



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:35 pm BST

PDB ID : 3D9G  
Title : Nitroalkane oxidase: wild type crystallized in a trapped state forming a cyanoadduct with FAD  
Authors : Heroux, A.; Bozinovski, D.M.; Valley, M.P.; Fitzpatrick, P.F.; Orville, A.M.  
Deposited on : 2008-05-27  
Resolution : 2.15 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 : 2.11  
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) : 2.11

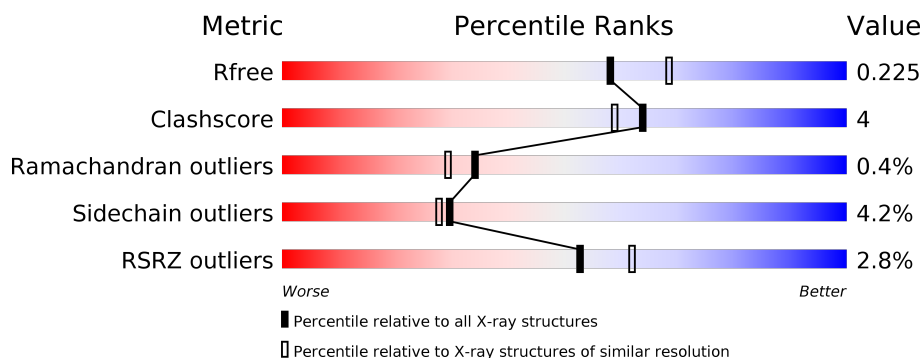
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	438	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	438	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	C	438	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>..</div> </div> </div>
1	D	438	<div> <div></div> <div> <div></div> <div>86%</div> <div>10%</div> <div>..</div> </div> </div>

2 Entry composition ⓘ

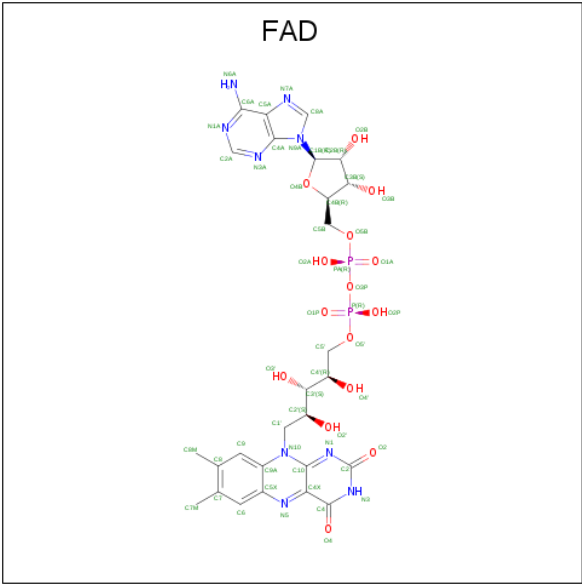
There are 5 unique types of molecules in this entry. The entry contains 14353 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitroalkane oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	1	0
			3315	2100	568	626	21			
1	B	431	Total	C	N	O	S	0	1	0
			3320	2103	569	627	21			
1	C	430	Total	C	N	O	S	0	0	0
			3307	2095	567	625	20			
1	D	430	Total	C	N	O	S	0	1	0
			3315	2100	568	626	21			

- 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>).



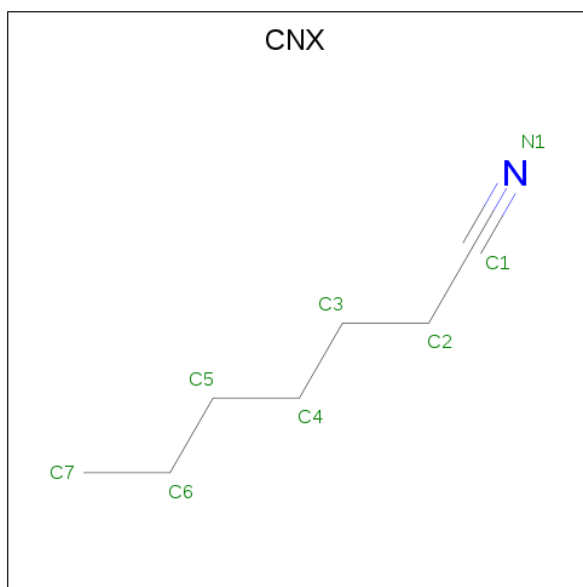
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
2	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

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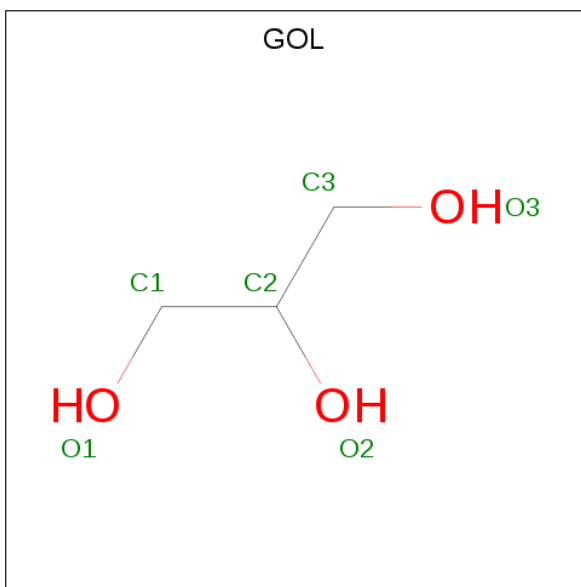
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is heptanenitrile (three-letter code: CNX) (formula:  $C_7H_{13}N$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			8	7	1		
3	B	1	Total	C	N	0	0
			8	7	1		
3	C	1	Total	C	N	0	0
			8	7	1		
3	D	1	Total	C	N	0	0
			8	7	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

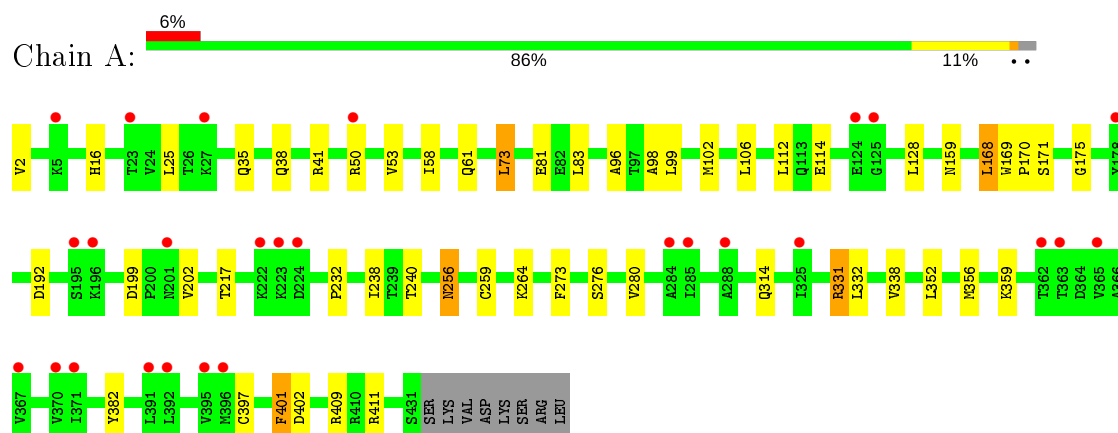
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total	O	0	0
			204	204		
5	B	194	Total	O	0	0
			194	194		
5	C	219	Total	O	0	0
			219	219		
5	D	223	Total	O	0	0
			223	223		

