Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 02:57 pm GMT

PDB ID	:	2VFS
Title	:	Alditol Oxidase from Streptomyces coelicolor A3(2): Complex with Xylitol
Authors	:	Forneris, F.; Mattevi, A.
Deposited on	:	2007-11-05
Resolution	:	1.60 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

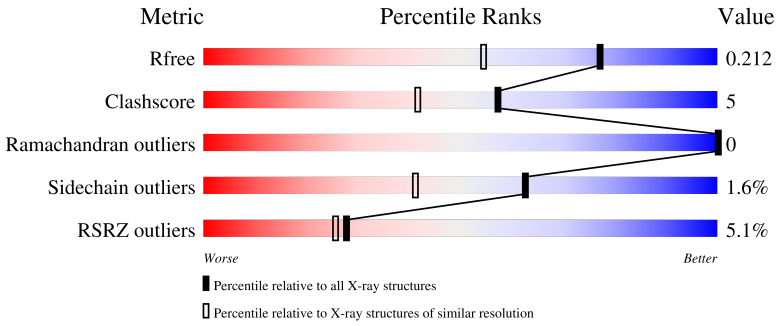
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

2 Entry composition (i)

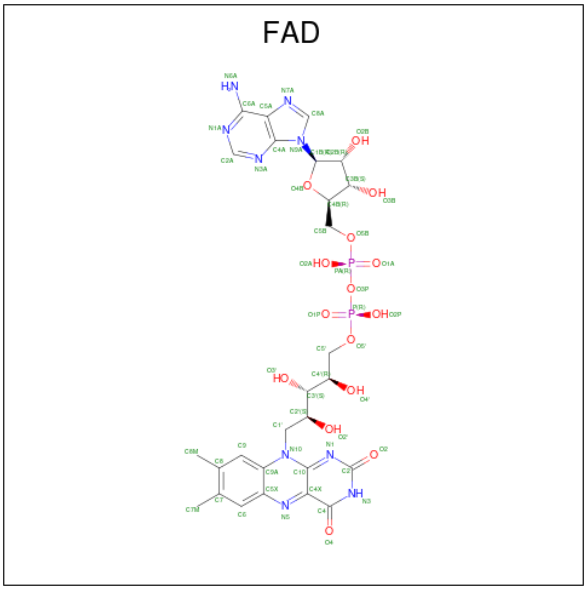
There are 5 unique types of molecules in this entry. The entry contains 3524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XYLITOL OXIDASE.

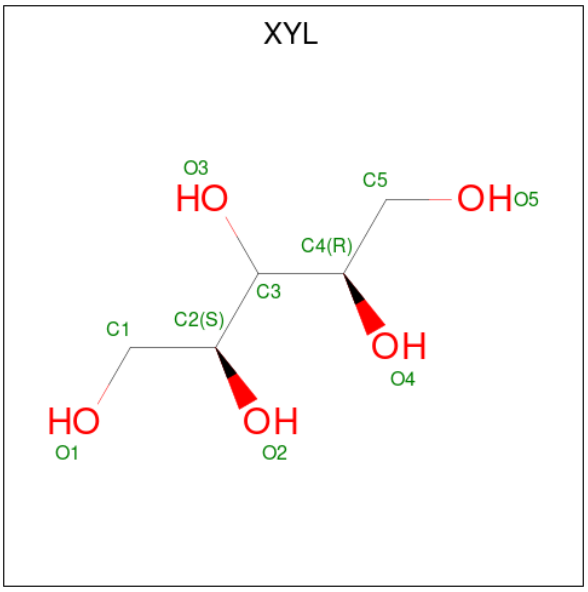
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	1	0
			3104	1973	552	570	9			

- 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		

- Molecule 3 is Xylitol (three-letter code: XYL) (formula: $C_5H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	356	Total O 356 356	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.96Å 67.08Å 59.81Å 90.00° 94.83° 90.00°	Depositor
Resolution (Å)	33.54 – 1.60 33.54 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (33.54-1.60) 94.1 (33.54-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.211 0.174 , 0.212	Depositor DCC
R_{free} test set	2626 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3524	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, XYL, 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	0.86	0/3185	0.73	1/4356 (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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	LEU	CA-CB-CG	7.22	131.90	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	417	ALA	Peptide

