



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2021 – 03:09 PM EDT

PDB ID : 3D9D  
Title : Nitroalkane oxidase: mutant D402N crystallized with 1-nitrohexane  
Authors : Heroux, A.; Bozinovski, D.M.; Valley, M.P.; Fitzpatrick, P.F.; Orville, A.M.  
Deposited on : 2008-05-27  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 2.23.2  
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) : 2.23.2



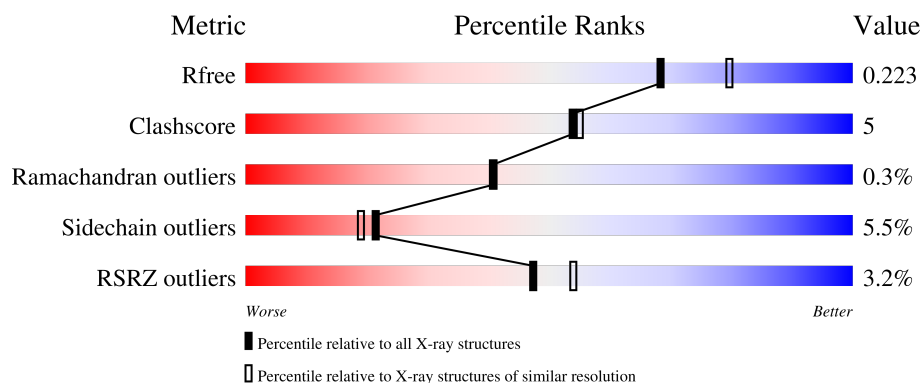
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>4%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	438	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	438	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>..</div> </div> </div>
1	D	438	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	N6C	B	600	-	-	X	-



## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14165 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.

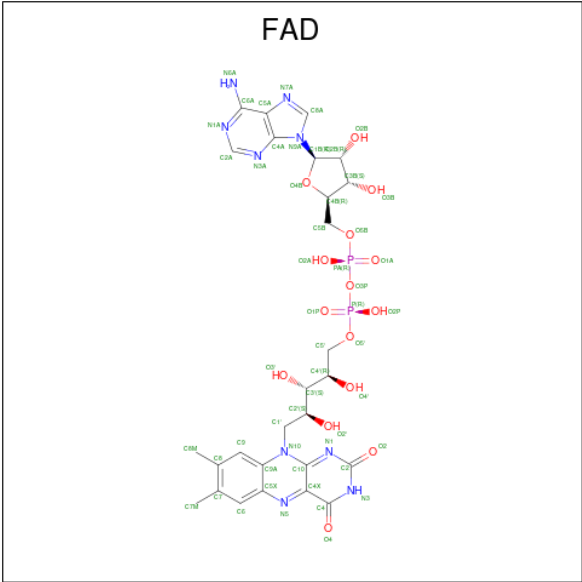
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3312	2098	567	627	20			
1	B	431	Total	C	N	O	S	0	0	0
			3300	2092	565	623	20			
1	C	430	Total	C	N	O	S	0	0	0
			3301	2092	565	624	20			
1	D	431	Total	C	N	O	S	0	0	0
			3306	2095	566	625	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	ASN	ASP	engineered mutation	UNP Q8X1D8
B	402	ASN	ASP	engineered mutation	UNP Q8X1D8
C	402	ASN	ASP	engineered mutation	UNP Q8X1D8
D	402	ASN	ASP	engineered mutation	UNP Q8X1D8

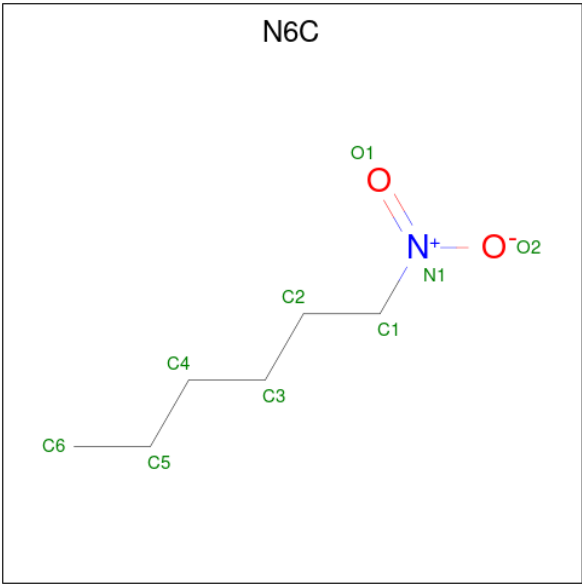
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).





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

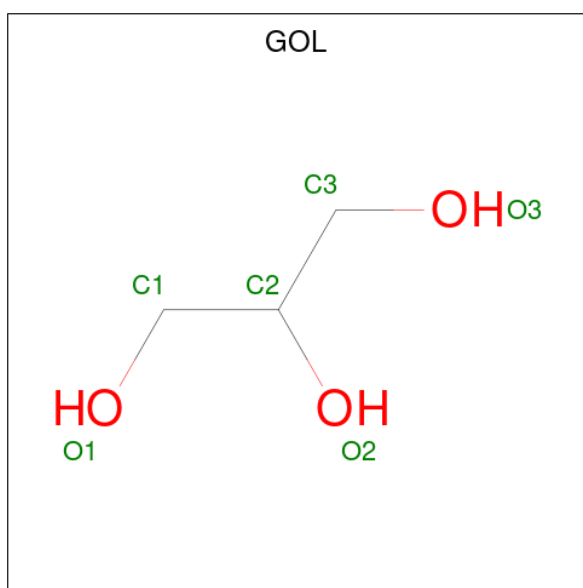
- Molecule 3 is 1-nitrohexane (three-letter code: N6C) (formula:  $C_6H_{13}NO_2$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		

- 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	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		



- Molecule 5 is water.

