wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2023 – 04:34 AM EDT

PDB ID	:	3AD7
Title	:	Heterotetrameric Sarcosine Oxidase from Corynebacterium sp. U-96 in complex with methylthio acetate
Authors	:	Suzuki, H.; Moriguchi, T.; Ida, K.
Deposited on	:	2010-01-15
Resolution	:	2.20 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:

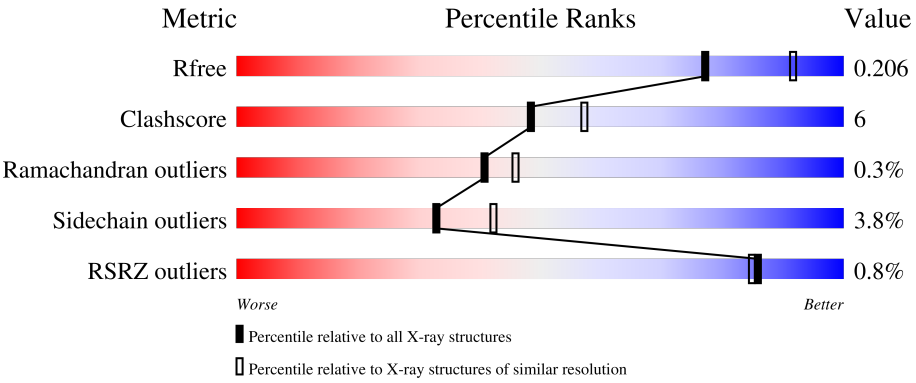
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	964	88% 11%
2	B	404	89% 9%
3	C	203	86% 9%
4	D	99	89% 8%

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
8	FMN	B	406	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 13623 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 Subunit alpha of sarcosine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	963	Total	C	N	O	S	0	0	0
			7229	4507	1287	1413	22			

- Molecule 2 is a protein called Subunit beta of sarcosine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3108	1981	541	576	10			

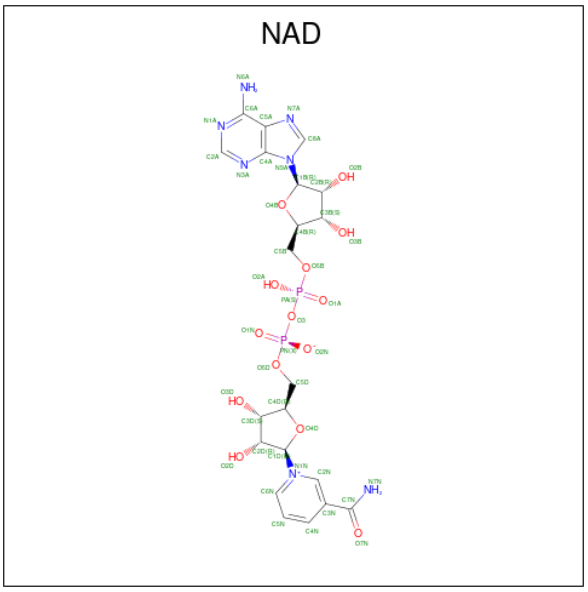
- Molecule 3 is a protein called Subunit gamma of sarcosine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	195	Total	C	N	O	S	0	0	0
			1433	902	257	271	3			

- Molecule 4 is a protein called Subunit delta of sarcosine oxidase.

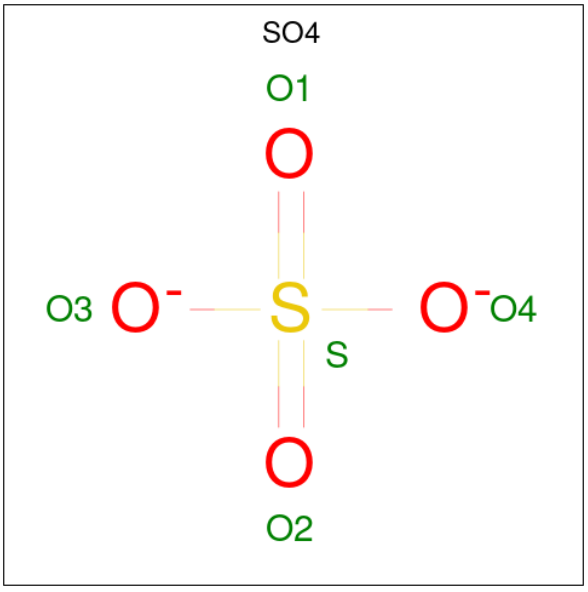
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	91	Total	C	N	O	S	0	0	0
			749	476	135	133	5			

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	O	S		0	0
			5	4	1			
6	A	1	Total	O	S		0	0
			5	4	1			
6	A	1	Total	O	S		0	0
			5	4	1			