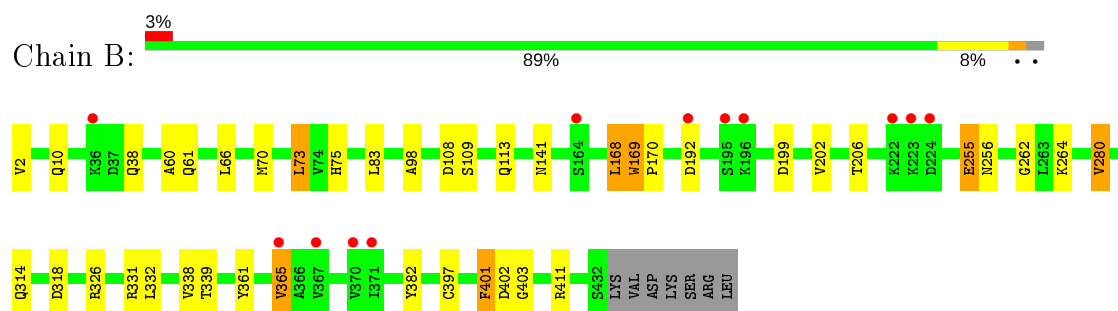
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

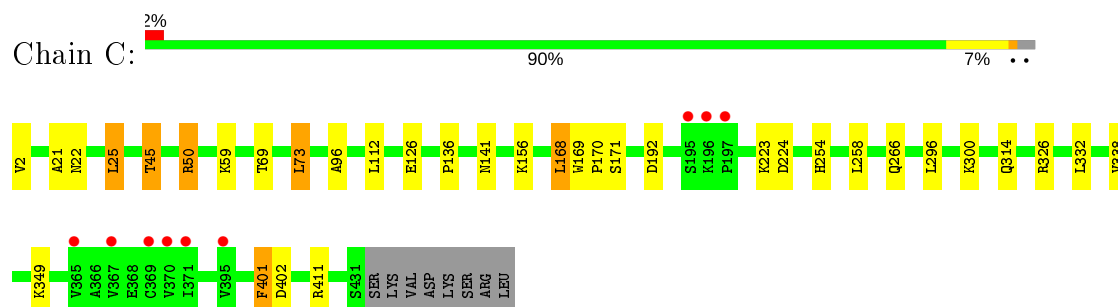
#### • Molecule 1: Nitroalkane oxidase



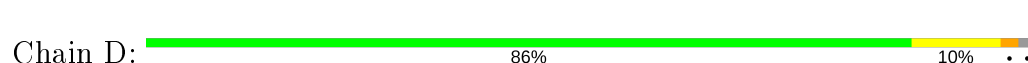
#### • Molecule 1: Nitroalkane oxidase

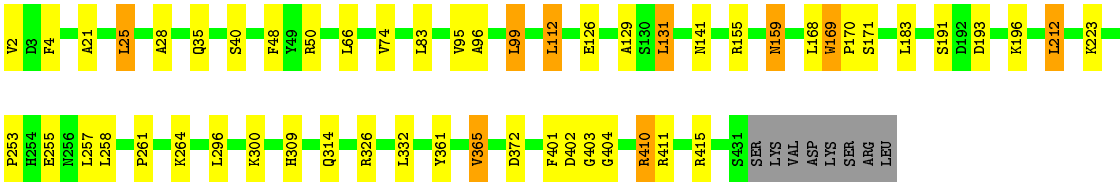


#### • Molecule 1: Nitroalkane oxidase



#### • Molecule 1: Nitroalkane oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.26Å 109.26Å 343.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.15 49.32 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.0 (50.00-2.15) 94.0 (49.32-2.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194 , 0.233 0.191 , 0.225	Depositor DCC
$R_{free}$ test set	6137 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 31.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14353	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, FAD, CNX

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	0.50	0/3384	0.61	1/4592 (0.0%)
1	B	0.50	0/3389	0.62	2/4599 (0.0%)
1	C	0.52	0/3376	0.59	0/4581
1	D	0.51	0/3384	0.63	2/4592 (0.0%)
All	All	0.51	0/13533	0.61	5/18364 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	331	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	D	410	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	D	410	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	331	ARG	NE-CZ-NH1	5.83	123.22	120.30

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	3315	0	3328	30	0
1	B	3320	0	3330	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3307	0	3319	23	0
1	D	3315	0	3328	32	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0
2	C	53	0	31	5	0
2	D	53	0	31	3	0
3	A	8	0	12	3	0
3	B	8	0	12	4	0
3	C	8	0	12	4	0
3	D	8	0	12	3	0
4	A	6	0	8	1	0
4	D	6	0	8	2	0
5	A	204	0	0	1	0
5	B	194	0	0	3	0
5	C	219	0	0	5	0
5	D	223	0	0	3	0
All	All	14353	0	13493	114	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 4.