4.2 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	3104	0	3081	30	0
2	A	53	0	30	5	0
3	A	10	0	12	1	0
4	A	1	0	0	0	0
5	A	356	0	0	9	1
All	All	3524	0	3123	30	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:O	5:A:2128:HOH:O	1.57	1.21
1:A:21:LEU:HD13	1:A:32[B]:LEU:CD1	1.94	0.96
1:A:21:LEU:HD13	1:A:32[B]:LEU:HD11	1.49	0.94
1:A:21:LEU:CD1	1:A:32[B]:LEU:HD11	1.97	0.94
1:A:46:HIS:CE1	2:A:1423:FAD:C8M	2.66	0.76
1:A:21:LEU:HD13	1:A:32[B]:LEU:HD13	1.70	0.73
1:A:21:LEU:HD12	1:A:59:VAL:HG11	1.69	0.73
1:A:83:GLY:O	5:A:2087:HOH:O	2.10	0.69
1:A:260:GLU:OE2	1:A:276:ARG:NH1	2.25	0.68
1:A:260:GLU:OE1	5:A:2236:HOH:O	2.12	0.66
1:A:46:HIS:ND1	2:A:1423:FAD:HM81	2.03	0.63
1:A:107:LEU:HD22	2:A:1423:FAD:HM73	1.82	0.62
1:A:21:LEU:HD12	1:A:32[B]:LEU:HD11	1.82	0.61
1:A:295:ARG:NH2	5:A:2128:HOH:O	1.82	0.58
1:A:227:LYS:HZ1	1:A:274:HIS:HD2	1.52	0.58
1:A:260:GLU:HG3	5:A:2250:HOH:O	2.06	0.55
1:A:21:LEU:HD12	1:A:59:VAL:CG1	2.34	0.55
1:A:17:ALA:HA	5:A:2014:HOH:O	2.09	0.53
1:A:46:HIS:ND1	2:A:1423:FAD:C8	2.66	0.52
1:A:274:HIS:HE1	1:A:320:GLU:OE2	1.93	0.52
1:A:227:LYS:NZ	1:A:274:HIS:HD2	2.06	0.52
1:A:343:HIS:CE1	3:A:1424:XYL:H11	2.45	0.51
1:A:21:LEU:CD1	1:A:32[B]:LEU:CD1	2.68	0.50
1:A:46:HIS:CG	2:A:1423:FAD:C8M	2.81	0.49
1:A:297:HIS:HD2	5:A:2120:HOH:O	1.99	0.45
1:A:16:THR:HG21	1:A:56:ASP:OD1	2.18	0.43
1:A:53:GLU:HG2	5:A:2053:HOH:O	2.19	0.43
1:A:71:ASP:HB2	5:A:2074:HOH:O	2.18	0.42
1:A:362:GLU:O	1:A:365:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:HZ1	1:A:274:HIS:CD2	2.34	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2255:HOH:O	5:A:2312:HOH:O[4_546]	2.09	0.11

4.3 Torsion angles

4.3.1 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	413/422 (98%)	403 (98%)	10 (2%)	0	100 100

There are no Ramachandran outliers to report.

4.3.2 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	315/322 (98%)	310 (98%)	5 (2%)	62 41

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	103	ASN
1	A	111	SER
1	A	228	ARG
1	A	348	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	103	ASN
1	A	185	HIS
1	A	274	HIS
1	A	297	HIS

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\|>2$
2	FAD	A	1423	1	53,58,58	1.38	5 (9%)	68,89,89	1.28	5 (7%)
3	XYL	A	1424	-	9,9,9	0.88	1 (11%)	11,11,11	1.09	1 (9%)

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	1423	1	-	0/30/50/50	0/6/6/6
3	XYL	A	1424	-	-	0/12/12/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1423	FAD	C4X-N5	5.44	1.41	1.30
2	A	1423	FAD	C2A-N3A	3.65	1.38	1.32
2	A	1423	FAD	C2A-N1A	3.32	1.40	1.33
2	A	1423	FAD	C10-N1	3.23	1.39	1.33
2	A	1423	FAD	C5'-C4'	2.29	1.55	1.51
3	A	1424	XYL	C4-C3	2.10	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1423	FAD	N3A-C2A-N1A	-4.63	121.44	128.68
2	A	1423	FAD	C4X-C10-N10	3.55	121.67	116.48
2	A	1423	FAD	C5A-C6A-N6A	3.53	125.72	120.35
2	A	1423	FAD	O3'-C3'-C2'	3.01	116.09	108.81
2	A	1423	FAD	C10-C4X-N5	-2.48	119.59	124.86
3	A	1424	XYL	O1-C1-C2	2.05	115.54	111.07

There are no chirality outliers.

