wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 03:48 AM JST

PDB ID	:	4YTZ / pdb_00004ytz
Title	:	Rat xanthine oxidoreductase, C-terminal deletion protein variant, crystal grown without dithiothreitol
Authors	:	Nishino, T.; Okamoto, K.; Kawaguchi, Y.; Matsumura, T.; Eger, B.T.; Pai, E.F.; Nishino, T.
Deposited on	:	2015-03-18
Resolution	:	2.30 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*
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:

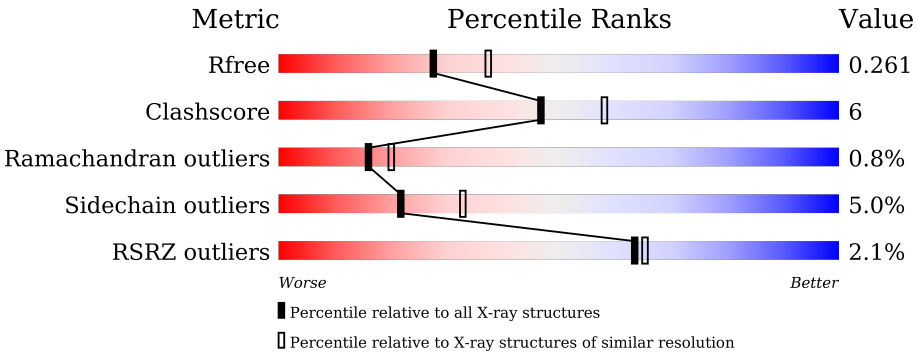
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 >=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 <=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	1315	2% 80% 16%
1	B	1315	2% 82% 13%

2 Entry composition

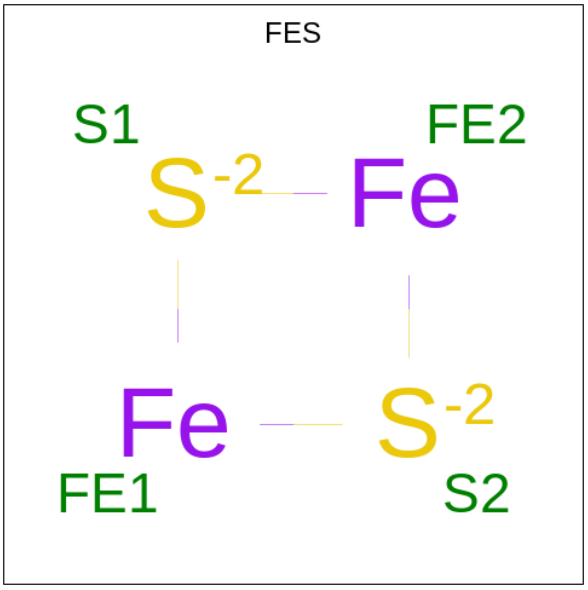
There are 7 unique types of molecules in this entry. The entry contains 20067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xanthine dehydrogenase/oxidase.

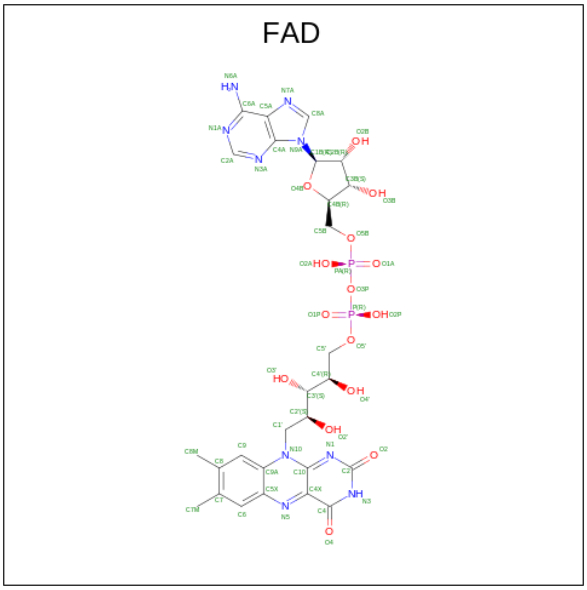
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1289	Total	C	N	O	S	0	0	0
			9964	6314	1714	1873	63			
1	B	1273	Total	C	N	O	S	0	0	0
			9840	6232	1696	1849	63			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