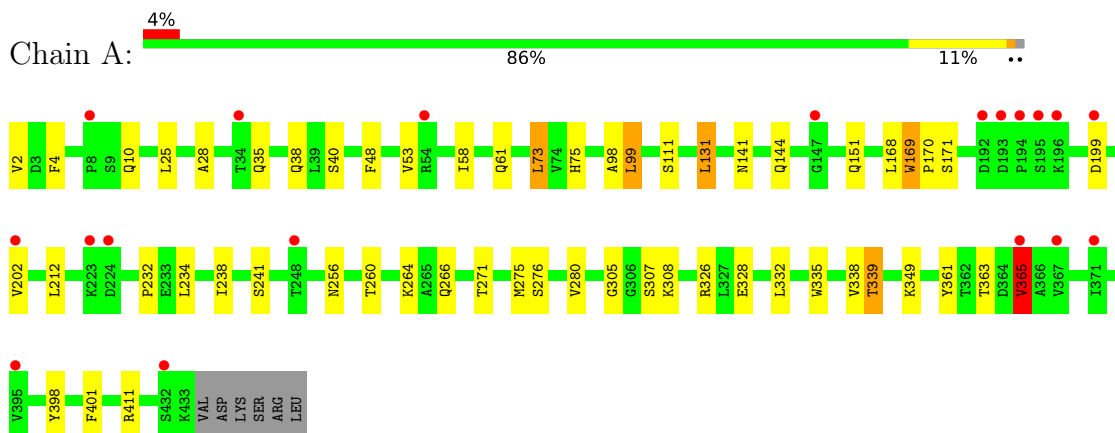
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total 160	O 160	0	0
5	B	150	Total 150	O 150	0	0
5	C	167	Total 167	O 167	0	0
5	D	173	Total 173	O 173	0	0



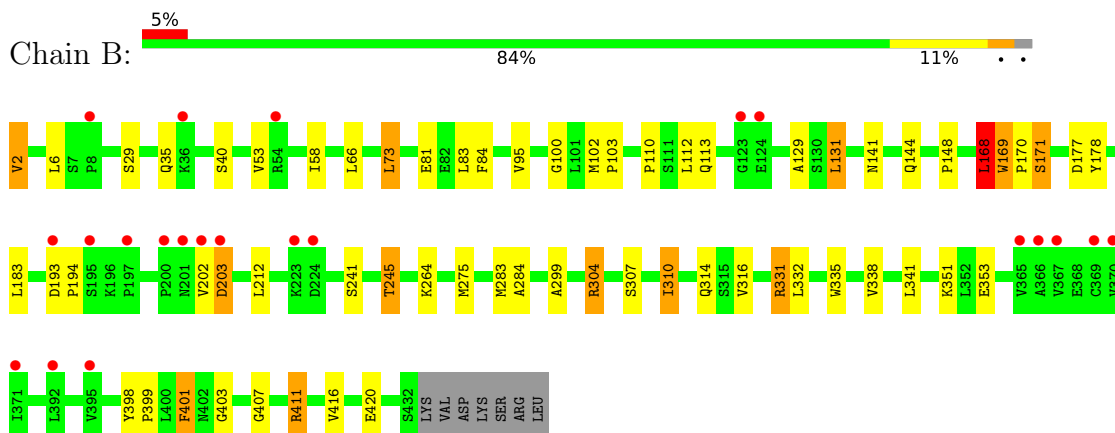
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

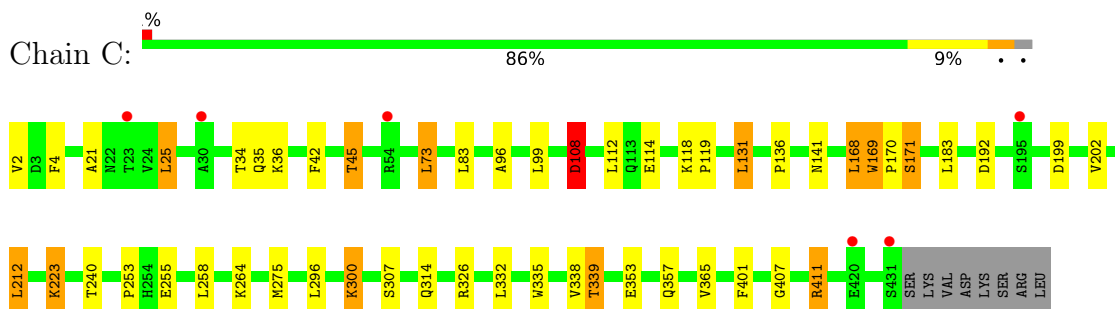
#### • Molecule 1: Nitroalkane oxidase



#### • Molecule 1: Nitroalkane oxidase

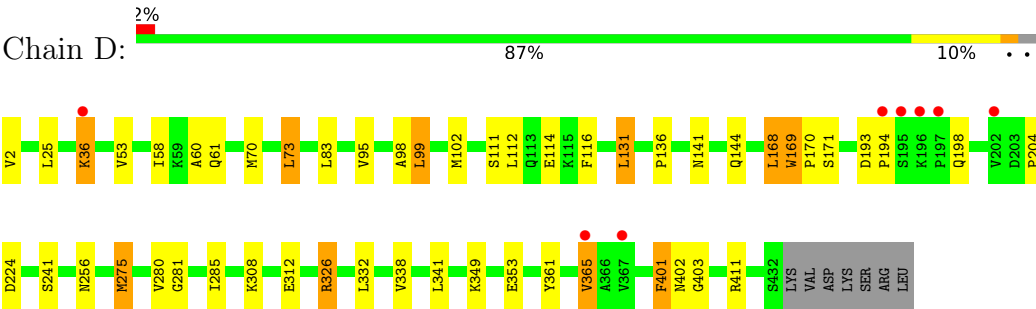


#### • Molecule 1: Nitroalkane oxidase





● Molecule 1: Nitroalkane oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.88Å 107.88Å 338.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 48.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.9 (50.00-2.10) 91.9 (48.66-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.180 , 0.219 0.185 , 0.223	Depositor DCC
$R_{free}$ test set	6169 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14165	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, GOL, N6C