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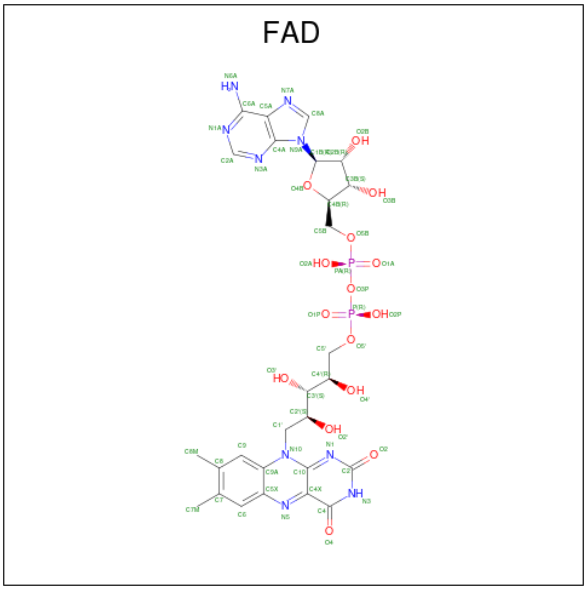
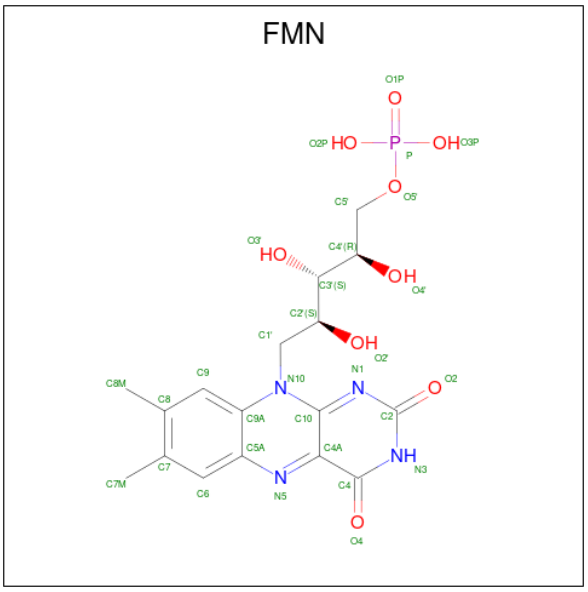
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



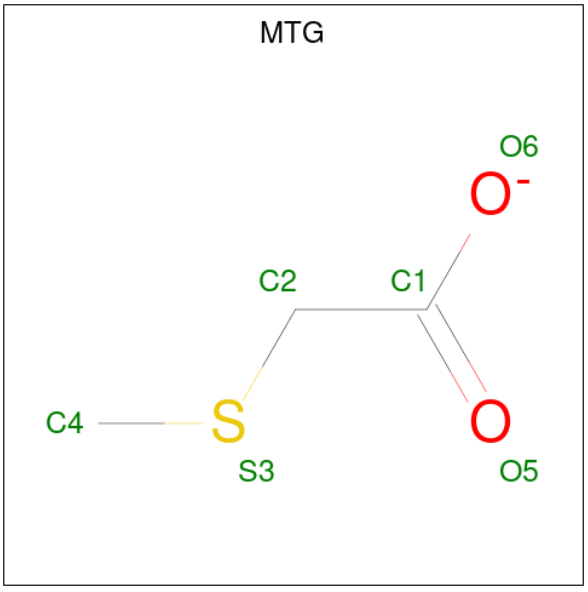
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 8 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 9 is [METHYLTHIO]ACETATE (three-letter code: MTG) (formula: $C_3H_5O_2S$).



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

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total Zn 1 1	0	0

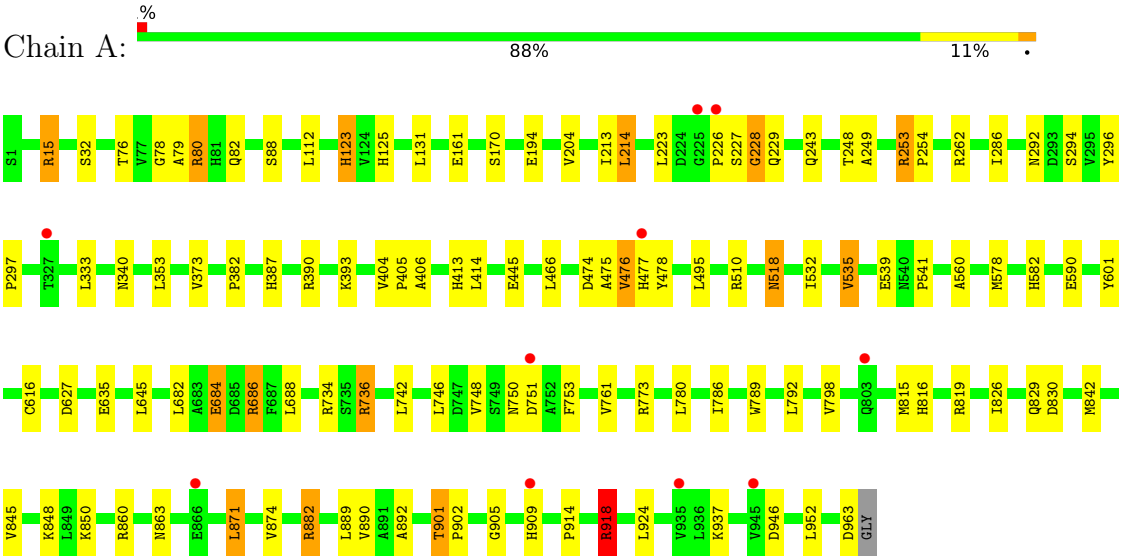
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	558	Total O 558 558	0	0
11	B	184	Total O 184 184	0	0
11	C	117	Total O 117 117	0	0
11	D	65	Total O 65 65	0	0