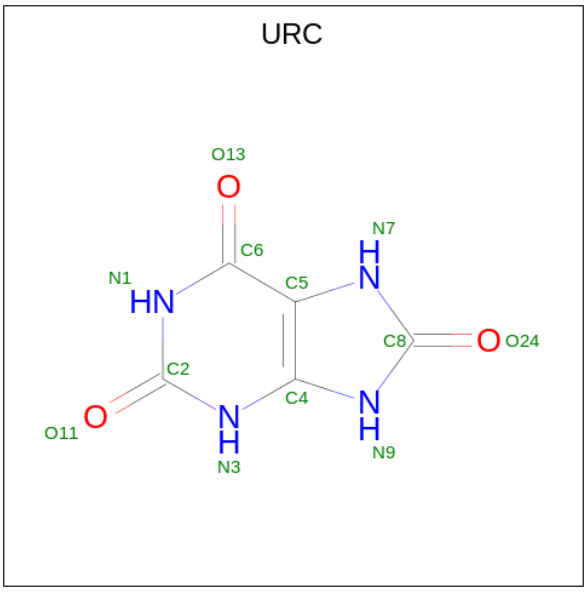
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Fe	S		0	0
			4	2	2			
2	A	1	Total	Fe	S		0	0
			4	2	2			
2	B	1	Total	Fe	S		0	0
			4	2	2			
2	B	1	Total	Fe	S		0	0
			4	2	2			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is URIC ACID (CCD ID: URC) (formula: $C_5H_4N_4O_3$).



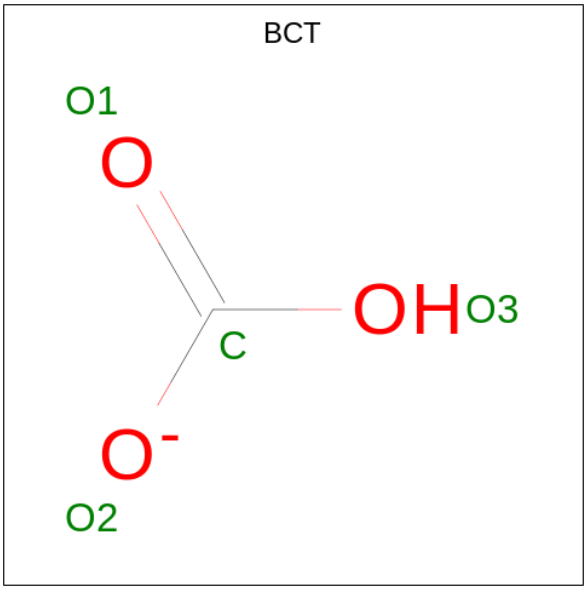
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	5	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 12 5 4 3	0	0

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0
6	B	2	Total Ca 2 2	0	0

- Molecule 7 is water.

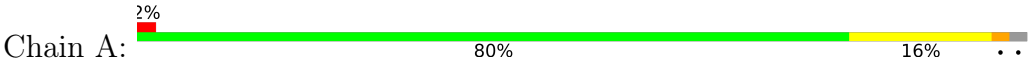
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	40	Total O 40 40	0	0
7	B	65	Total O 65 65	0	0