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	0.68	0/3381	0.71	1/4589 (0.0%)
1	B	0.67	0/3369	0.76	4/4575 (0.1%)
1	C	0.69	0/3370	0.73	2/4574 (0.0%)
1	D	0.69	0/3375	0.72	1/4581 (0.0%)
All	All	0.68	0/13495	0.73	8/18319 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	B	331	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	365	VAL	CG1-CB-CG2	5.79	120.16	110.90
1	B	168	LEU	CA-CB-CG	5.59	128.15	115.30
1	D	326	ARG	NE-CZ-NH1	-5.59	117.51	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	108	ASP	CA

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3312	0	3317	35	0
1	B	3300	0	3295	46	0
1	C	3301	0	3310	37	2
1	D	3306	0	3312	31	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
2	C	53	0	31	3	0
2	D	53	0	31	2	0
3	A	9	0	13	2	0
3	B	9	0	13	7	0
3	C	9	0	13	0	0
3	D	9	0	13	2	0
4	A	12	0	16	1	0
4	B	12	0	16	1	0
4	C	12	0	16	2	0
4	D	12	0	16	1	0
5	A	160	0	0	2	0
5	B	150	0	0	2	0
5	C	167	0	0	4	1
5	D	173	0	0	1	0
All	All	14165	0	13474	143	2

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 5.

The worst 5 of 143 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:203:ASP:HB3	5:B:785:HOH:O	1.40	1.19
1:B:102:MET:HE1	1:B:275:MET:HG3	1.36	1.06
1:B:245:THR:HG23	5:B:851:HOH:O	1.74	0.88
1:A:141:ASN:HD21	2:A:500:FAD:H61A	1.20	0.86
1:D:275:MET:HE3	1:D:341:LEU:HD13	1.58	0.83

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLU:OE1	5:C:840:HOH:O[6_554]	1.71	0.49
1:C:108:ASP:OD2	1:C:264:LYS:NZ[6_554]	2.11	0.09

## 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	430/438 (98%)	424 (99%)	5 (1%)	1 (0%)	47	49
1	B	429/438 (98%)	419 (98%)	8 (2%)	2 (0%)	29	26
1	C	428/438 (98%)	418 (98%)	9 (2%)	1 (0%)	47	49
1	D	429/438 (98%)	422 (98%)	5 (1%)	2 (0%)	29	26
All	All	1716/1752 (98%)	1683 (98%)	27 (2%)	6 (0%)	41	41

5 of 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

### 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	355/363 (98%)	338 (95%)	17 (5%)	25	24
1	B	351/363 (97%)	331 (94%)	20 (6%)	20	18
1	C	354/363 (98%)	335 (95%)	19 (5%)	22	20
1	D	354/363 (98%)	332 (94%)	22 (6%)	18	15
All	All	1414/1452 (97%)	1336 (94%)	78 (6%)	21	19

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	36	LYS
1	D	312	GLU
1	D	83	LEU
1	D	212	LEU
1	D	365	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	207	GLN
1	D	198	GLN
1	C	256	ASN
1	D	113	GLN
1	D	266	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	N6C	B	600	-	6,8,8	0.29	0	4,8,8	0.61	0
2	FAD	A	500	-	51,58,58	1.43	6 (11%)	60,89,89	1.62	7 (11%)
3	N6C	D	600	-	6,8,8	0.30	0	4,8,8	0.74	0
4	GOL	A	700	-	5,5,5	0.43	0	5,5,5	0.51	0
4	GOL	B	701	-	5,5,5	0.38	0	5,5,5	0.28	0
4	GOL	B	700	-	5,5,5	0.36	0	5,5,5	0.32	0
2	FAD	B	500	-	51,58,58	1.45	8 (15%)	60,89,89	1.63	8 (13%)
4	GOL	C	700	-	5,5,5	0.45	0	5,5,5	0.49	0
4	GOL	C	701	-	5,5,5	0.43	0	5,5,5	0.34	0
4	GOL	D	700	-	5,5,5	0.60	0	5,5,5	0.46	0
4	GOL	A	701	-	5,5,5	0.40	0	5,5,5	0.77	0
3	N6C	A	600	-	6,8,8	0.39	0	4,8,8	0.66	0
2	FAD	C	500	-	51,58,58	1.57	6 (11%)	60,89,89	2.00	9 (15%)
3	N6C	C	600	-	6,8,8	0.33	0	4,8,8	0.57	0
2	FAD	D	500	-	51,58,58	1.48	8 (15%)	60,89,89	1.78	9 (15%)
4	GOL	D	701	-	5,5,5	0.39	0	5,5,5	0.52	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
3	N6C	B	600	-	-	2/5/6/6	-
2	FAD	A	500	-	-	5/30/50/50	0/6/6/6
3	N6C	D	600	-	-	3/5/6/6	-
4	GOL	A	700	-	-	0/4/4/4	-
4	GOL	B	701	-	-	0/4/4/4	-
4	GOL	B	700	-	-	0/4/4/4	-
2	FAD	B	500	-	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	700	-	-	0/4/4/4	-
4	GOL	C	701	-	-	0/4/4/4	-
4	GOL	D	700	-	-	0/4/4/4	-
4	GOL	A	701	-	-	2/4/4/4	-
3	N6C	A	600	-	-	2/5/6/6	-
2	FAD	C	500	-	-	5/30/50/50	0/6/6/6
3	N6C	C	600	-	-	2/5/6/6	-
2	FAD	D	500	-	-	4/30/50/50	0/6/6/6
4	GOL	D	701	-	-	0/4/4/4	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	FAD	C10-N1	6.02	1.41	1.33
2	C	500	FAD	C4X-N5	4.88	1.40	1.33
2	B	500	FAD	C10-N1	4.39	1.38	1.33
2	A	500	FAD	C4X-N5	4.38	1.39	1.33
2	A	500	FAD	C2A-N3A	4.28	1.39	1.32