All (114) 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:159:ASN:HD22	1:D:159:ASN:H	1.21	0.83
1:C:141:ASN:HD21	2:C:500:FAD:H61A	1.24	0.82
1:C:22:ASN:HB3	5:C:697:HOH:O	1.78	0.81
1:B:199:ASP:HB3	1:B:202:VAL:HG12	1.64	0.79
1:B:199:ASP:HB3	1:B:202:VAL:CG1	2.16	0.76
1:C:45:THR:HG23	5:C:685:HOH:O	1.86	0.76
1:C:168:LEU:C	1:C:170:PRO:HD3	2.07	0.75
1:C:402:ASP:HA	3:C:501:CNX:N1	2.04	0.73
1:B:73:LEU:HB3	1:B:338:VAL:HB	1.72	0.72
1:A:168:LEU:C	1:A:170:PRO:HD3	2.11	0.71
1:C:326:ARG:NH2	5:C:606:HOH:O	2.03	0.71
1:A:73:LEU:HB3	1:A:338:VAL:HB	1.73	0.69
1:C:73:LEU:HB3	1:C:338:VAL:HB	1.73	0.69
1:D:50:ARG:HD2	1:D:126:GLU:OE1	1.92	0.69
1:B:168:LEU:C	1:B:170:PRO:HD3	2.14	0.67
1:A:38:GLN:HG3	1:A:232:PRO:O	1.95	0.66
1:D:326:ARG:NH2	1:D:372:ASP:OD2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:VAL:N	4:D:701:GOL:HO3	1.96	0.64
1:D:95:VAL:HG22	3:D:501:CNX:H7A	1.79	0.63
1:C:22:ASN:CB	5:C:697:HOH:O	2.40	0.62
1:D:141:ASN:HD21	2:D:500:FAD:H61A	1.46	0.62
1:C:96:ALA:HB1	1:C:171:SER:HB2	1.79	0.62
1:D:253:PRO:HB2	1:D:255:GLU:HG2	1.81	0.62
1:B:326:ARG:HB3	1:B:365:VAL:HG13	1.82	0.61
1:D:35:GLN:HE21	1:D:40:SER:HB3	1.66	0.61
1:B:141:ASN:HD21	2:B:500:FAD:H61A	1.49	0.60
1:D:96:ALA:HB1	1:D:171:SER:HB2	1.83	0.60
1:C:45:THR:CG2	5:C:685:HOH:O	2.48	0.60
1:A:168:LEU:O	1:A:170:PRO:HD3	2.00	0.60
1:A:402:ASP:HA	3:A:501:CNX:N1	2.17	0.60
1:A:16:HIS:HD2	5:A:846:HOH:O	1.85	0.59
1:B:339:THR:HG21	1:D:4:PHE:HD1	1.67	0.58
1:B:61:GLN:HE21	1:B:98:ALA:HB2	1.68	0.58
1:D:402:ASP:HA	3:D:501:CNX:N1	2.19	0.58
1:B:255:GLU:HG3	5:B:682:HOH:O	2.03	0.57
1:B:314:GLN:HB2	1:C:314:GLN:HB2	1.88	0.56
2:C:500:FAD:O4	3:C:501:CNX:H2A	2.05	0.55
1:A:53:VAL:HG22	1:A:58:ILE:HG13	1.88	0.55
1:B:264:LYS:HE3	5:B:659:HOH:O	2.07	0.54
1:A:96:ALA:HB1	1:A:171:SER:HB2	1.90	0.54
1:A:276:SER:HB2	3:A:501:CNX:H7B	1.89	0.53
2:C:500:FAD:H6	3:C:501:CNX:H3	1.91	0.53
1:A:38:GLN:HE22	1:A:238:ILE:HA	1.73	0.52
1:A:382:TYR:CZ	1:B:397:CYS:HB2	2.45	0.52
1:D:326:ARG:HB3	1:D:365:VAL:HG13	1.91	0.52
1:C:141:ASN:ND2	2:C:500:FAD:H61A	2.02	0.51
1:A:259:CYS:HB2	1:A:264:LYS:HD3	1.92	0.51
1:A:314:GLN:HB2	1:D:314:GLN:HB2	1.93	0.51
1:D:99:LEU:HD22	1:D:131:LEU:HD23	1.92	0.51
1:B:280:VAL:HG23	3:B:501:CNX:H7A	1.94	0.50
1:B:402:ASP:HA	3:B:501:CNX:N1	2.27	0.50
1:A:199:ASP:HB3	1:A:202:VAL:HG12	1.94	0.50
1:A:256:ASN:N	1:A:256:ASN:HD22	2.08	0.50
1:C:50:ARG:HG3	1:C:126:GLU:OE1	2.12	0.49
1:C:21:ALA:HA	1:C:25:LEU:HB2	1.93	0.49
1:A:273:PHE:CD1	4:A:700:GOL:H12	2.47	0.49
1:B:168:LEU:O	1:B:170:PRO:HD3	2.13	0.49
1:D:296:LEU:O	1:D:300:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:HE21	1:A:98:ALA:HB2	1.79	0.48
1:C:96:ALA:HB1	1:C:171:SER:CB	2.43	0.48
1:A:401:PHE:CD2	1:A:401:PHE:C	2.87	0.47
1:B:206:THR:O	1:B:262:GLY:HA2	2.13	0.47
1:C:168:LEU:O	1:C:170:PRO:HD3	2.13	0.47
1:A:102[B]:MET:HE3	1:A:106:LEU:HG	1.95	0.47
1:A:199:ASP:HB3	1:A:202:VAL:CG1	2.45	0.47
1:D:21:ALA:HA	1:D:25:LEU:HB2	1.96	0.47
1:D:74:VAL:HB	4:D:701:GOL:H2	1.96	0.47
1:C:296:LEU:O	1:C:300:LYS:HG3	2.15	0.46
1:C:401:PHE:CD2	1:C:401:PHE:C	2.86	0.46
1:D:112:LEU:HD23	1:D:258:LEU:HD12	1.97	0.46
1:D:193:ASP:OD1	1:D:196:LYS:HE2	2.16	0.46
2:A:500:FAD:O4	3:A:501:CNX:H2A	2.16	0.46
1:C:112:LEU:HD23	1:C:258:LEU:HD12	1.97	0.45
1:D:257:LEU:HD21	1:D:261:PRO:HD3	1.98	0.45
1:B:168:LEU:O	1:B:169:TRP:HB2	2.16	0.45
1:C:402:ASP:CA	3:C:501:CNX:N1	2.77	0.45
1:D:159:ASN:H	1:D:159:ASN:ND2	2.01	0.45
1:A:35:GLN:HB2	1:A:41:ARG:HG2	1.99	0.45
1:D:309:HIS:HE1	5:D:909:HOH:O	1.98	0.45
1:A:53:VAL:HG22	1:A:58:ILE:CG1	2.46	0.44
1:A:81:GLU:OE2	1:A:331:ARG:HD3	2.18	0.44
1:D:155:ARG:HB3	1:D:191:SER:O	2.17	0.44
1:A:170:PRO:HA	2:A:500:FAD:C4	2.47	0.44
1:D:169:TRP:N	1:D:170:PRO:HD2	2.33	0.44
1:B:361:TYR:O	1:B:365:VAL:HB	2.18	0.44
1:A:397:CYS:HB2	1:B:382:TYR:CZ	2.52	0.44
1:D:159:ASN:N	1:D:159:ASN:HD22	1.98	0.44
1:D:361:TYR:O	1:D:365:VAL:HB	2.17	0.44
1:B:402:ASP:N	3:B:501:CNX:N1	2.66	0.43
1:A:352:LEU:O	1:A:356:MET:HG2	2.19	0.43
1:A:128:LEU:HD12	1:A:175:GLY:HA2	2.00	0.43
1:D:28:ALA:HA	1:D:48:PHE:CZ	2.54	0.43
2:D:500:FAD:H52A	2:D:500:FAD:O2P	2.18	0.43
1:D:169:TRP:N	1:D:170:PRO:CD	2.82	0.43
1:B:401:PHE:CD2	1:B:401:PHE:C	2.92	0.43
1:B:10:GLN:HG3	1:B:75:HIS:CE1	2.54	0.42
1:D:404:GLY:HA3	5:D:716:HOH:O	2.18	0.42
2:C:500:FAD:H52A	2:C:500:FAD:O2P	2.20	0.42
1:C:136:PRO:HA	1:C:168:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ARG:NH2	5:D:810:HOH:O	2.36	0.42
1:B:109:SER:O	1:B:113:GLN:HG3	2.20	0.41
1:C:59:LYS:HE2	1:C:69:THR:HG23	2.02	0.41
1:D:183:LEU:HD11	1:D:212:LEU:HG	2.01	0.41
1:A:382:TYR:OH	1:B:397:CYS:HB2	2.21	0.41
1:A:359:LYS:HD2	1:A:409:ARG:HG3	2.02	0.41
1:B:108:ASP:HB3	5:B:689:HOH:O	2.20	0.41
2:D:500:FAD:O4	3:D:501:CNX:H2A	2.21	0.41
1:B:318:ASP:HA	1:D:410:ARG:HH21	1.84	0.41
1:B:402:ASP:CA	3:B:501:CNX:N1	2.84	0.41
1:A:240:THR:HG21	2:A:500:FAD:HM72	2.03	0.41
1:C:156:LYS:HE3	1:C:254:HIS:ND1	2.36	0.41
1:B:38:GLN:HE21	1:B:38:GLN:HB2	1.70	0.40
1:B:60:ALA:O	1:B:70:MET:HB2	2.21	0.40
1:D:129:ALA:HA	1:D:183:LEU:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/438 (98%)	423 (99%)	5 (1%)	1 (0%)	47	46
1	B	430/438 (98%)	422 (98%)	6 (1%)	2 (0%)	29	22
1	C	428/438 (98%)	420 (98%)	7 (2%)	1 (0%)	47	46
1	D	429/438 (98%)	419 (98%)	8 (2%)	2 (0%)	29	22
All	All	1716/1752 (98%)	1684 (98%)	26 (2%)	6 (0%)	34	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	TRP
1	B	169	TRP
1	C	169	TRP
1	D	169	TRP
1	D	403	GLY
1	B	403	GLY

