	B	196	ARG	3.9
1	A	182	THR	3.9
1	B	190	SER	3.9
1	B	218	ALA	3.8
1	C	201	ARG	3.7
1	B	186	GLU	3.6
1	C	234	PHE	3.6
1	A	188	LEU	3.6
1	B	187	GLU	3.5
1	C	190	SER	3.5
1	C	205	MET	3.5
1	C	170	SER	3.5
1	B	244	THR	3.5
1	B	239	ARG	3.5
1	C	204	ALA	3.4
1	B	202	PHE	3.4
1	B	241	HIS	3.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	244	THR	3.4
1	C	182	THR	3.3
1	A	253	TRP	3.3
1	B	254	LEU	3.3
1	A	179	MET	3.2
1	C	253	TRP	3.2
1	B	246	PHE	3.2
1	C	169	PRO	3.2
1	A	243	GLY	3.2
1	A	205	MET	3.2
1	B	253	TRP	3.1
1	C	180	GLU	3.1
1	A	221	VAL	3.0
1	C	198	THR	3.0
1	C	183	ALA	3.0
1	B	200	GLN	3.0
1	B	198	THR	2.9
1	B	211	VAL	2.9
1	C	191	VAL	2.9
1	C	254	LEU	2.8
1	C	237	GLN	2.8
1	C	187	GLU	2.8
1	C	199	GLN	2.8
1	B	215	VAL	2.8
1	B	216	VAL	2.8
1	C	211	VAL	2.8
1	C	256	ARG	2.7
1	A	203	GLY	2.7
1	B	208	GLY	2.7
1	B	210	GLY	2.7
1	B	199	GLN	2.7
1	C	175	LEU	2.7
1	A	220	GLY	2.6
1	C	206	PRO	2.6
1	B	214	VAL	2.6
1	C	423	ALA	2.6
1	C	219	GLU	2.5
1	B	209	ASP	2.5
1	C	80	THR	2.5
1	C	196	ARG	2.5
1	A	250	SER	2.5
1	C	172	VAL	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	40	SER	2.5
1	A	249	HIS	2.4
1	A	180	GLU	2.4
1	C	233	GLU	2.4
1	B	231	LEU	2.4
1	A	192	MET	2.4
1	A	212	PHE	2.3
1	C	174	THR	2.3
1	B	182	THR	2.3
1	A	183	ALA	2.3
1	C	467	PRO	2.3
1	A	254	LEU	2.3
1	B	203	GLY	2.2
1	A	176	LEU	2.2
1	C	230	THR	2.2
1	B	197	LYS	2.2
1	B	242	ALA	2.2
1	C	185	GLN	2.2
1	C	2	PHE	2.2
1	B	230	THR	2.2
1	C	85	ARG	2.2
1	C	212	PHE	2.2
1	A	174	THR	2.1
1	C	251	PRO	2.1
1	A	189	THR	2.1
1	A	423	ALA	2.1
1	B	217	PRO	2.1
1	C	217	PRO	2.0
1	C	218	ALA	2.0
1	A	185	GLN	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

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.

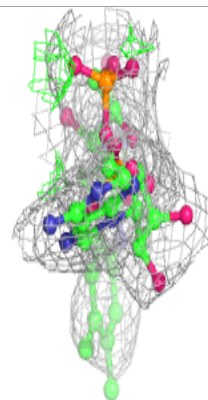
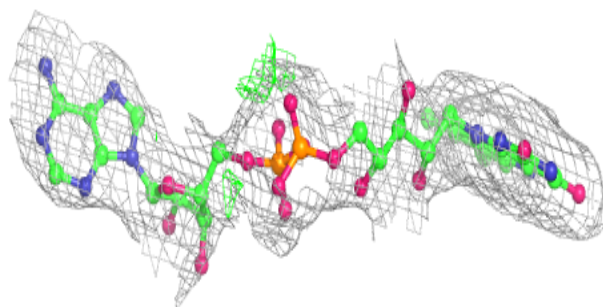
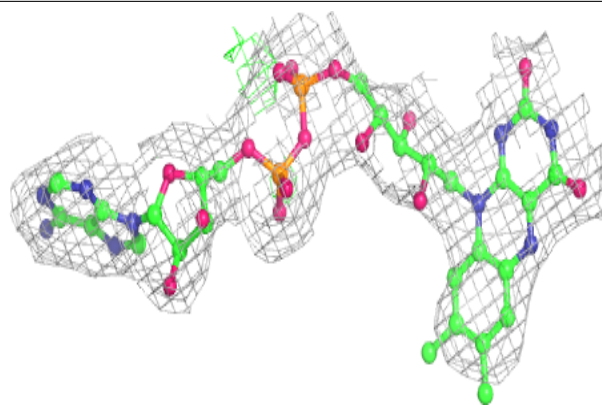
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	B	506	1/1	0.77	0.17	85,85,85,85	0
3	CL	C	502	1/1	0.79	0.26	67,67,67,67	0
3	CL	A	503	1/1	0.88	0.27	65,65,65,65	0
3	CL	B	503	1/1	0.89	0.30	57,57,57,57	0
3	CL	A	504	1/1	0.90	0.49	66,66,66,66	0
3	CL	B	505	1/1	0.92	0.19	49,49,49,49	0
3	CL	B	504	1/1	0.93	0.14	56,56,56,56	0
2	FAD	B	501	53/53	0.94	0.22	24,43,56,61	0
2	FAD	A	501	53/53	0.94	0.18	32,44,57,63	0
3	CL	A	502	1/1	0.95	0.27	35,35,35,35	0
2	FAD	C	501	53/53	0.95	0.19	18,46,72,78	0
4	GOL	B	502	6/6	0.95	0.12	24,30,42,44	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.