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FAD	C4-N3-C2	7.77	121.70	115.14
2	D	500	FAD	N3A-C2A-N1A	-6.05	119.22	128.68
2	A	500	FAD	N3A-C2A-N1A	-5.85	119.53	128.68
2	D	500	FAD	C4-N3-C2	5.52	119.81	115.14
2	C	500	FAD	N3A-C2A-N1A	-5.41	120.23	128.68

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	GOL	C1-C2-C3-O3
3	B	600	N6C	C1-C2-C3-C4
3	D	600	N6C	C1-C2-C3-C4
3	A	600	N6C	C1-C2-C3-C4
2	A	500	FAD	C2'-C3'-C4'-C5'

There are no ring outliers.

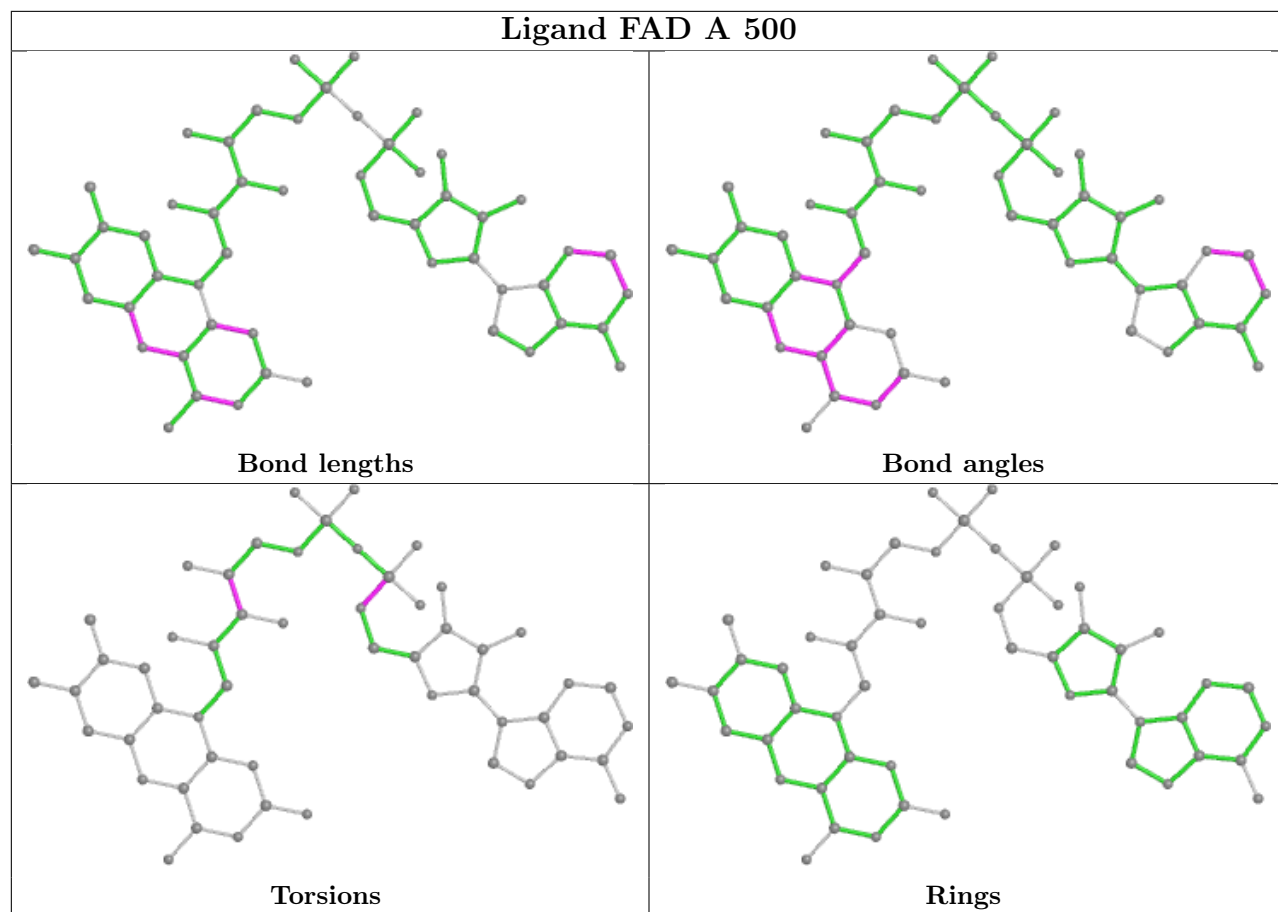
11 monomers are involved in 25 short contacts:



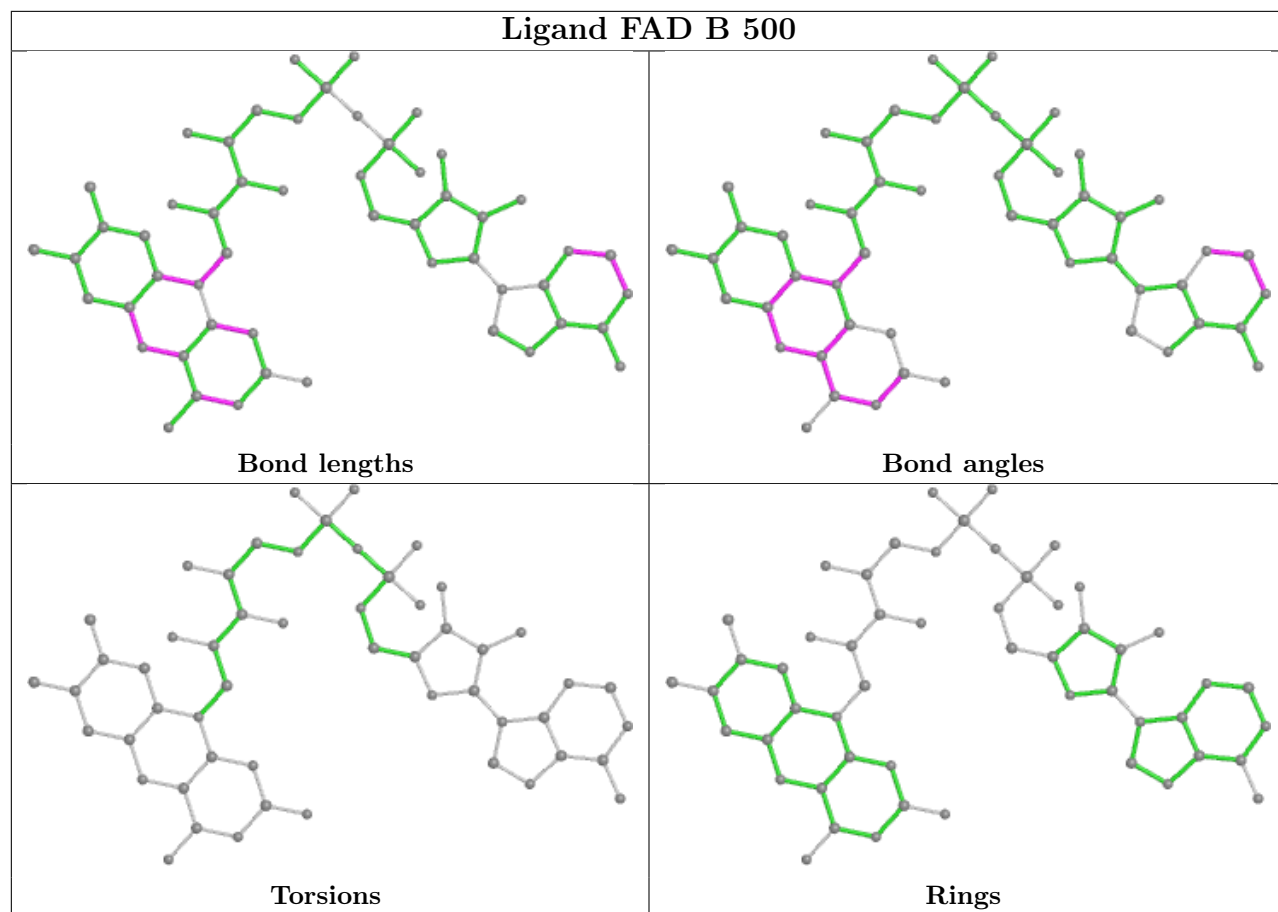
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	600	N6C	7	0
2	A	500	FAD	3	0
3	D	600	N6C	2	0
4	B	701	GOL	1	0
2	B	500	FAD	2	0
4	C	701	GOL	2	0
4	A	701	GOL	1	0
3	A	600	N6C	2	0
2	C	500	FAD	3	0
2	D	500	FAD	2	0
4	D	701	GOL	1	0

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.