### 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	356/363 (98%)	339 (95%)	17 (5%)	25	22
1	B	356/363 (98%)	344 (97%)	12 (3%)	37	35
1	C	355/363 (98%)	341 (96%)	14 (4%)	32	30
1	D	356/363 (98%)	340 (96%)	16 (4%)	27	24
All	All	1423/1452 (98%)	1364 (96%)	59 (4%)	30	29

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	25	LEU
1	A	50	ARG
1	A	73	LEU
1	A	83	LEU
1	A	99	LEU
1	A	112	LEU
1	A	114	GLU
1	A	159	ASN
1	A	168	LEU
1	A	192	ASP
1	A	217	THR
1	A	256	ASN
1	A	280	VAL
1	A	332	LEU
1	A	401	PHE

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Mol	Chain	Res	Type
1	A	411	ARG
1	B	66	LEU
1	B	73	LEU
1	B	83	LEU
1	B	168	LEU
1	B	192	ASP
1	B	255	GLU
1	B	256	ASN
1	B	280	VAL
1	B	332	LEU
1	B	365	VAL
1	B	401	PHE
1	B	411	ARG
1	C	2	VAL
1	C	25	LEU
1	C	45	THR
1	C	50	ARG
1	C	73	LEU
1	C	168	LEU
1	C	192	ASP
1	C	223	LYS
1	C	224	ASP
1	C	266	GLN
1	C	332	LEU
1	C	349	LYS
1	C	401	PHE
1	C	411	ARG
1	D	2	VAL
1	D	25	LEU
1	D	66	LEU
1	D	83	LEU
1	D	99	LEU
1	D	112	LEU
1	D	131	LEU
1	D	159	ASN
1	D	168	LEU
1	D	212	LEU
1	D	223	LYS
1	D	264	LYS
1	D	332	LEU
1	D	365	VAL
1	D	401	PHE

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Mol	Chain	Res	Type
1	D	411	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	38	GLN
1	A	43	GLN
1	A	61	GLN
1	A	113	GLN
1	A	137	ASN
1	A	159	ASN
1	A	198	GLN
1	A	256	ASN
1	B	22	ASN
1	B	35	GLN
1	B	38	GLN
1	B	113	GLN
1	B	137	ASN
1	B	141	ASN
1	B	198	GLN
1	B	237	HIS
1	B	256	ASN
1	B	266	GLN
1	B	357	GLN
1	C	22	ASN
1	C	43	GLN
1	C	113	GLN
1	C	137	ASN
1	C	141	ASN
1	C	144	GLN
1	C	198	GLN
1	C	357	GLN
1	D	16	HIS
1	D	22	ASN
1	D	35	GLN
1	D	43	GLN
1	D	113	GLN
1	D	137	ASN
1	D	141	ASN
1	D	144	GLN
1	D	159	ASN

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Mol	Chain	Res	Type
1	D	198	GLN
1	D	256	ASN
1	D	266	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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	B	500	3	51,58,58	1.58	4 (7%)	60,89,89	1.75	8 (13%)
4	GOL	D	701	-	5,5,5	0.35	0	5,5,5	0.26	0
2	FAD	A	500	3	51,58,58	1.45	3 (5%)	60,89,89	1.61	9 (15%)
2	FAD	C	500	3	51,58,58	1.52	6 (11%)	60,89,89	1.64	7 (11%)
3	CNX	D	501	2	7,7,7	0.72	0	6,6,6	1.38	1 (16%)
3	CNX	A	501	2	7,7,7	0.34	0	6,6,6	0.90	0
3	CNX	C	501	2	7,7,7	0.50	0	6,6,6	1.20	1 (16%)
2	FAD	D	500	3	51,58,58	1.54	4 (7%)	60,89,89	1.60	8 (13%)
3	CNX	B	501	2	7,7,7	0.45	0	6,6,6	1.18	1 (16%)
4	GOL	A	700	-	5,5,5	0.44	0	5,5,5	0.20	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	B	500	3	-	4/30/50/50	0/6/6/6
4	GOL	D	701	-	-	2/4/4/4	-
2	FAD	A	500	3	-	4/30/50/50	0/6/6/6
2	FAD	C	500	3	-	4/30/50/50	0/6/6/6
3	CNX	D	501	2	-	3/5/5/5	-
3	CNX	A	501	2	-	3/5/5/5	-
3	CNX	C	501	2	-	4/5/5/5	-
2	FAD	D	500	3	-	5/30/50/50	0/6/6/6
3	CNX	B	501	2	-	2/5/5/5	-
4	GOL	A	700	-	-	2/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	FAD	C4X-N5	7.48	1.44	1.33
2	B	500	FAD	C4X-N5	7.22	1.43	1.33
2	A	500	FAD	C4X-N5	6.88	1.43	1.33
2	C	500	FAD	C4X-N5	6.84	1.43	1.33
2	B	500	FAD	C5X-N5	4.79	1.43	1.35
2	D	500	FAD	C5X-N5	4.60	1.42	1.35
2	C	500	FAD	C5X-N5	4.51	1.42	1.35
2	A	500	FAD	C5X-N5	4.47	1.42	1.35
2	B	500	FAD	O4B-C1B	3.47	1.45	1.41
2	C	500	FAD	C9A-N10	3.37	1.43	1.38
2	A	500	FAD	C9A-N10	3.20	1.42	1.38
2	D	500	FAD	C9A-N10	2.73	1.42	1.38
2	D	500	FAD	O4B-C1B	2.68	1.44	1.41
2	C	500	FAD	C4X-C10	2.63	1.41	1.38
2	B	500	FAD	C9A-N10	2.51	1.41	1.38
2	C	500	FAD	C2-N3	-2.11	1.34	1.38
2	C	500	FAD	O4B-C1B	2.03	1.43	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	C4-N3-C2	7.63	121.58	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	FAD	C4-N3-C2	6.90	120.97	115.14
2	A	500	FAD	C4-N3-C2	6.52	120.65	115.14
2	C	500	FAD	C4-N3-C2	6.39	120.54	115.14
2	B	500	FAD	N3A-C2A-N1A	-5.45	120.17	128.68
2	A	500	FAD	N3A-C2A-N1A	-5.23	120.50	128.68
2	D	500	FAD	N3A-C2A-N1A	-5.18	120.58	128.68
2	C	500	FAD	N3A-C2A-N1A	-4.81	121.15	128.68
2	C	500	FAD	C9A-N10-C10	-3.72	117.03	121.91
2	D	500	FAD	C9A-N10-C10	-3.67	117.10	121.91
2	B	500	FAD	C1'-N10-C9A	3.65	121.17	118.29
2	B	500	FAD	C4-C4X-C10	-3.61	117.56	119.95
2	B	500	FAD	C9A-N10-C10	-3.50	117.32	121.91
2	C	500	FAD	C1'-N10-C9A	3.48	121.03	118.29
2	C	500	FAD	C1'-N10-C10	3.41	121.47	118.41
2	D	500	FAD	C4X-N5-C5X	-3.41	113.36	116.77
2	A	500	FAD	C1'-N10-C9A	3.40	120.97	118.29
2	B	500	FAD	C4X-N5-C5X	-3.36	113.41	116.77
2	A	500	FAD	C9A-N10-C10	-3.25	117.65	121.91
2	D	500	FAD	C4X-C4-N3	-3.01	119.32	123.43
2	C	500	FAD	C4X-C4-N3	-2.91	119.45	123.43
2	A	500	FAD	C4-C4X-C10	-2.85	118.06	119.95
2	C	500	FAD	C4X-N5-C5X	-2.80	113.98	116.77
3	C	501	CNX	C2-C1-N1	-2.78	161.35	176.53
2	B	500	FAD	C1'-N10-C10	2.69	120.82	118.41
3	D	501	CNX	C2-C1-N1	-2.68	161.93	176.53
2	D	500	FAD	C1'-N10-C10	2.59	120.73	118.41
2	B	500	FAD	C4X-C4-N3	-2.58	119.91	123.43
2	D	500	FAD	C4-C4X-C10	-2.55	118.26	119.95
2	A	500	FAD	C3B-C2B-C1B	2.47	104.70	100.98
2	A	500	FAD	C4A-C5A-N7A	-2.43	106.87	109.40
2	A	500	FAD	C4X-N5-C5X	-2.41	114.36	116.77
3	B	501	CNX	C2-C1-N1	-2.34	163.79	176.53
2	A	500	FAD	C4X-C4-N3	-2.33	120.25	123.43
2	D	500	FAD	C3B-C2B-C1B	2.12	104.17	100.98