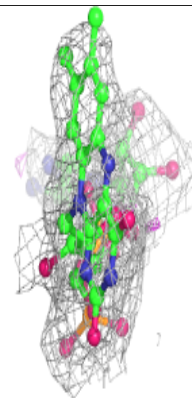
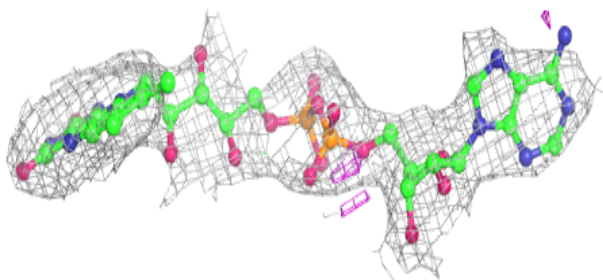
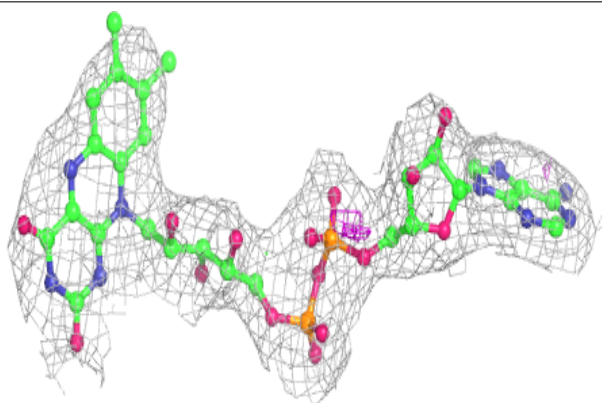


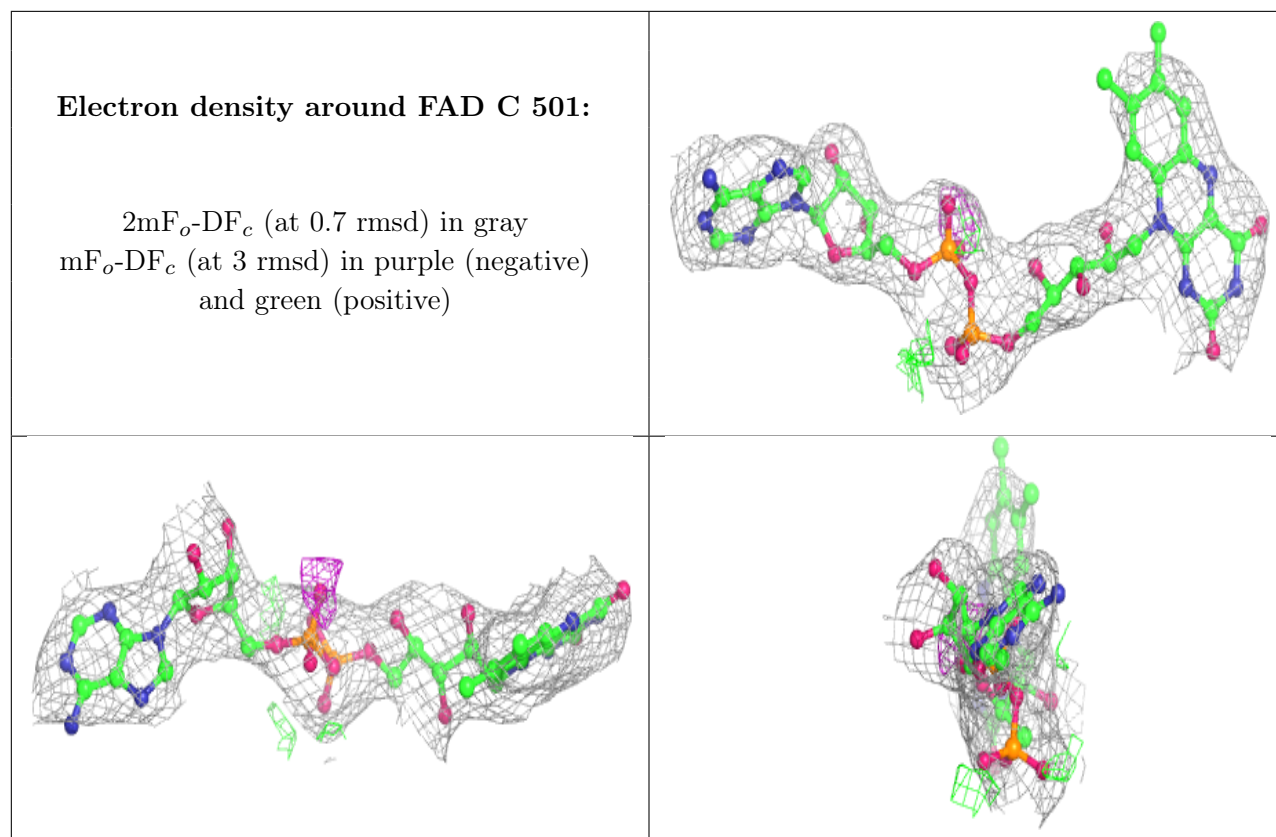
**Electron density around FAD B 501:**

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

**Electron density around FAD 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.