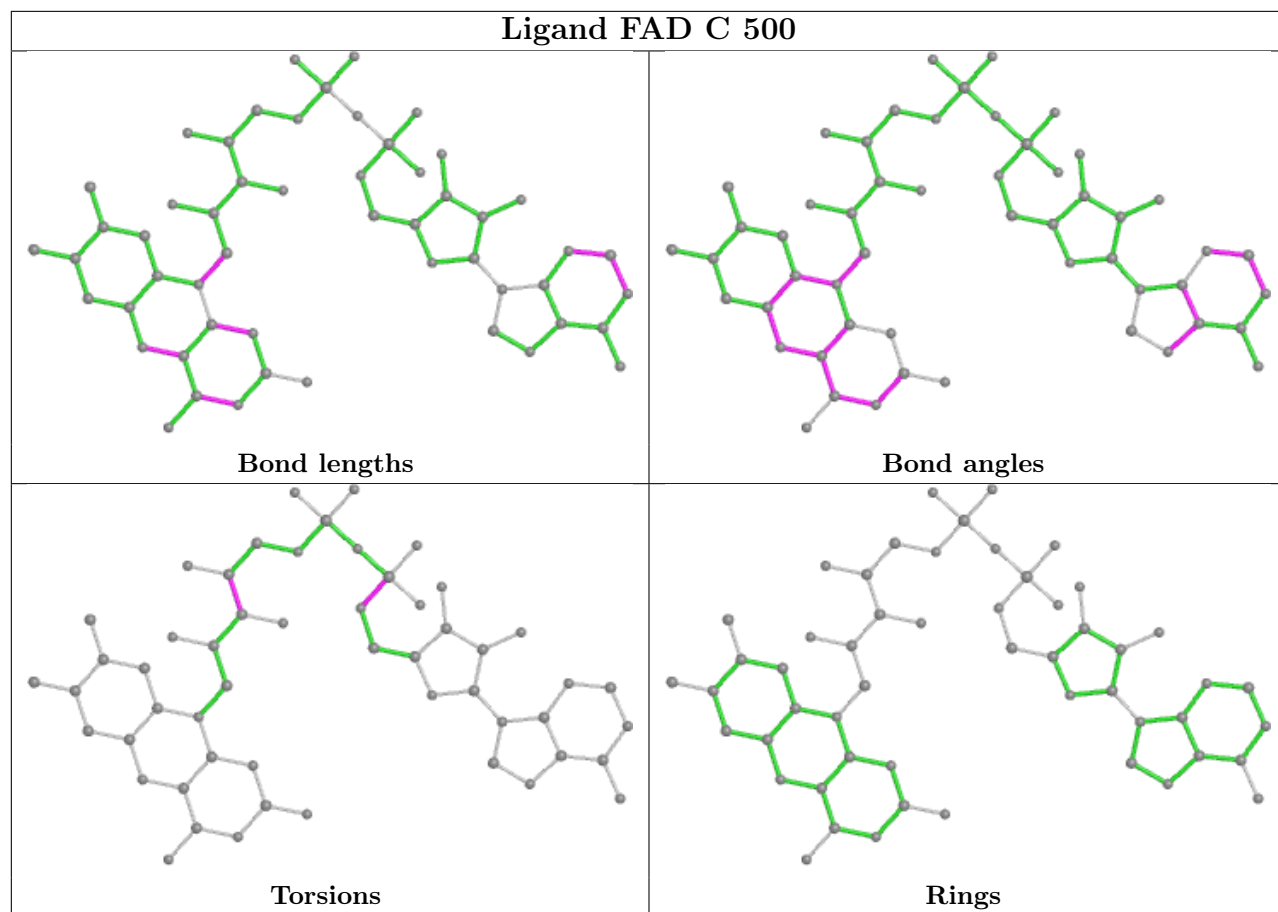




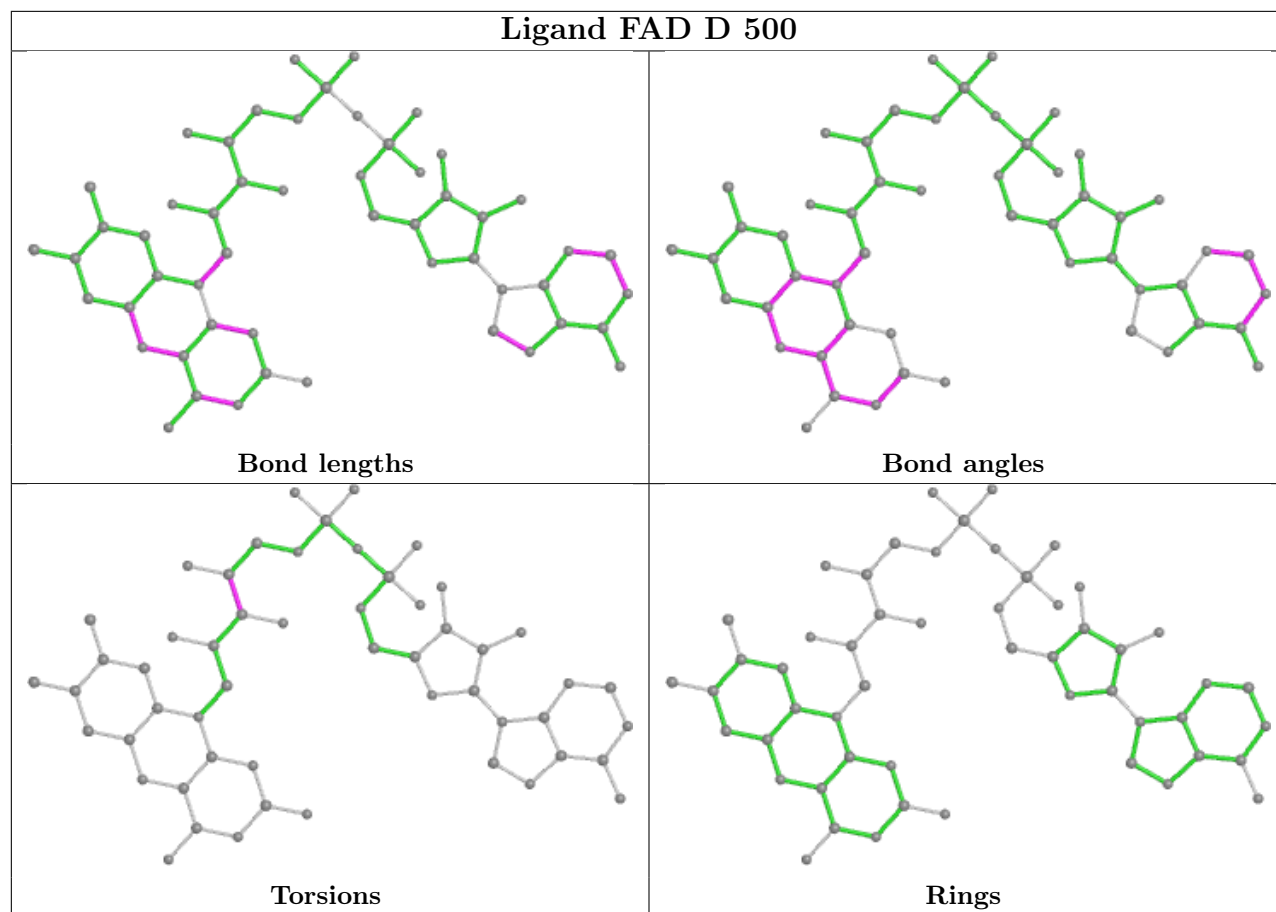












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	432/438 (98%)	0.18	19 (4%)	34 40	25, 36, 51, 63	1 (0%)
1	B	431/438 (98%)	0.25	22 (5%)	28 33	25, 37, 51, 61	1 (0%)
1	C	430/438 (98%)	-0.05	6 (1%)	75 78	24, 33, 49, 66	1 (0%)
1	D	431/438 (98%)	-0.05	9 (2%)	63 68	25, 33, 47, 57	2 (0%)
All	All	1724/1752 (98%)	0.08	56 (3%)	47 54	24, 35, 49, 66	5 (0%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	195	SER	4.2
1	A	224	ASP	4.0
1	A	371	ILE	3.9
1	A	195	SER	3.8
1	C	431	SER	3.7