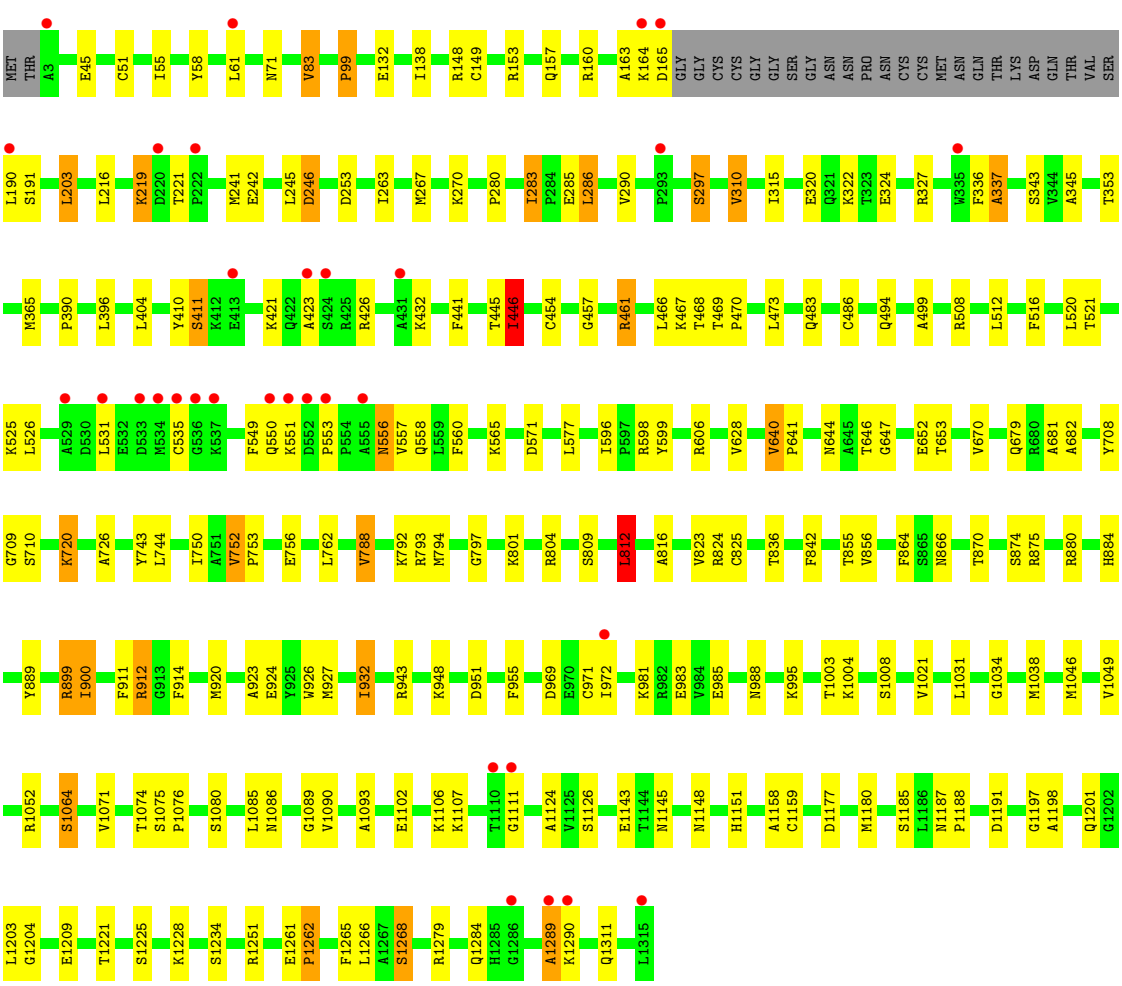
3 Residue-property plots (i)

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: Xanthine dehydrogenase/oxidase

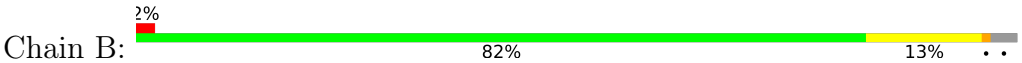
Chain A:

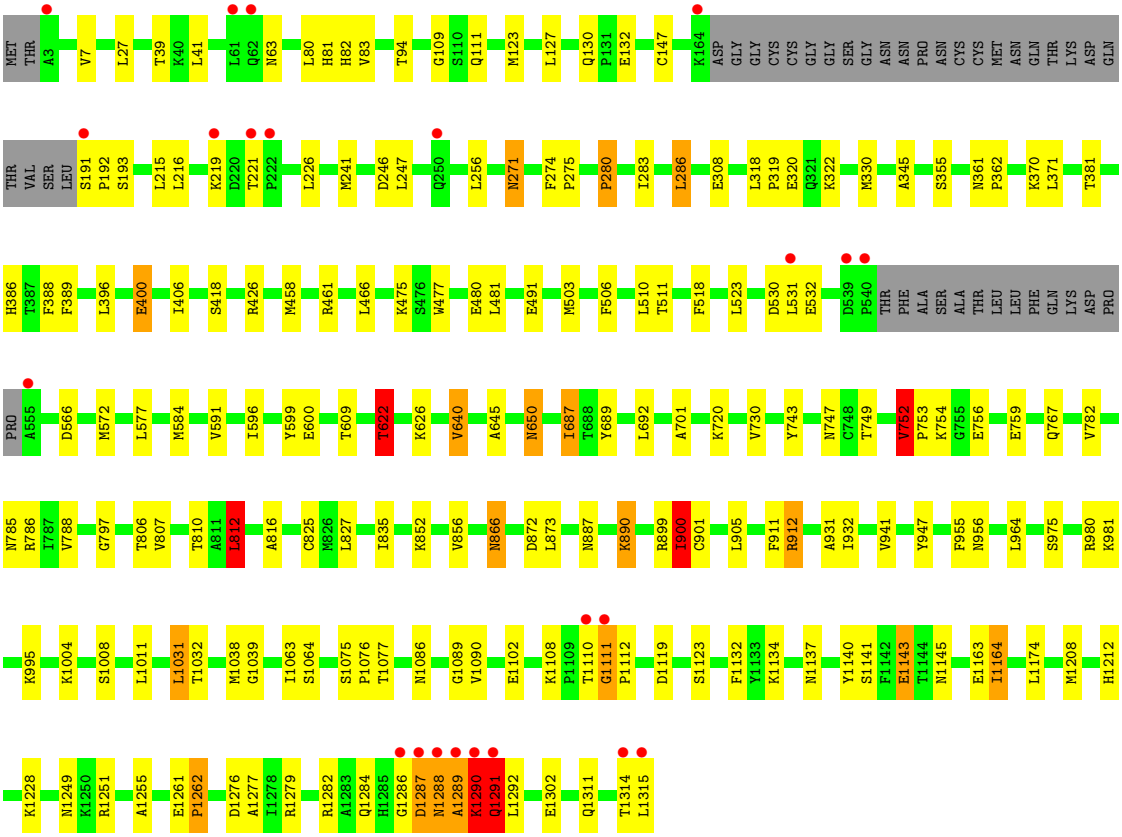




• Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:




MET THR A3 V7 L27 T39 K40 L41 L61 Q62 N63 L80 H81 H82 V83 T94 G109 S110 Q111 M123 L127 Q130 P131 E132 C147 K164 ASP GLY GLY CYS CYS GLY GLY SER GLY ASN ASN PRO ASN CYS CYS MET ASN GLN THR LYS ASP GLN
THR VAL SER LEU S191 P192 S193 L215 L216 K219 D220 T221 P222 L226 M241 D246 L247 Q250 L256 N271 F274 P275 P280 I283 L286 E308 L318 P319 E320 Q321 K322 M330 A345 S355 N361 P362 K370 L371 T381
H386 T387 F388 F389 L396 E400 I406 S418 R426 M458 R461 L466 K475 S476 W477 E480 L481 E491 M503 F506 L510 T511 F518 L523 D530 L531 E532 D539 P540 THR PHE ALA SER ALA THR LEU LEU PHE GLN LYS ASP PRO
PRO A555 D566 M572 L577 M584 V591 I596 Y599 E600 T609 T622 K626 V640 A645 N650 I687 T688 Y689 L692 A701 K720 V730 Y743 N747 C748 T749 V752 P753 K754 G755 E756 E759 Q767 V782
N785 R786 T787 V788 G797 T806 V807 T810 A811 L812 A816 C825 M826 L827 I835 K852 V856 N866 D872 L873 N887 K890 R899 I900 C901 L905 F911 R912 A931 I932 V941 Y947 F955 N956 L964 S975 R980 K981
K995 K1004 S1008 L1011 L1031 T1032 M1038 G1039 I1063 S1064 S1075 P1076 T1077 N1086 G1089 V1090 E1102 K1108 P1109 T1110 G1111 P1112 D1119 S1123 F1132 Y1133 K1134 N1137 Y1140 S1141 F1142 E1143 T1144 N1145 E1163 I1164 L1174 M1208 H1212
K1228 N1249 K1250 R1251 A1255 E1261 P1262 D1276 A1277 I1278 R1279 R1282 A1283 Q1284 H1285 G1286 D1287 N1288 A1289 K1290 Q1291 L1292 E1302 Q1311 T1314 L1315

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.17Å 139.12Å 223.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.30 29.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.87-2.30) 96.8 (29.87-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.207 , 0.265 0.206 , 0.261	Depositor DCC
R_{free} test set	5404 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 21.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20067	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FAD, URC, BCT, FES

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	1.14	8/10174 (0.1%)	1.14	29/13767 (0.2%)
1	B	1.22	15/10045 (0.1%)	1.18	19/13588 (0.1%)
All	All	1.18	23/20219 (0.1%)	1.16	48/27355 (0.2%)

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	B	0	1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	905	LEU	CA-C	7.04	1.59	1.52
1	A	310	VAL	CA-CB	6.48	1.62	1.54
1	B	1064	SER	CA-C	6.38	1.60	1.52
1	B	355	SER	C-O	-5.89	1.16	1.24
1	A	446	ILE	CA-CB	5.78	1.61	1.54

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	ASN	N-CA-C	8.25	122.65	112.58
1	B	1291	GLN	N-CA-C	-7.98	93.79	110.80
1	A	812	LEU	CA-CB-CG	-7.77	89.11	116.30
1	A	1111	GLY	CA-C-N	-7.42	112.68	120.03
1	A	1111	GLY	C-N-CA	-7.42	112.68	120.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1111	GLY	Peptide

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	9964	0	9968	118	0
1	B	9840	0	9841	118	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	53	0	31	2	0
3	B	53	0	31	2	0
4	A	12	0	4	0	0
4	B	12	0	4	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	40	0	0	0	0
7	B	65	0	0	0	0
All	All	20067	0	19879	228	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 6.