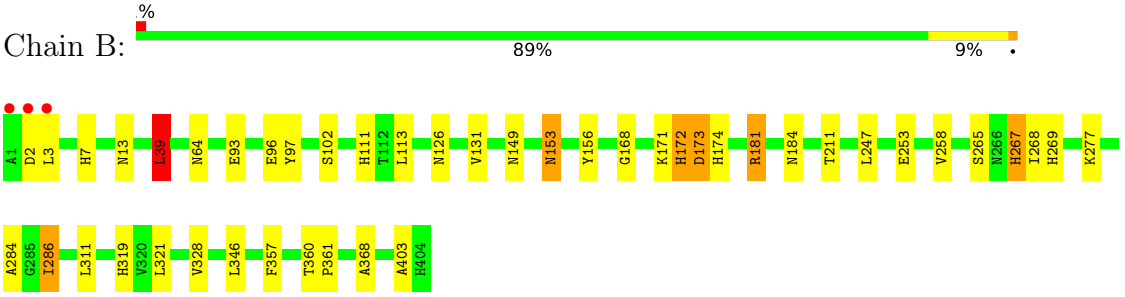
3 Residue-property plots (i)

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.

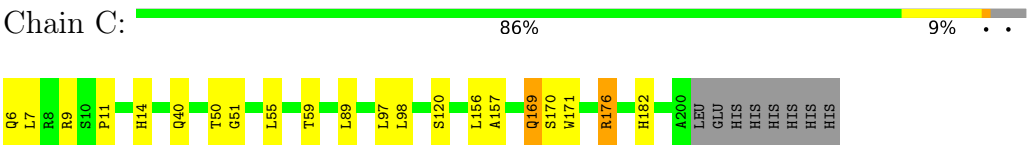
• Molecule 1: Subunit alpha of sarcosine oxidase



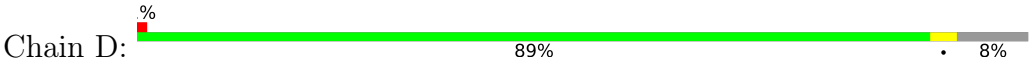
• Molecule 2: Subunit beta of sarcosine oxidase

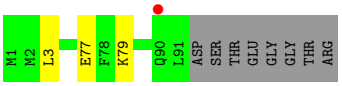


• Molecule 3: Subunit gamma of sarcosine oxidase



• Molecule 4: Subunit delta of sarcosine oxidase




M1
M2
L3
E77
F78
K79
Q90
L91
ASP
SER
THR
GLU
GLY
GLY
THR
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	198.95Å 198.95Å 196.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.53 – 2.20 39.53 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.53-2.20) 100.0 (39.53-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	6.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.205 0.170 , 0.206	Depositor DCC
R_{free} test set	5804 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13623	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: ZN, NAD, FAD, SO4, FMN, MTG

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	0.82	0/7361	0.79	10/10017 (0.1%)
2	B	0.84	0/3189	0.74	3/4340 (0.1%)
3	C	0.88	0/1461	0.86	2/1998 (0.1%)
4	D	0.85	0/772	0.82	1/1040 (0.1%)
All	All	0.84	0/12783	0.79	16/17395 (0.1%)

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
2	B	0	1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	176	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	A	15	ARG	NE-CZ-NH2	-9.47	115.56	120.30
3	C	176	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	A	214	LEU	CA-CB-CG	-7.76	97.46	115.30
1	A	918	ARG	NE-CZ-NH1	6.72	123.66	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	268	ILE	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	7229	0	7104	100	0
2	B	3108	0	3035	41	0
3	C	1433	0	1434	12	0
4	D	749	0	706	1	0
5	A	44	0	26	4	0
6	A	25	0	0	0	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	B	53	0	31	3	0
8	B	31	0	19	10	0
9	B	6	0	5	0	0
10	D	1	0	0	0	0
11	A	558	0	0	12	0
11	B	184	0	0	6	0
11	C	117	0	0	2	0
11	D	65	0	0	0	0
All	All	13623	0	12360	151	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 151 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)
2:B:172:HIS:NE2	8:B:406:FMN:C8M	1.79	1.44
1:A:829:GLN:HB2	1:A:909:HIS:HE1	1.10	1.17
2:B:172:HIS:NE2	8:B:406:FMN:HM83	0.82	1.14
1:A:829:GLN:HB2	1:A:909:HIS:CE1	1.87	1.10
1:A:882:ARG:HG2	1:A:882:ARG:HH11	1.14	1.07

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	961/964 (100%)	936 (97%)	21 (2%)	4 (0%)	34 37
2	B	402/404 (100%)	392 (98%)	9 (2%)	1 (0%)	47 55
3	C	193/203 (95%)	187 (97%)	6 (3%)	0	100 100
4	D	89/99 (90%)	88 (99%)	1 (1%)	0	100 100
All	All	1645/1670 (98%)	1603 (97%)	37 (2%)	5 (0%)	41 46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	476	VAL
1	A	228	GLY
1	A	406	ALA
2	B	284	ALA