### 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.

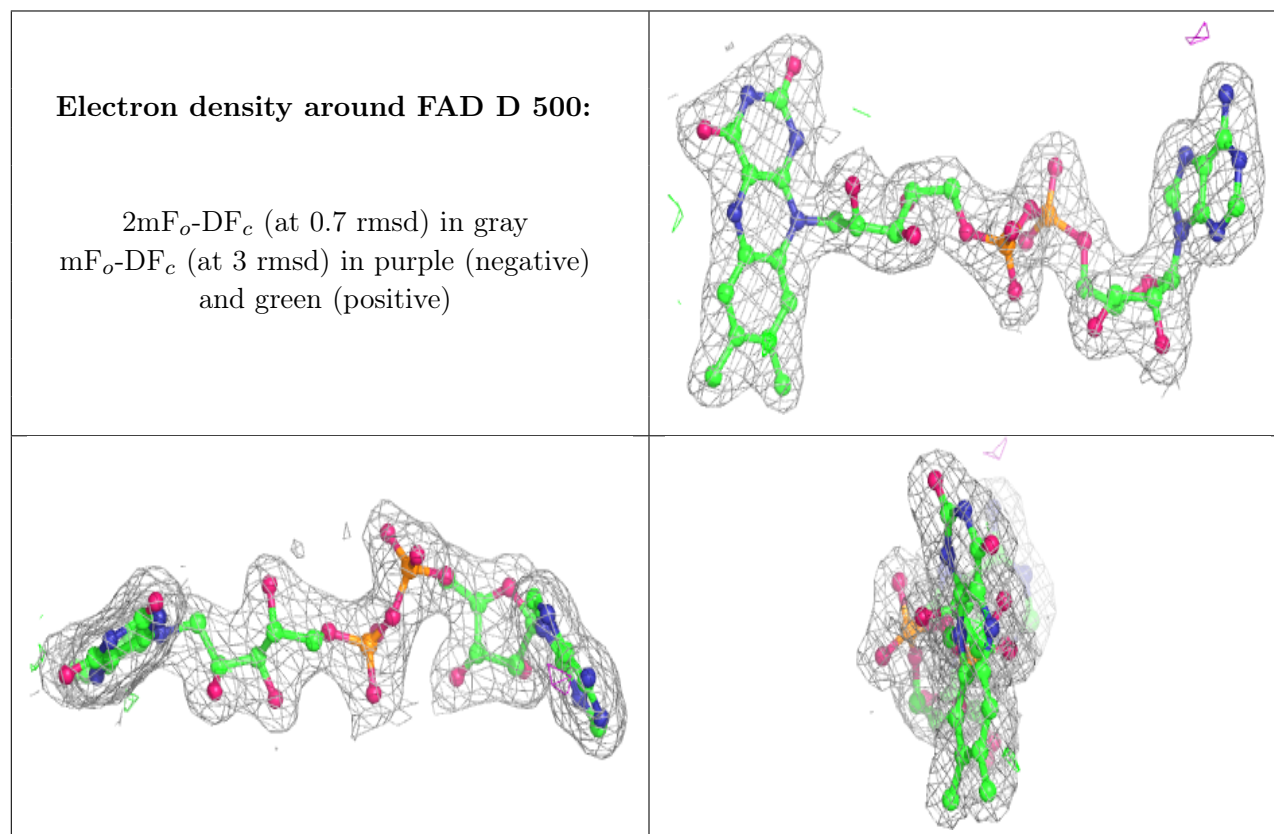
### 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
3	N6C	C	600	9/9	0.85	0.23	46,48,53,55	0
3	N6C	D	600	9/9	0.86	0.20	43,44,45,46	0
3	N6C	A	600	9/9	0.87	0.21	48,50,51,52	0
3	N6C	B	600	9/9	0.88	0.23	53,55,56,58	0
4	GOL	B	701	6/6	0.91	0.13	56,58,58,58	0
4	GOL	D	701	6/6	0.92	0.21	53,54,55,56	0
4	GOL	C	701	6/6	0.93	0.12	48,54,55,56	0
4	GOL	A	701	6/6	0.94	0.16	52,54,55,57	0
4	GOL	A	700	6/6	0.94	0.12	35,37,37,38	0
4	GOL	D	700	6/6	0.95	0.11	29,31,32,33	0
4	GOL	B	700	6/6	0.96	0.12	35,38,38,39	0
2	FAD	D	500	53/53	0.97	0.10	23,27,31,32	0
4	GOL	C	700	6/6	0.97	0.11	29,32,33,35	0
2	FAD	A	500	53/53	0.97	0.10	25,30,34,36	0
2	FAD	B	500	53/53	0.97	0.09	27,31,34,38	0
2	FAD	C	500	53/53	0.98	0.12	23,28,31,33	0

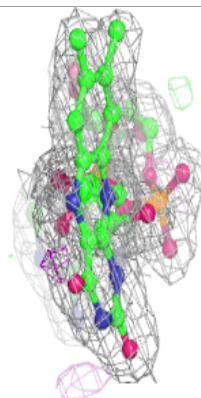
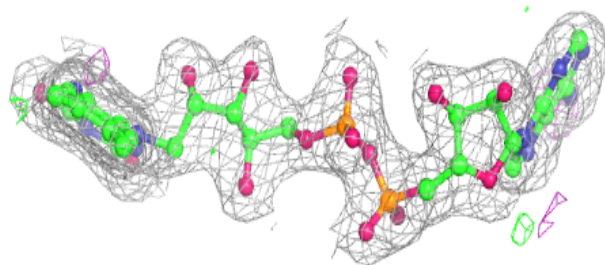
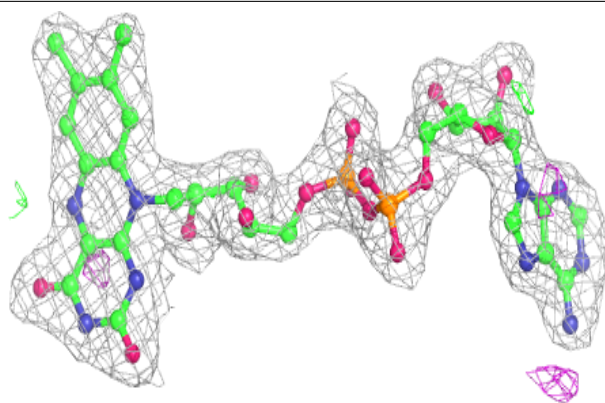
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