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	700	GOL	C1-C2-C3-O3
4	A	700	GOL	O2-C2-C3-O3
2	B	500	FAD	O3'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
2	B	500	FAD	C2'-C3'-C4'-O4'
2	A	500	FAD	C2'-C3'-C4'-O4'
2	A	500	FAD	O3'-C3'-C4'-O4'
2	A	500	FAD	C2'-C3'-C4'-C5'
3	B	501	CNX	C2-C3-C4-C5
3	C	501	CNX	C2-C3-C4-C5
2	B	500	FAD	O3'-C3'-C4'-C5'
2	A	500	FAD	O3'-C3'-C4'-C5'
2	D	500	FAD	C2'-C3'-C4'-C5'
3	C	501	CNX	C1-C2-C3-C4
3	A	501	CNX	C2-C3-C4-C5
3	A	501	CNX	C4-C5-C6-C7
3	D	501	CNX	C4-C5-C6-C7
2	C	500	FAD	O3'-C3'-C4'-O4'
3	C	501	CNX	C4-C5-C6-C7
2	C	500	FAD	C2'-C3'-C4'-O4'
2	D	500	FAD	C2'-C3'-C4'-O4'
3	D	501	CNX	C1-C2-C3-C4
3	A	501	CNX	C1-C2-C3-C4
2	D	500	FAD	O3'-C3'-C4'-C5'
2	B	500	FAD	C2'-C3'-C4'-C5'
2	D	500	FAD	O3'-C3'-C4'-O4'
4	D	701	GOL	O1-C1-C2-C3
3	B	501	CNX	C1-C2-C3-C4
2	C	500	FAD	O3'-C3'-C4'-C5'
2	C	500	FAD	C2'-C3'-C4'-C5'
3	D	501	CNX	C2-C3-C4-C5
2	D	500	FAD	O4B-C4B-C5B-O5B
3	C	501	CNX	C3-C4-C5-C6
4	D	701	GOL	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 25 short contacts:

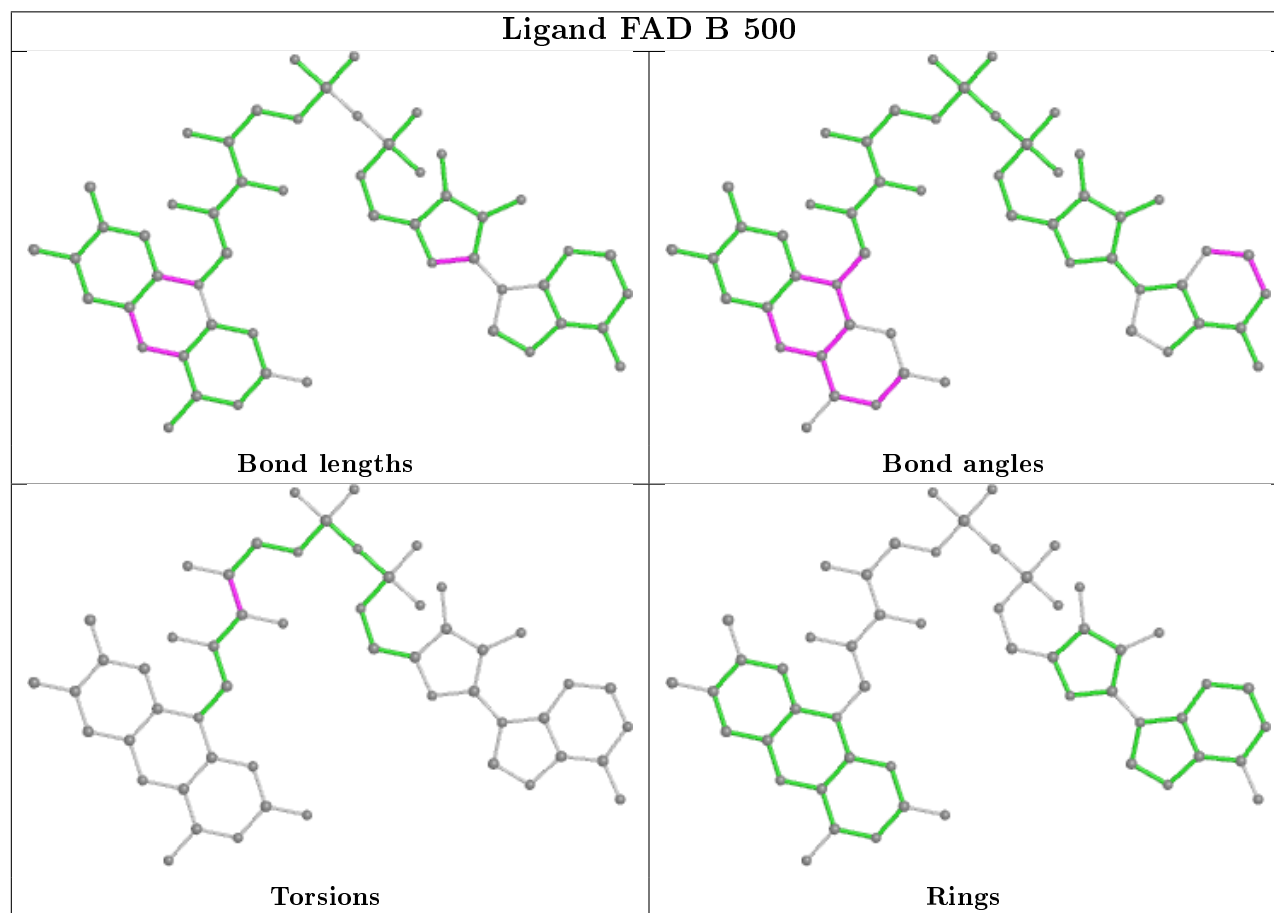
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	FAD	1	0
4	D	701	GOL	2	0
2	A	500	FAD	3	0
2	C	500	FAD	5	0
3	D	501	CNX	3	0
3	A	501	CNX	3	0
3	C	501	CNX	4	0