There are no torsion outliers.

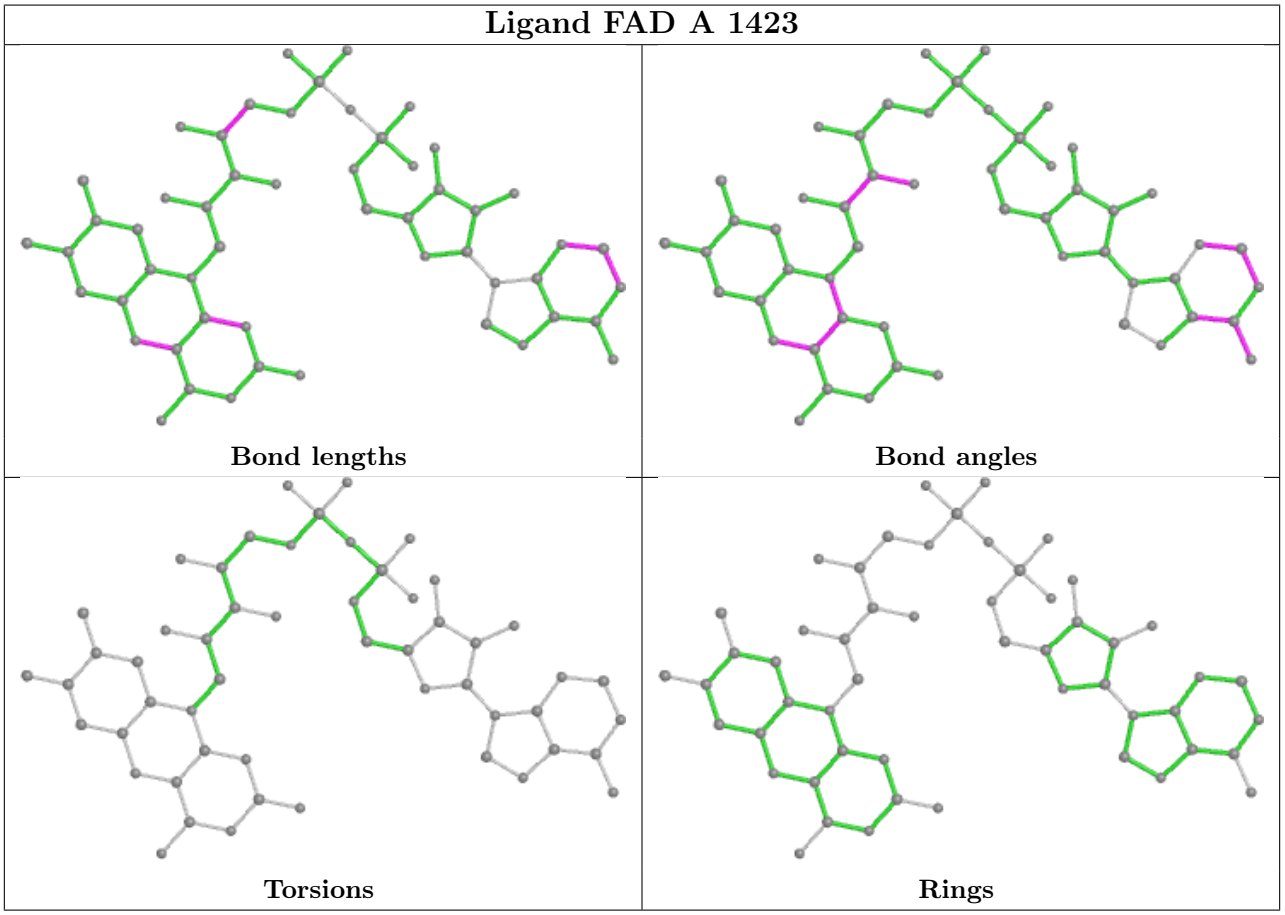
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1423	FAD	5	0
3	A	1424	XYL	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FAD A 1423