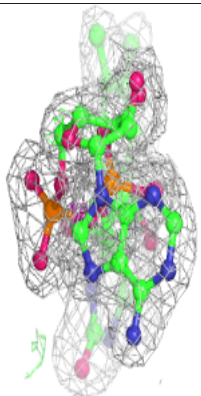
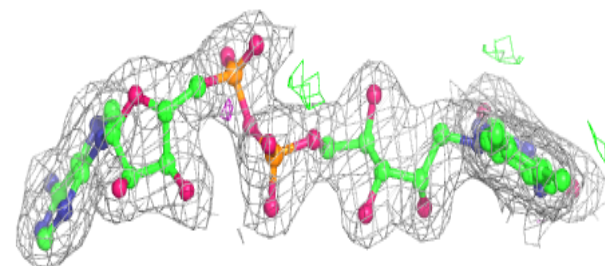
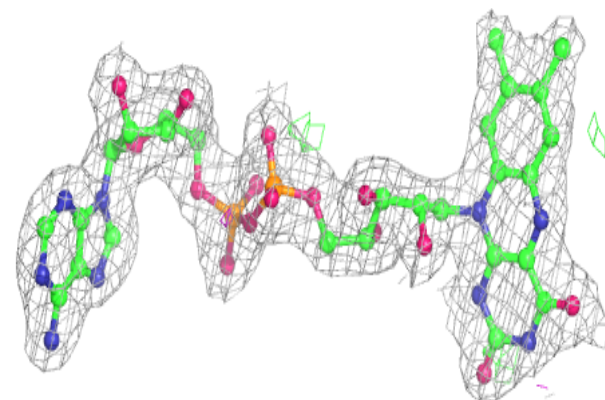


**Electron density around FAD A 500:**

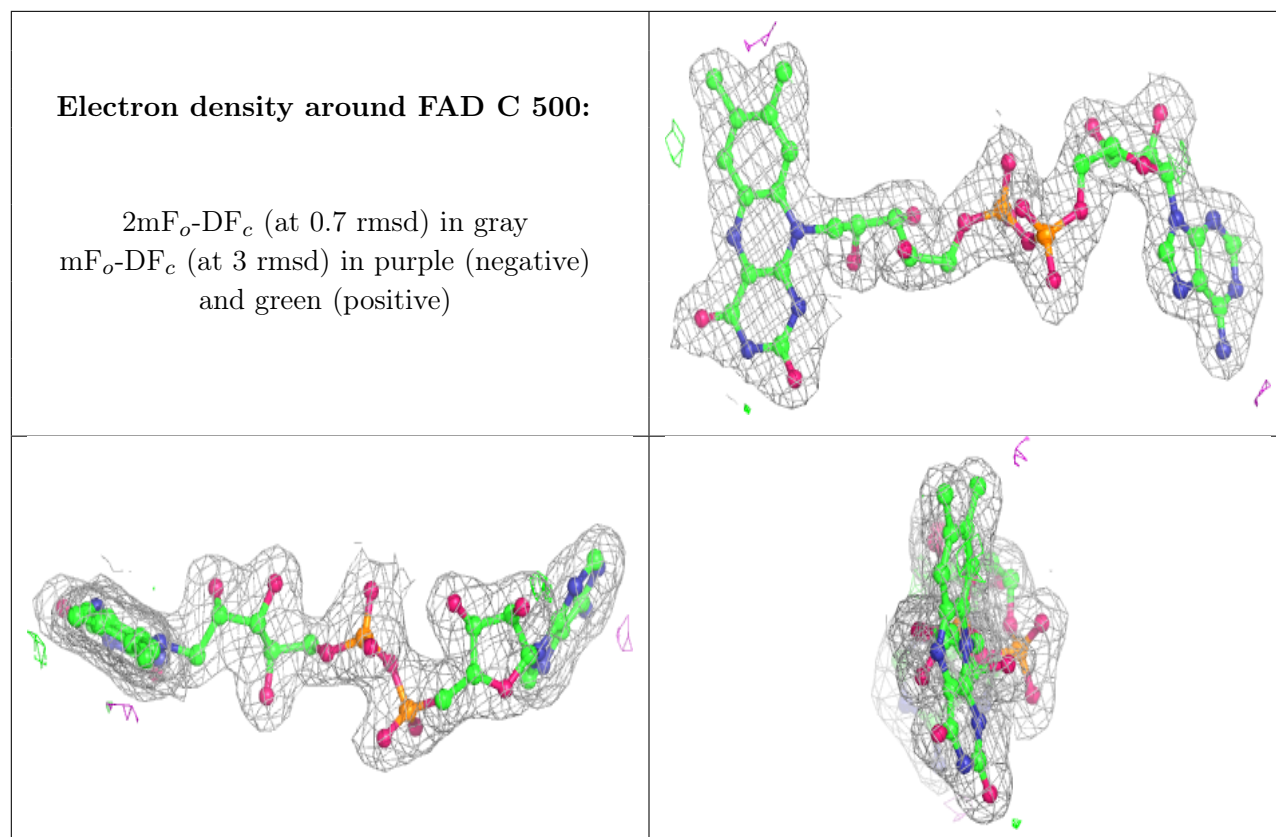
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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.