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	747/747 (100%)	714 (96%)	33 (4%)	28 35
2	B	319/319 (100%)	309 (97%)	10 (3%)	40 51
3	C	143/151 (95%)	137 (96%)	6 (4%)	30 38
4	D	75/81 (93%)	75 (100%)	0	100 100
All	All	1284/1298 (99%)	1235 (96%)	49 (4%)	33 42

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	882	ARG
2	B	97	TYR
1	A	889	LEU
1	A	918	ARG
2	B	172	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	40	GLN
3	C	158	ASN
1	A	543	GLN
1	A	540	ASN
3	C	169	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\#\|Z\|>2$
6	SO4	C	2564	-	4,4,4	0.36	0	6,6,6	0.33	0
7	FAD	B	405	-	53,58,58	1.31	5 (9%)	68,89,89	1.37	13 (19%)
8	FMN	B	406	-	33,33,33	1.87	10 (30%)	48,50,50	2.17	14 (29%)
6	SO4	D	2566	-	4,4,4	0.17	0	6,6,6	0.18	0
5	NAD	A	965	-	42,48,48	1.72	5 (11%)	50,73,73	1.60	7 (14%)
6	SO4	A	2563	-	4,4,4	0.16	0	6,6,6	0.32	0
6	SO4	B	2568	-	4,4,4	0.16	0	6,6,6	0.34	0
6	SO4	A	2559	-	4,4,4	0.20	0	6,6,6	0.15	0
6	SO4	B	2569	-	4,4,4	0.10	0	6,6,6	0.44	0
6	SO4	A	2567	-	4,4,4	0.11	0	6,6,6	0.40	0
6	SO4	A	2560	-	4,4,4	0.28	0	6,6,6	0.40	0
6	SO4	A	2571	-	4,4,4	0.18	0	6,6,6	0.44	0
9	MTG	B	801	-	5,5,5	0.83	0	4,5,5	1.78	1 (25%)

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
9	MTG	B	801	-	-	1/3/3/3	-
7	FAD	B	405	-	-	3/30/50/50	0/6/6/6
8	FMN	B	406	-	-	9/18/18/18	0/3/3/3
5	NAD	A	965	-	-	4/26/62/62	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	965	NAD	O7N-C7N	6.93	1.37	1.24
5	A	965	NAD	C2N-N1N	5.28	1.41	1.35
8	B	406	FMN	O5'-C5'	-5.06	1.25	1.44
7	B	405	FAD	C4X-N5	5.04	1.40	1.30
8	B	406	FMN	C4A-N5	4.64	1.39	1.30

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	406	FMN	C5'-C4'-C3'	-6.33	99.98	112.20
8	B	406	FMN	O4'-C4'-C5'	-6.23	95.92	109.92
5	A	965	NAD	O4B-C1B-C2B	-5.93	98.26	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	406	FMN	O5'-P-O1P	4.57	119.29	106.47
7	B	405	FAD	N3A-C2A-N1A	-4.41	121.79	128.68

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	406	FMN	C1'-C2'-C3'-C4'
8	B	406	FMN	O3'-C3'-C4'-C5'
8	B	406	FMN	C3'-C4'-C5'-O5'
8	B	406	FMN	C5'-O5'-P-O3P
8	B	406	FMN	C2'-C3'-C4'-C5'

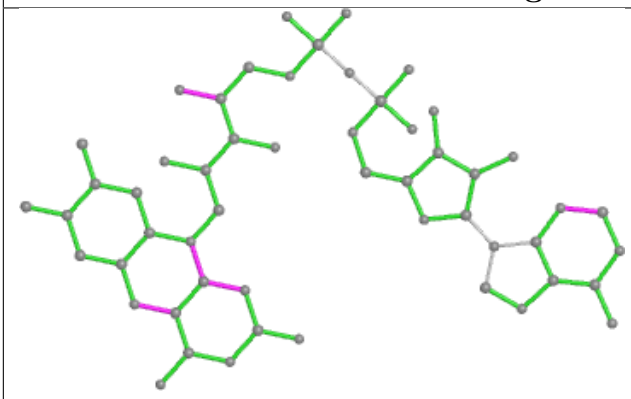
There are no ring outliers.

3 monomers are involved in 17 short contacts:

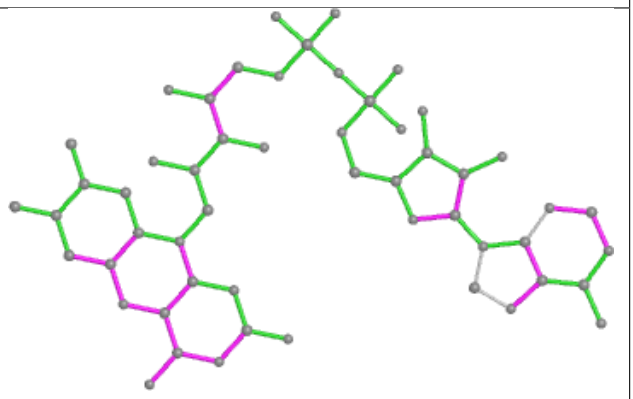
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	405	FAD	3	0
8	B	406	FMN	10	0
5	A	965	NAD	4	0

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.