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	414/422 (98%)	0.30	21 (5%) 28 26	9, 17, 30, 44	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	GLY	6.4
1	A	417	ALA	5.6
1	A	16	THR	5.5
1	A	55	GLY	5.0
1	A	5	THR	4.9
1	A	56	ASP	4.1
1	A	235	ASP	4.0
1	A	17	ALA	3.8
1	A	75	ALA	3.5
1	A	20	LEU	3.5
1	A	74	THR	2.9
1	A	236	GLY	2.8
1	A	351	ALA	2.6
1	A	154	GLU	2.6
1	A	233	PRO	2.6
1	A	105	ALA	2.4
1	A	18	LYS	2.4
1	A	76	ALA	2.3
1	A	359	ARG	2.2
1	A	120	THR	2.1
1	A	415	VAL	2.0

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

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

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

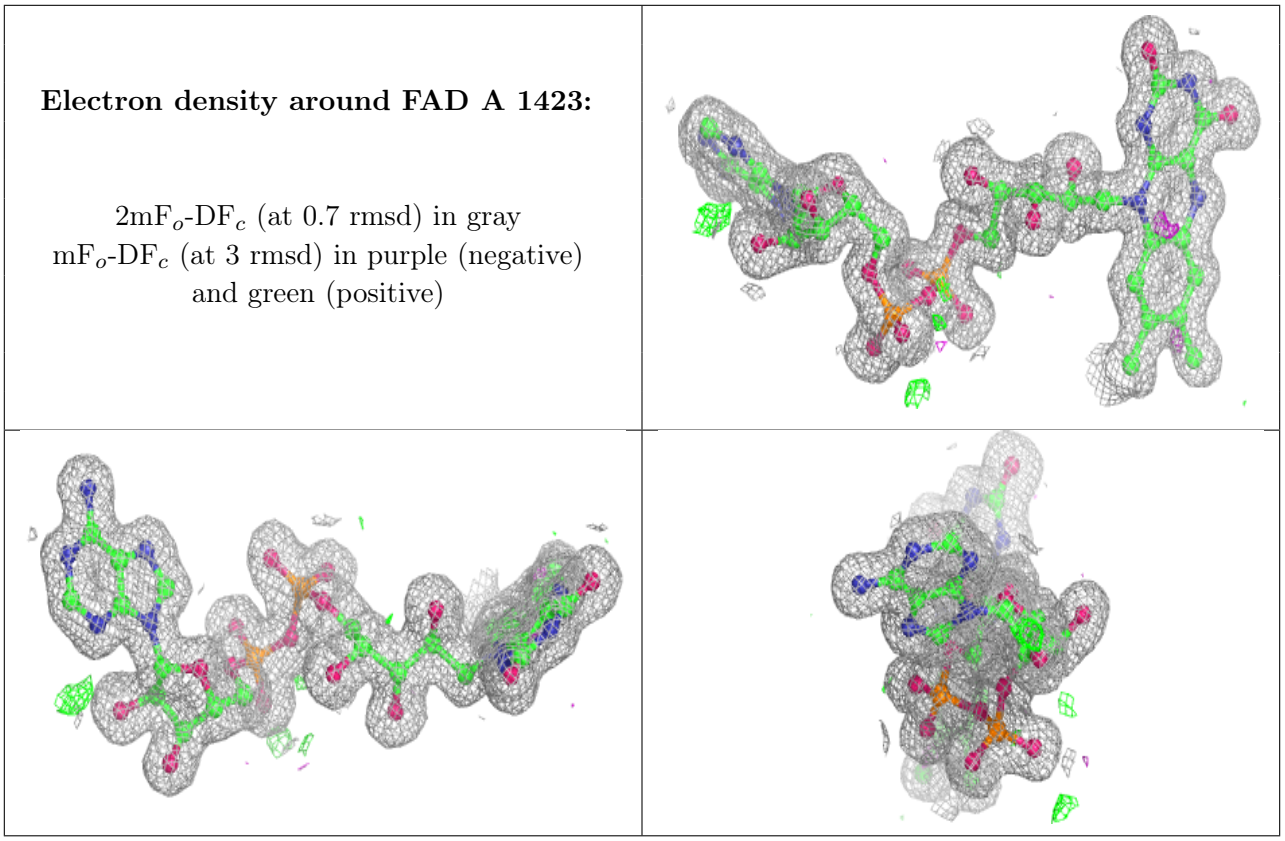
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	A	1423	53/53	0.97	0.12	8,10,12,15	0
3	XYL	A	1424	10/10	0.97	0.15	13,15,16,17	0
4	CL	A	1425	1/1	0.99	0.03	20,20,20,20	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 1423:

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



5.5 Other polymers (i)

There are no such residues in this entry.