The worst 5 of 228 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:1291:GLN:O	1:B:1291:GLN:HG3	1.64	0.96
1:B:1282:ARG:HE	1:B:1290:LYS:CB	1.76	0.96
1:B:1282:ARG:HE	1:B:1290:LYS:HB3	1.30	0.96
1:A:191:SER:HB2	1:A:560:PHE:O	1.71	0.90
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.38	0.88

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	1285/1315 (98%)	1218 (95%)	59 (5%)	8 (1%)	21	27
1	B	1267/1315 (96%)	1213 (96%)	42 (3%)	12 (1%)	14	17
All	All	2552/2630 (97%)	2431 (95%)	101 (4%)	20 (1%)	16	20

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	ALA
1	A	1008	SER
1	B	1008	SER
1	B	1287	ASP
1	B	1288	ASN

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	1088/1109 (98%)	1029 (95%)	59 (5%)	20	29
1	B	1074/1109 (97%)	1025 (95%)	49 (5%)	24	36
All	All	2162/2218 (98%)	2054 (95%)	108 (5%)	22	33

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1234	SER
1	B	400	GLU
1	B	1108	LYS
1	B	83	VAL
1	B	271	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	650	ASN
1	B	1284	GLN
1	B	705	ASN
1	B	1095	GLN
1	A	1088	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\#\|Z\|>2$
3	FAD	B	1403	-	56,58,58	1.27	5 (8%)	81,89,89	1.88	24 (29%)
2	FES	A	1401	1	0,4,4	-	-	-		
4	URC	B	1404	-	11,13,13	4.82	6 (54%)	12,19,19	2.76	5 (41%)
5	BCT	A	1405	-	2,3,3	0.90	0	2,3,3	0.54	0
2	FES	A	1402	1	0,4,4	-	-	-		
5	BCT	B	1405	-	2,3,3	0.95	0	2,3,3	1.34	0
4	URC	A	1404	-	11,13,13	4.76	4 (36%)	12,19,19	2.89	6 (50%)
2	FES	B	1401	1	0,4,4	-	-	-		
2	FES	B	1402	1	0,4,4	-	-	-		
3	FAD	A	1403	-	56,58,58	1.14	5 (8%)	81,89,89	1.57	18 (22%)

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	FAD	B	1403	-	-	2/34/50/50	0/6/6/6
2	FES	A	1401	1	-	-	0/1/1/1
4	URC	B	1404	-	-	-	0/2/2/2
2	FES	A	1402	1	-	-	0/1/1/1
4	URC	A	1404	-	-	-	0/2/2/2
2	FES	B	1401	1	-	-	0/1/1/1
2	FES	B	1402	1	-	-	0/1/1/1
3	FAD	A	1403	-	-	0/34/50/50	0/6/6/6

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1404	URC	O24-C8	11.76	1.48	1.23
4	A	1404	URC	O24-C8	11.63	1.47	1.23
4	A	1404	URC	O13-C6	8.38	1.39	1.23
4	B	1404	URC	O13-C6	7.50	1.37	1.23
4	B	1404	URC	O11-C2	6.21	1.36	1.23

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1404	URC	N7-C8-N9	6.02	116.71	107.19
3	B	1403	FAD	N3A-C2A-N1A	-5.96	119.28	128.60
4	B	1404	URC	N7-C8-N9	5.11	115.28	107.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1404	URC	N3-C2-N1	5.09	123.99	115.80
4	B	1404	URC	N3-C2-N1	4.81	123.54	115.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1403	FAD	O4B-C4B-C5B-O5B
3	B	1403	FAD	C3B-C4B-C5B-O5B

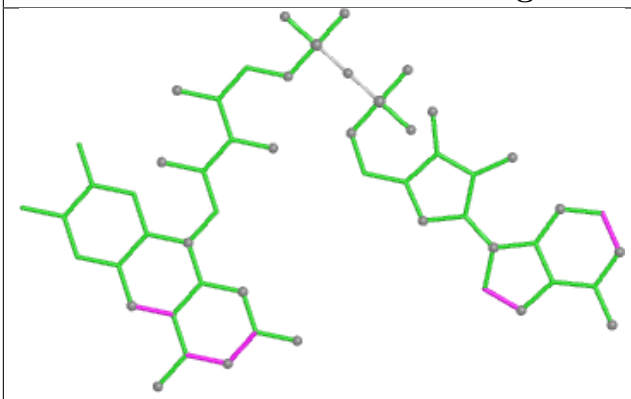
There are no ring outliers.