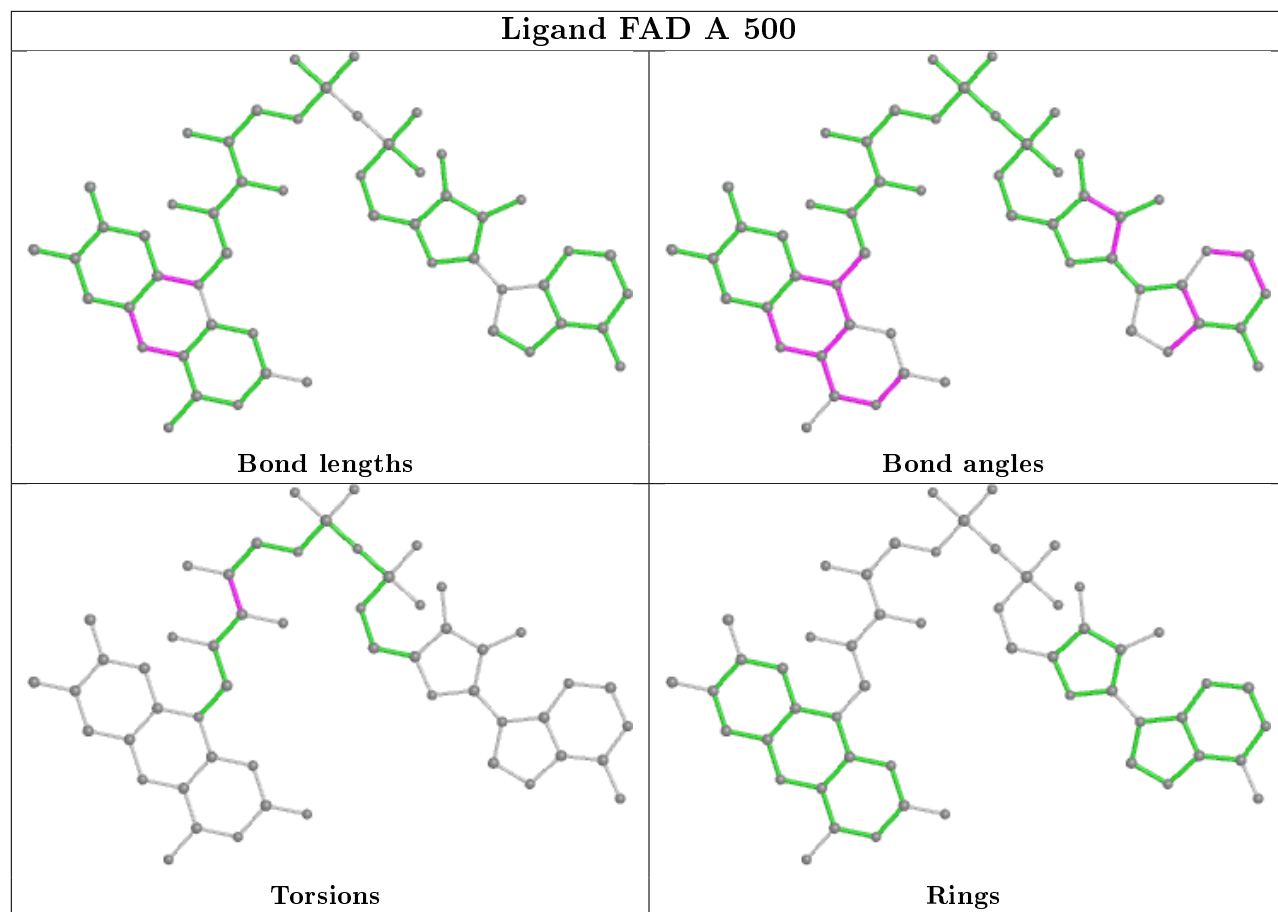
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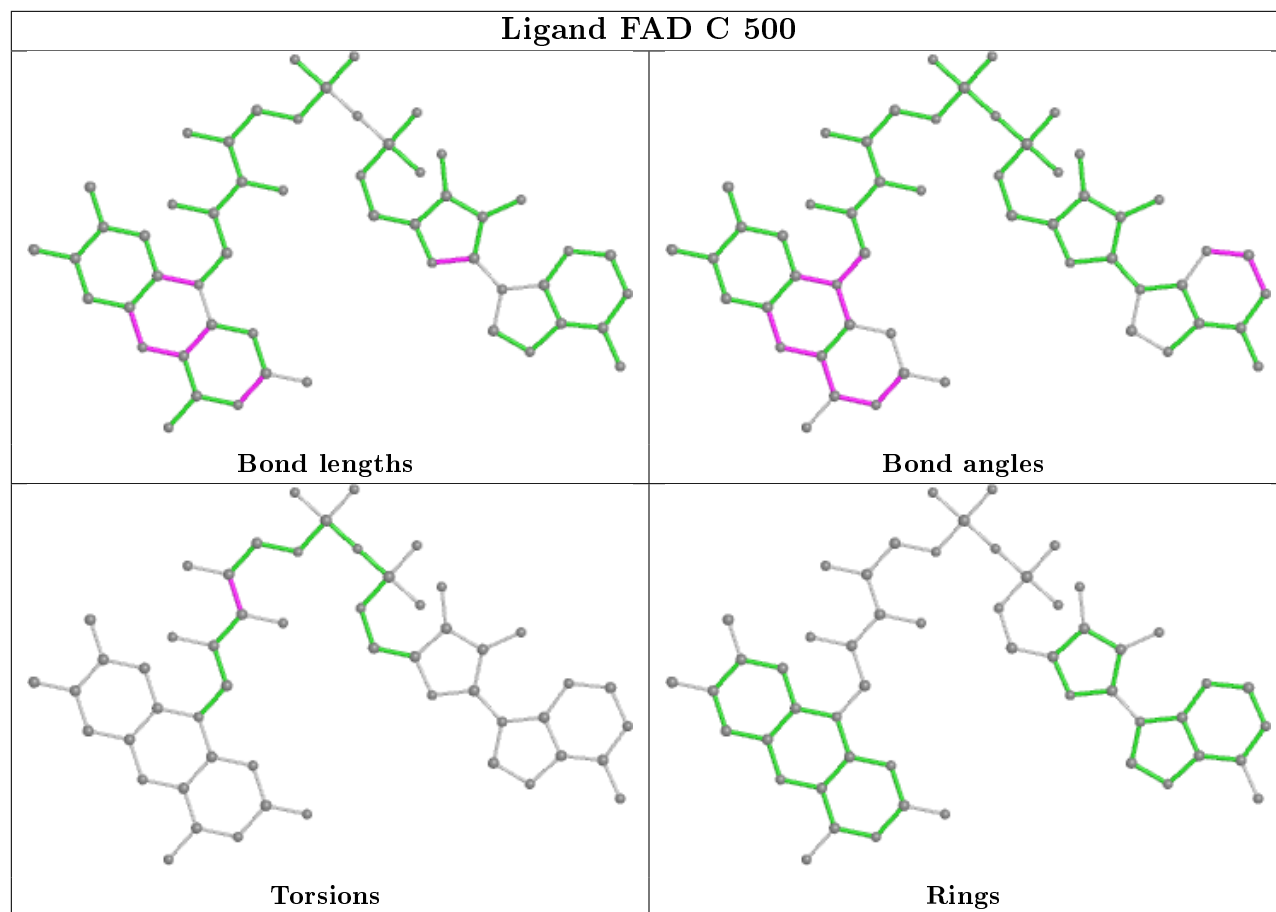
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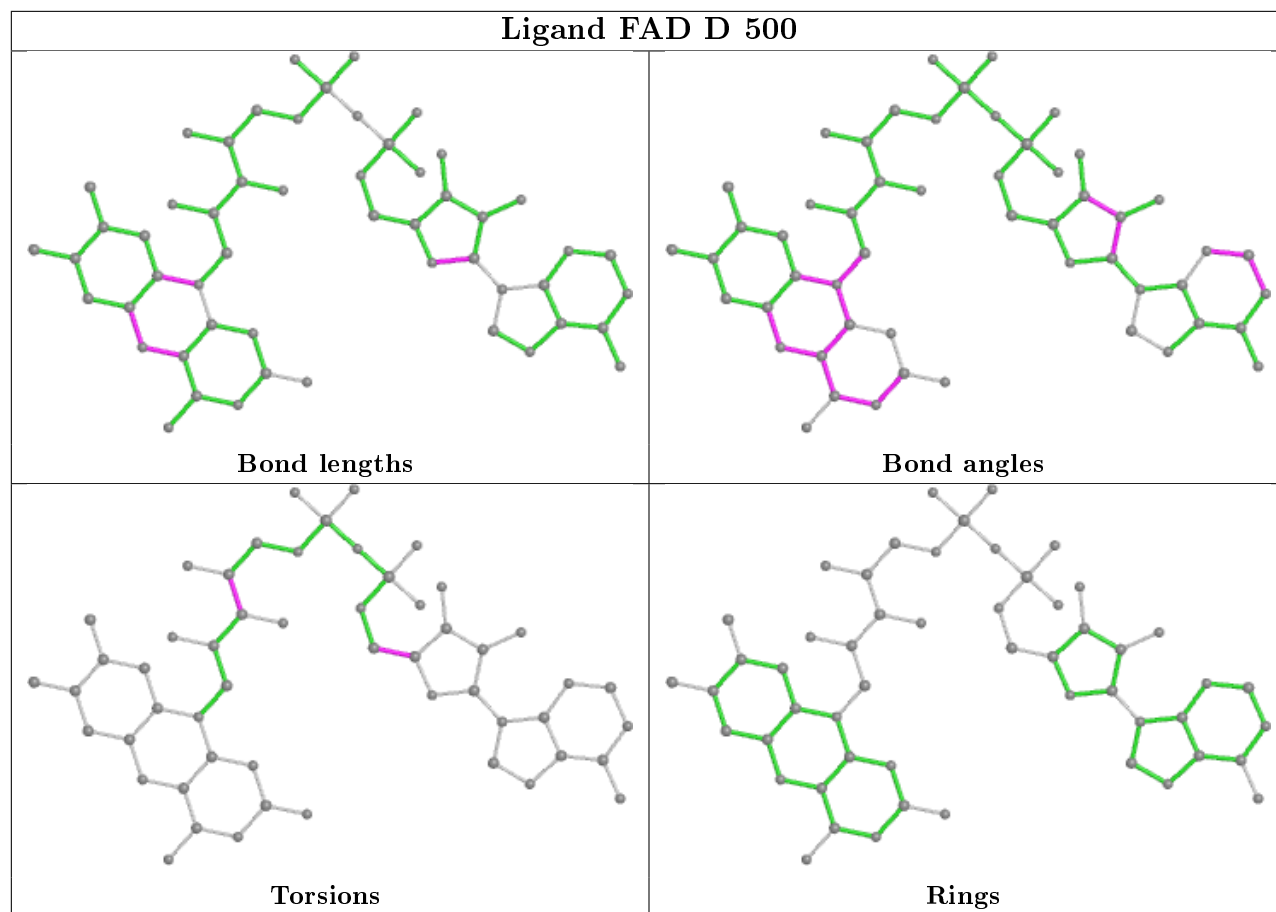
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	FAD	3	0
3	B	501	CNX	4	0
4	A	700	GOL	1	0