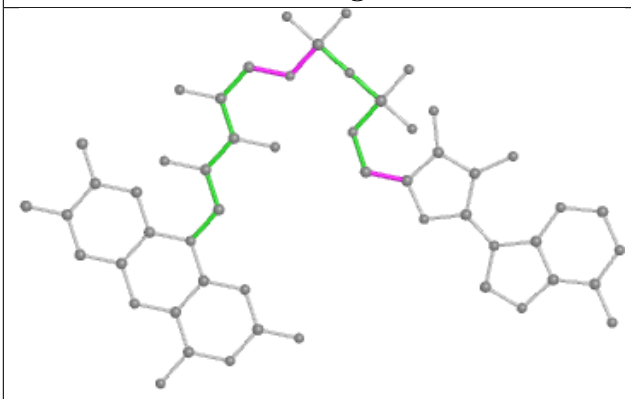
Ligand FAD B 405



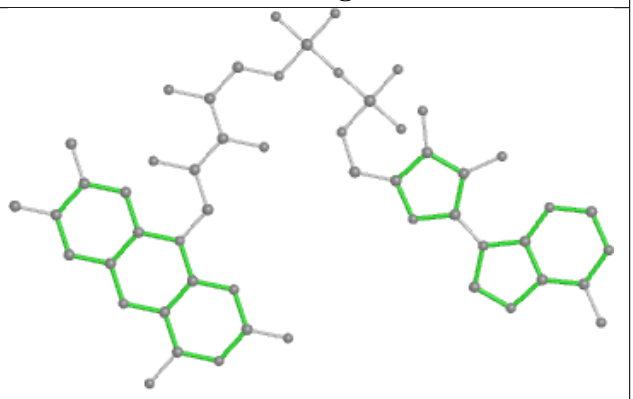
Bond lengths



Bond angles

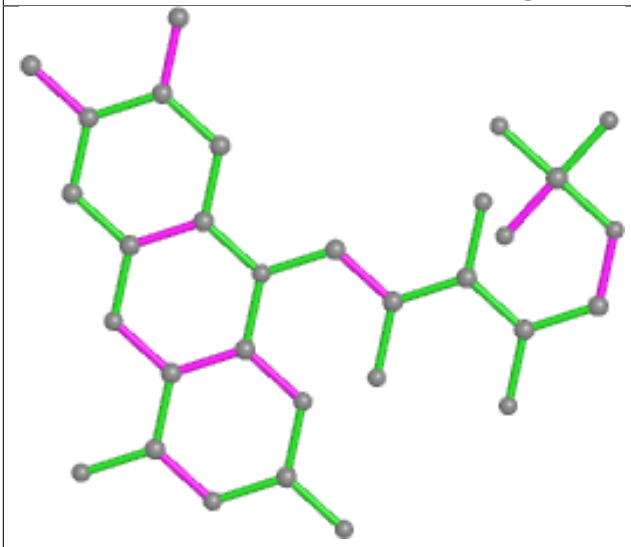


Torsions

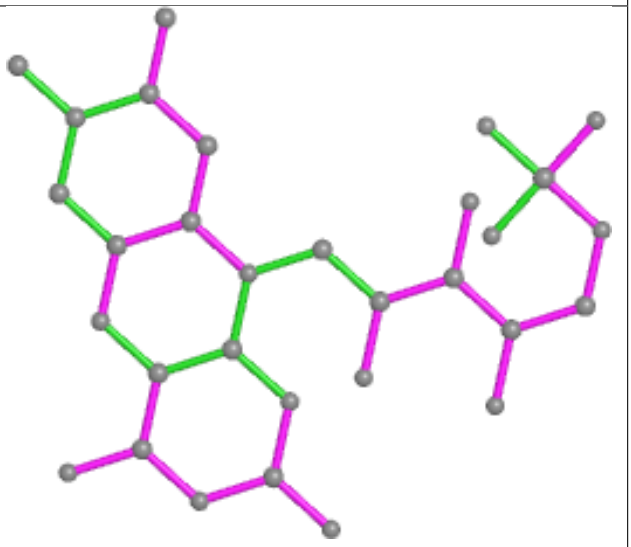


Rings

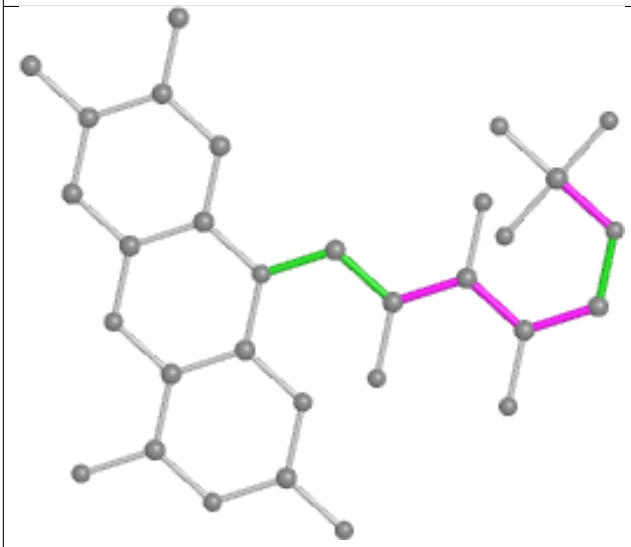
Ligand FMN B 406



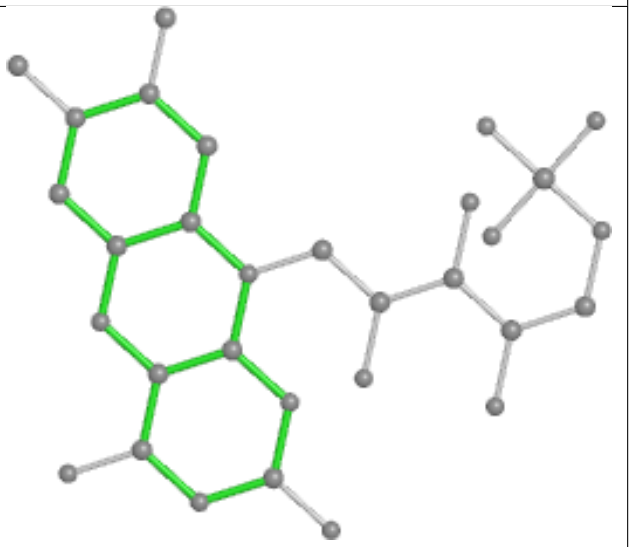
Bond lengths



Bond angles

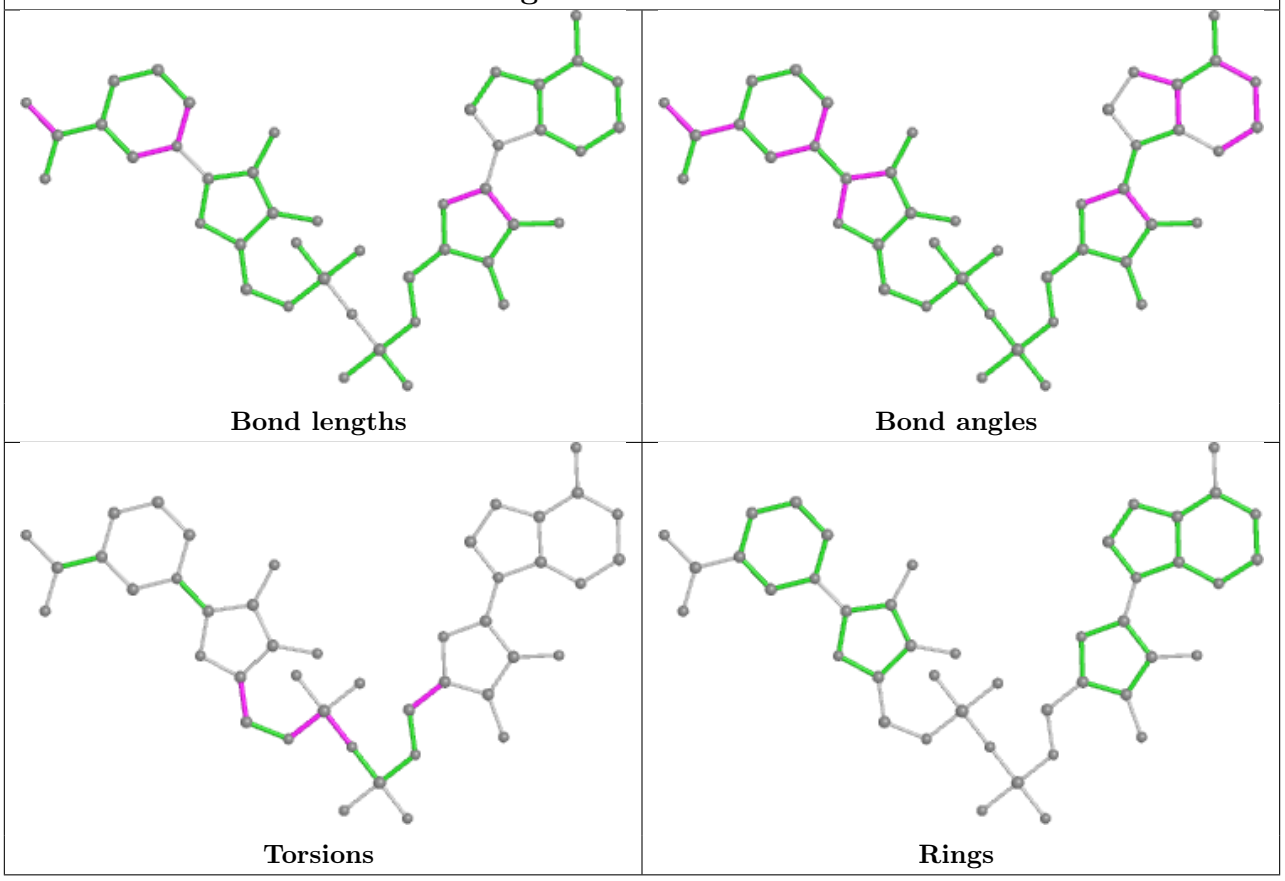


Torsions



Rings

Ligand NAD A 965



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^{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	963/964 (99%)	-0.53	10 (1%) 82 81	13, 26, 43, 61	0
2	B	404/404 (100%)	-0.59	3 (0%) 87 86	14, 26, 41, 64	0
3	C	195/203 (96%)	-0.71	0 100 100	16, 24, 41, 55	0
4	D	91/99 (91%)	-0.67	1 (1%) 80 79	18, 23, 42, 52	0
All	All	1653/1670 (98%)	-0.57	14 (0%) 86 85	13, 25, 43, 64	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	LEU	5.4
2	B	1	ALA	5.4
2	B	2	ASP	4.2
1	A	226	PRO	3.0
1	A	327	THR	2.9

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 monosaccharides in this entry.