2 monomers are involved in 4 short contacts:

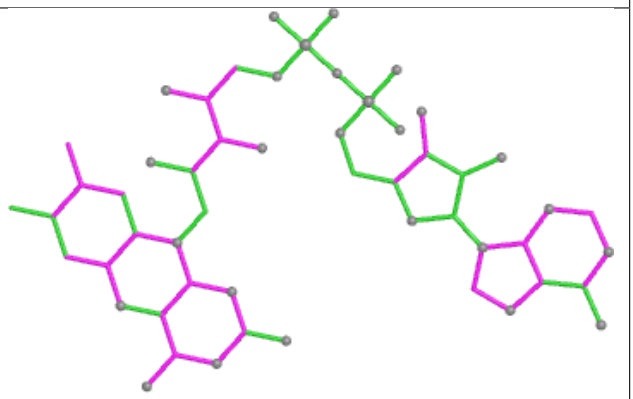
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1403	FAD	2	0
3	A	1403	FAD	2	0

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.

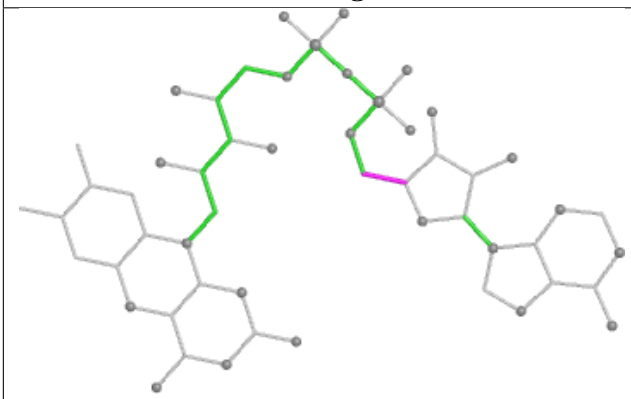
Ligand FAD B 1403



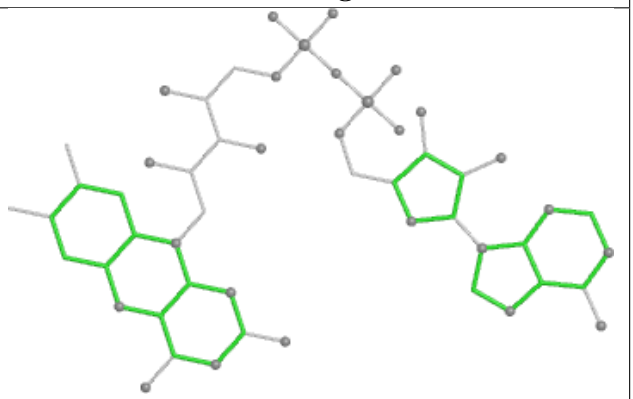
Bond lengths



Bond angles

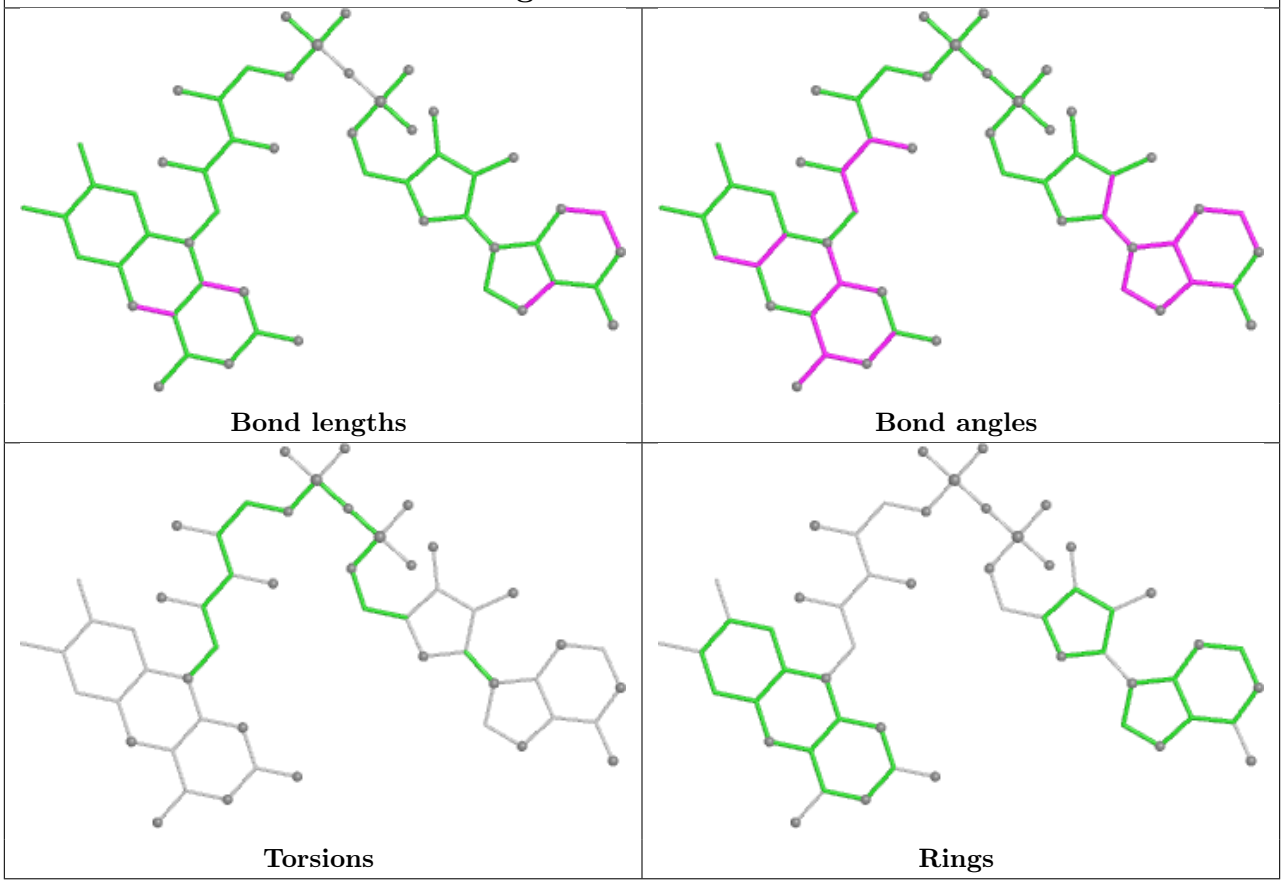


Torsions



Rings

Ligand FAD A 1403



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{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	1289/1315 (98%)	-0.06	32 (2%)	58	60	20, 35, 59, 94	0
1	B	1273/1315 (96%)	-0.33	23 (1%)	67	69	18, 30, 48, 75	0
All	All	2562/2630 (97%)	-0.19	55 (2%)	63	65	18, 32, 56, 94	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1315	LEU	6.2
1	A	536	GLY	5.5
1	A	1315	LEU	4.8
1	A	1289	ALA	4.6