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	430/438 (98%)	0.25	27 (6%) 20 27	27, 40, 52, 61	0
1	B	431/438 (98%)	0.06	12 (2%) 53 62	26, 37, 50, 58	0
1	C	430/438 (98%)	-0.08	9 (2%) 63 71	27, 35, 48, 59	0
1	D	430/438 (98%)	-0.09	0 100 100	26, 37, 51, 60	1 (0%)
All	All	1721/1752 (98%)	0.04	48 (2%) 53 62	26, 37, 50, 61	1 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	367	VAL	3.8
1	B	371	ILE	3.4
1	A	395	VAL	3.3
1	A	371	ILE	3.1
1	C	195	SER	3.0
1	A	195	SER	3.0
1	B	223	LYS	3.0
1	A	223	LYS	3.0
1	C	365	VAL	2.9
1	A	50	ARG	2.8
1	B	36	LYS	2.8
1	B	367	VAL	2.8
1	A	396	MET	2.8
1	B	224	ASP	2.7
1	A	178	TYR	2.7
1	C	196	LYS	2.7
1	A	363	THR	2.7
1	A	365	VAL	2.6
1	B	196	LYS	2.6
1	A	362	THR	2.5
1	A	284	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	369	CYS	2.5
1	A	370	VAL	2.4
1	A	392	LEU	2.4
1	C	197	PRO	2.3
1	C	371	ILE	2.3
1	B	164	SER	2.3
1	A	201	ASN	2.3
1	A	222	LYS	2.2
1	A	224	ASP	2.2
1	A	124	GLU	2.2
1	B	192	ASP	2.2
1	B	222	LYS	2.2
1	A	391	LEU	2.2
1	A	5	LYS	2.2
1	A	27	LYS	2.2
1	A	285	ILE	2.1
1	C	370	VAL	2.1
1	A	288	ALA	2.1
1	B	370	VAL	2.1
1	C	395	VAL	2.1
1	C	367	VAL	2.1
1	A	125	GLY	2.1
1	B	195	SER	2.0
1	A	325	ILE	2.0
1	B	365	VAL	2.0
1	A	196	LYS	2.0
1	A	23	THR	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 carbohydrates 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,

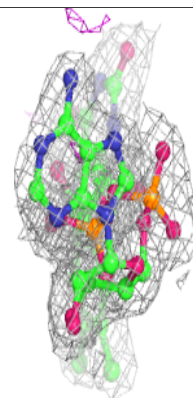
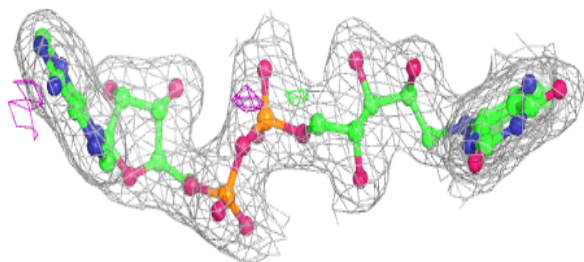
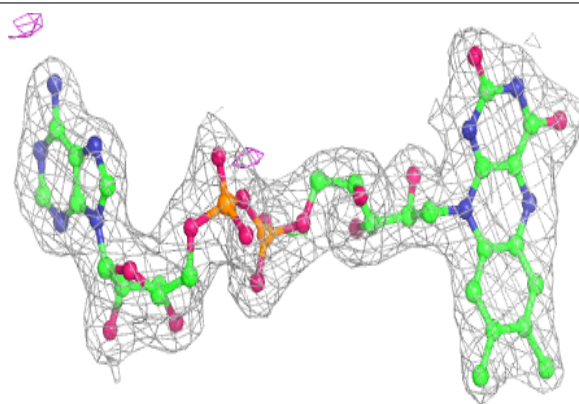
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	D	701	6/6	0.89	0.22	55,56,57,58	0
3	CNX	A	501	8/8	0.92	0.16	39,41,43,44	0
3	CNX	B	501	8/8	0.94	0.17	36,40,42,44	0
3	CNX	D	501	8/8	0.96	0.15	37,39,40,41	0
3	CNX	C	501	8/8	0.97	0.11	35,39,42,43	0
4	GOL	A	700	6/6	0.97	0.11	41,42,43,43	0
2	FAD	C	500	53/53	0.98	0.09	24,27,32,32	0
2	FAD	D	500	53/53	0.98	0.12	24,31,34,36	0
2	FAD	B	500	53/53	0.98	0.10	26,30,32,32	0
2	FAD	A	500	53/53	0.98	0.09	29,33,36,37	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.