6.4 Ligands

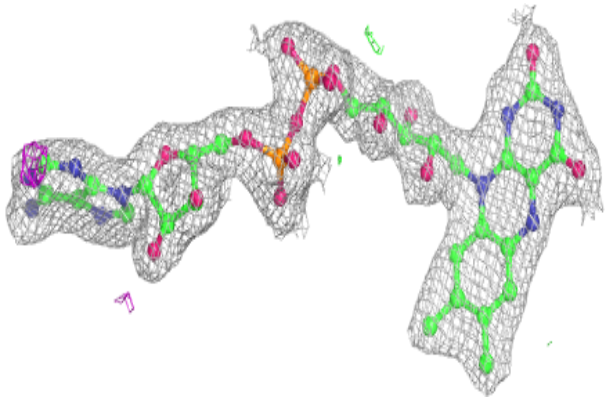
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

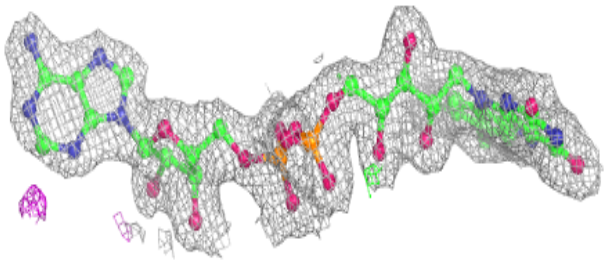
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MTG	B	801	6/6	0.92	0.18	48,49,50,54	0
6	SO4	A	2563	5/5	0.93	0.37	84,84,84,85	0
6	SO4	D	2566	5/5	0.96	0.21	89,89,90,90	0
6	SO4	A	2571	5/5	0.96	0.19	70,70,70,71	0
6	SO4	A	2560	5/5	0.97	0.12	49,50,52,52	0
7	FAD	B	405	53/53	0.97	0.10	19,24,27,28	0
6	SO4	B	2568	5/5	0.97	0.07	64,65,67,67	0
6	SO4	C	2564	5/5	0.98	0.17	35,35,38,38	0
8	FMN	B	406	31/31	0.98	0.12	12,15,21,23	0
6	SO4	B	2569	5/5	0.98	0.20	59,60,61,61	0
6	SO4	A	2567	5/5	0.99	0.06	33,34,38,40	0
5	NAD	A	965	44/44	0.99	0.11	11,16,21,26	0
6	SO4	A	2559	5/5	0.99	0.10	54,56,57,57	0
10	ZN	D	100	1/1	1.00	0.06	21,21,21,21	0

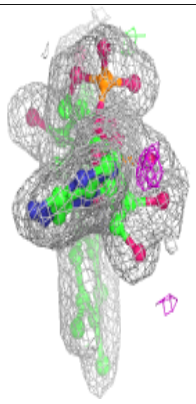
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 405:

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

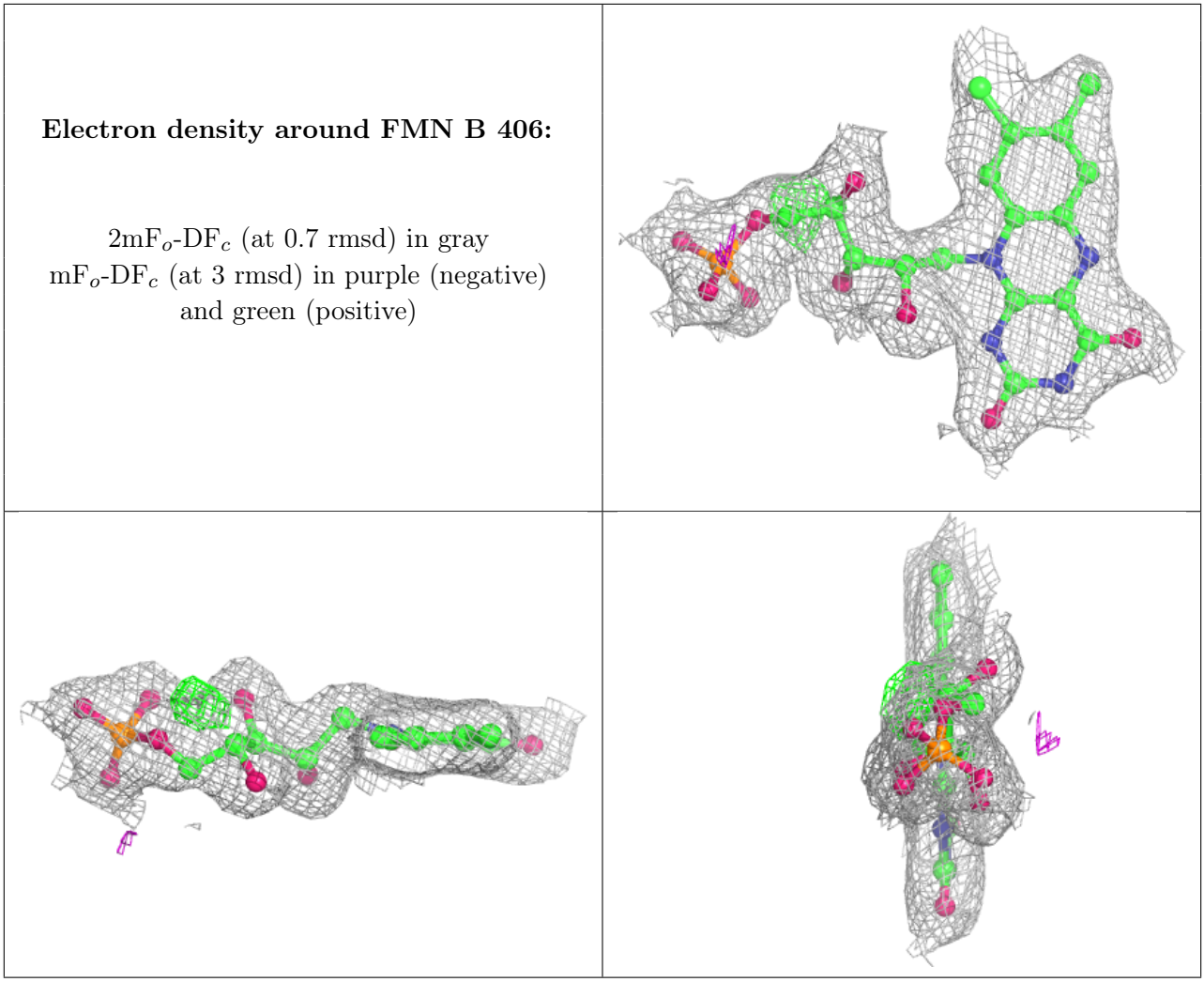






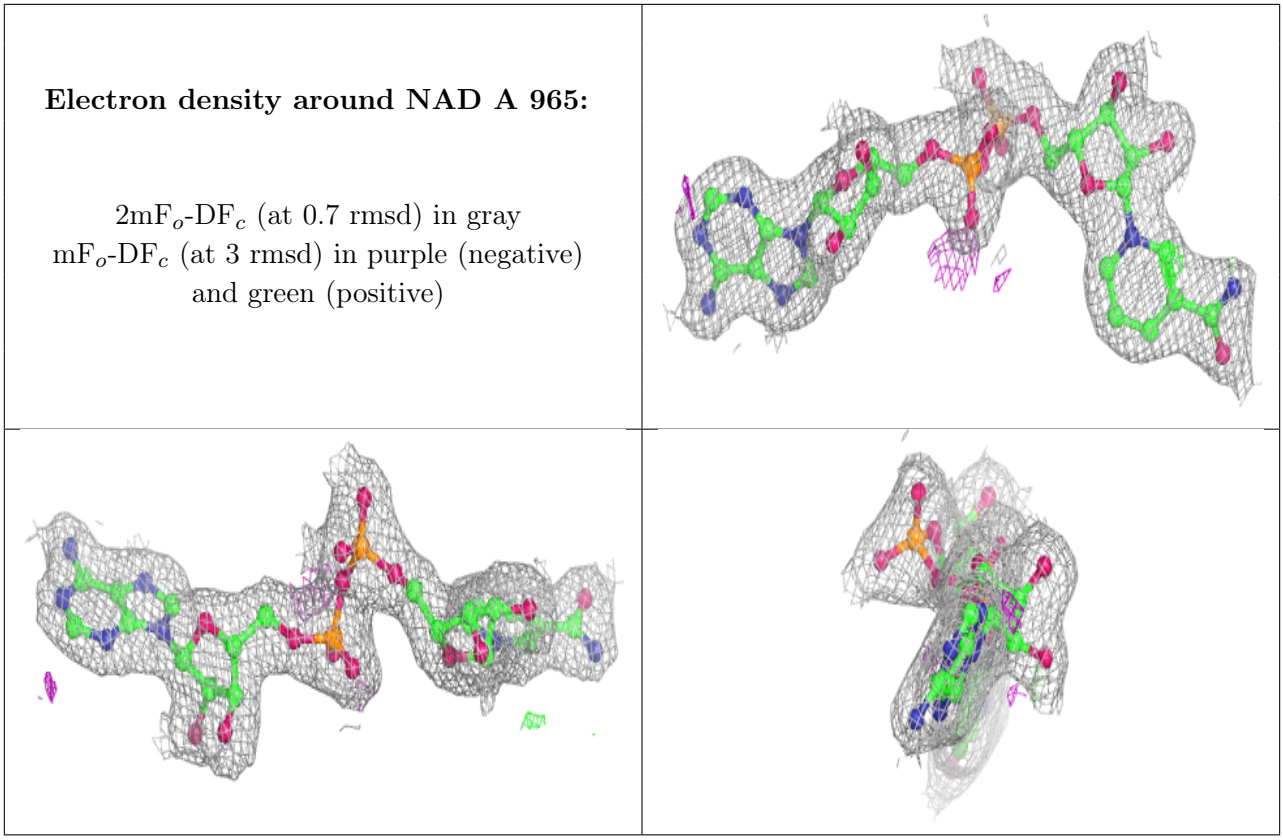
Electron density around FMN B 406:

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



Electron density around NAD A 965:

$2mF_o$-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.