1	A	534	MET	4.6

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

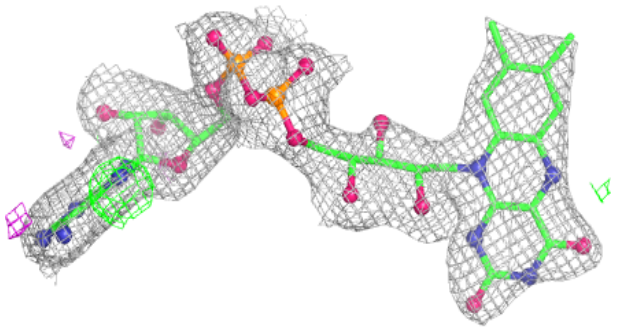
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

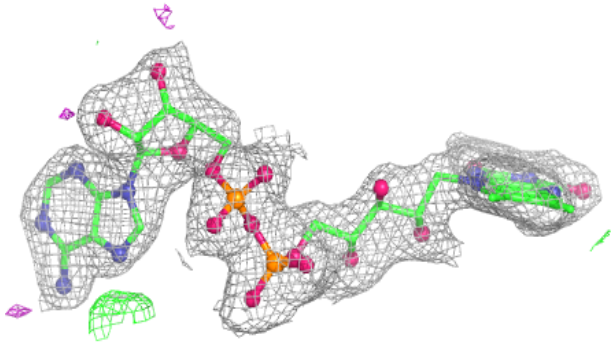
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	URC	A	1404	12/12	0.92	0.08	36,39,41,41	0
4	URC	B	1404	12/12	0.96	0.06	31,34,37,38	0
5	BCT	B	1405	4/4	0.96	0.06	23,24,24,25	0
5	BCT	A	1405	4/4	0.97	0.09	30,33,33,34	0
3	FAD	A	1403	53/53	0.97	0.07	28,35,40,44	0
3	FAD	B	1403	53/53	0.98	0.06	20,25,28,31	0
2	FES	A	1401	4/4	0.99	0.05	31,33,34,35	0
2	FES	A	1402	4/4	0.99	0.03	25,26,26,27	0
2	FES	B	1401	4/4	0.99	0.04	30,31,32,33	0
6	CA	A	1406	1/1	0.99	0.03	31,31,31,31	0
6	CA	A	1407	1/1	0.99	0.03	32,32,32,32	0
6	CA	B	1406	1/1	0.99	0.04	27,27,27,27	0
6	CA	B	1407	1/1	0.99	0.02	29,29,29,29	0
2	FES	B	1402	4/4	1.00	0.02	23,24,25,25	0