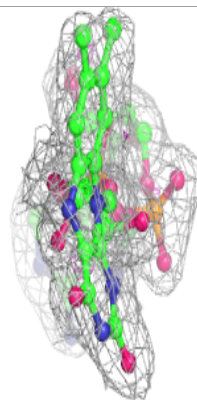
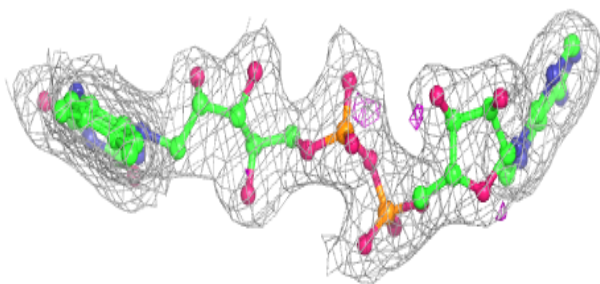
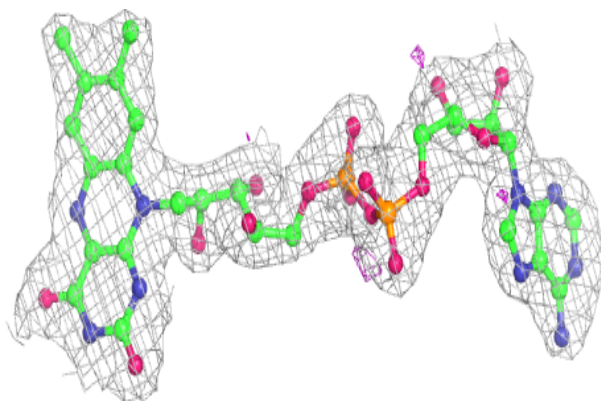
#### Electron density around FAD C 500:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

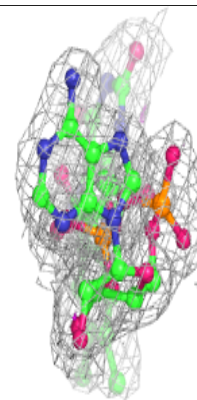
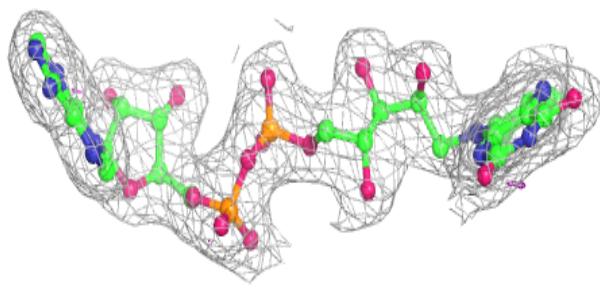
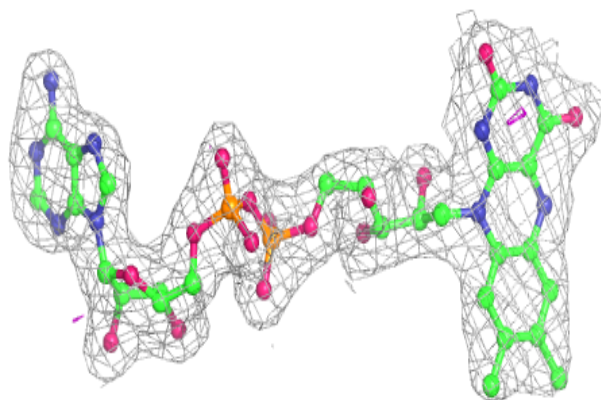


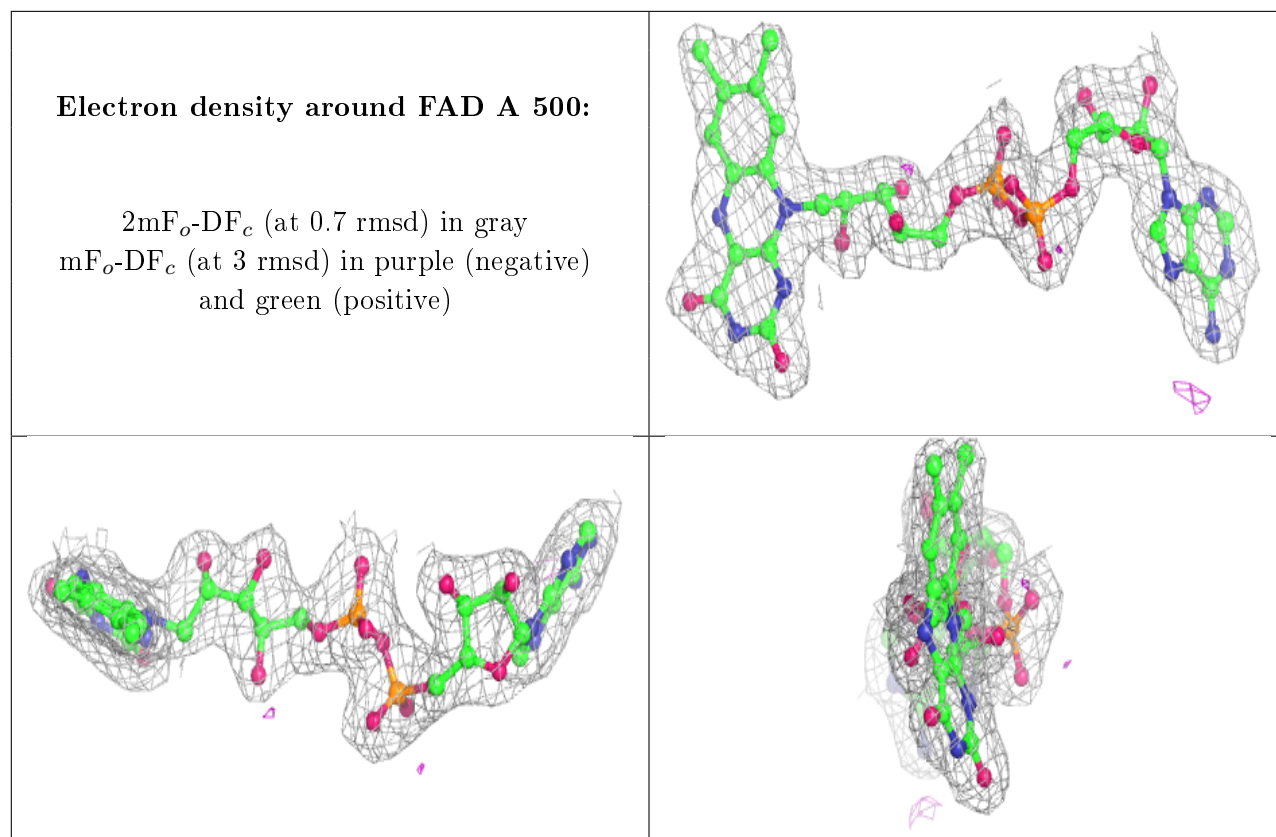
**Electron density around FAD D 500:**

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

**Electron density around FAD B 500:**

$2mF_o-DF_c$  (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.