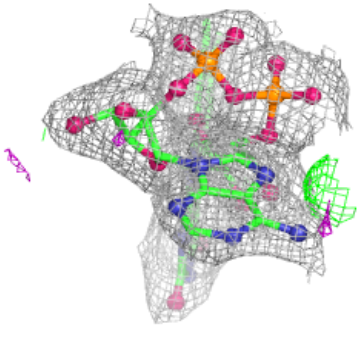
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 1403:

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

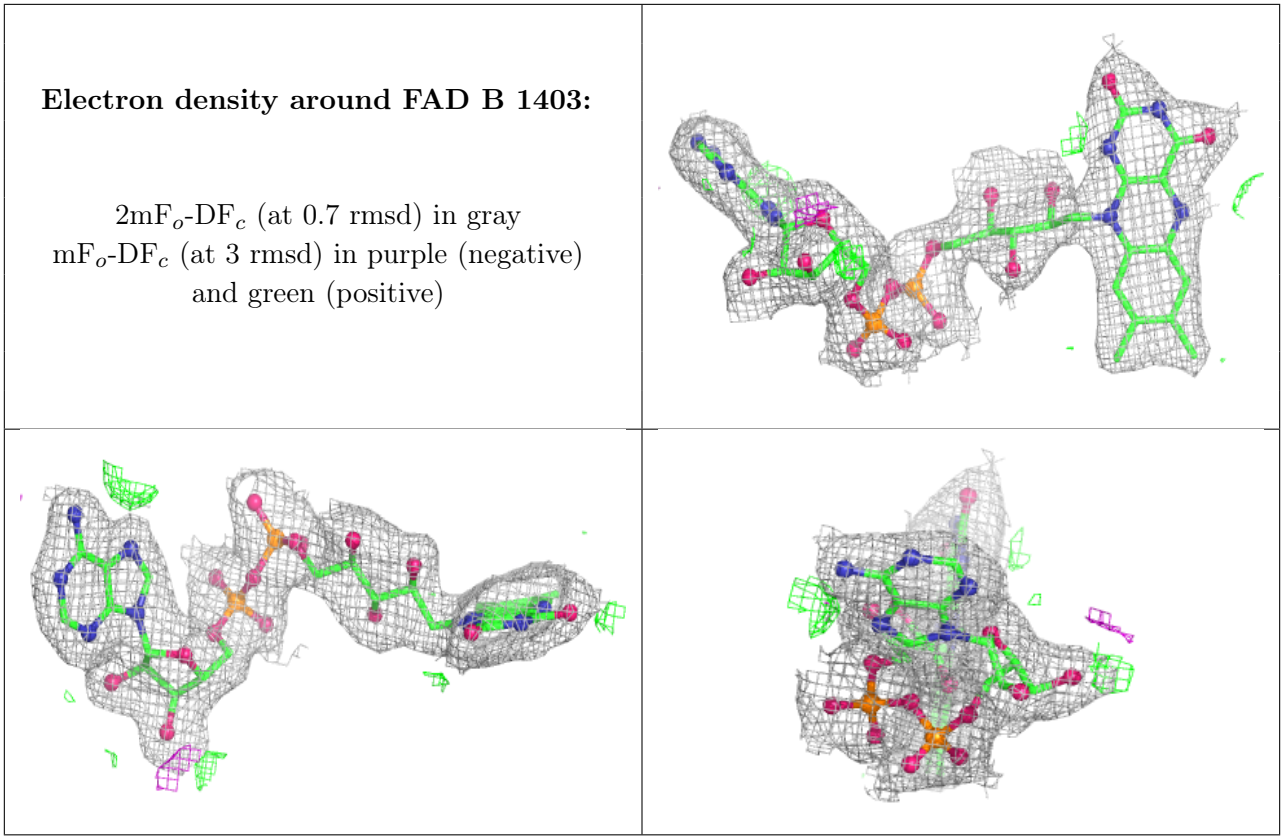






Electron density around FAD B 1403:

$2mF_o$-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.