



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 25, 2023 – 04:00 PM EDT

PDB ID : 3AD8
Title : Heterotetrameric Sarcosine Oxidase from *Corynebacterium* sp. U-96 in complex with pyrrole 2-carboxylate
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 ⓘ 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 ⓘ](#)) 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

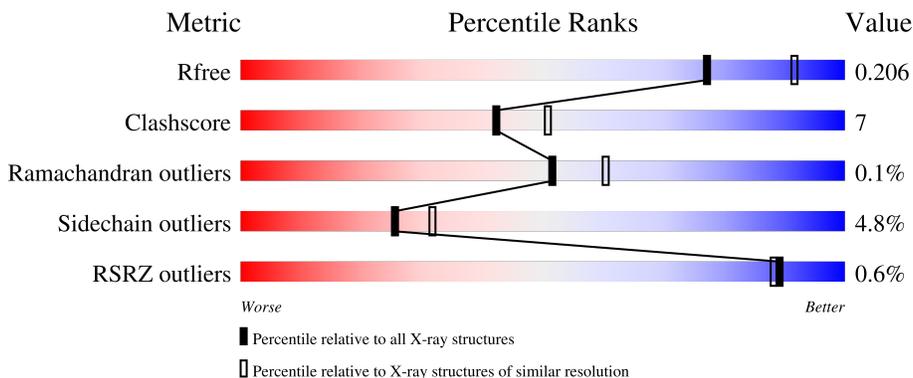
1 Overall quality at a glance

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 $\leq 5\%$. 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	964	 87% 11% .
2	B	404	 85% 12% .
3	C	203	 80% 13% . .
4	D	99	 87% 5% 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
6	SO4	A	2509	-	-	X	-
8	FMN	B	406	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 13736 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 SARCOSINE OXIDASE ALPHA SUBUNIT.

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

- Molecule 2 is a protein called SARCOSINE OXIDASE BETA SUBUNIT.

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

- Molecule 3 is a protein called SARCOSINE OXIDASE GAMMA SUBUNIT.

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

- Molecule 4 is a protein called SARCOSINE OXIDASE DELTA SUBUNIT.

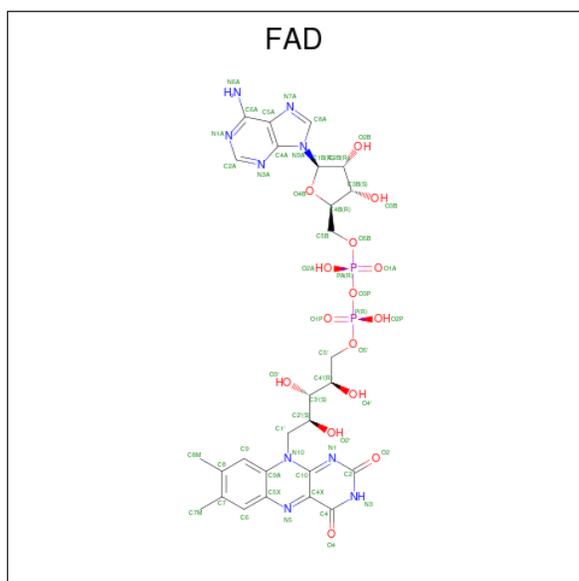
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	91	749	476	135	133	5	0	0	0

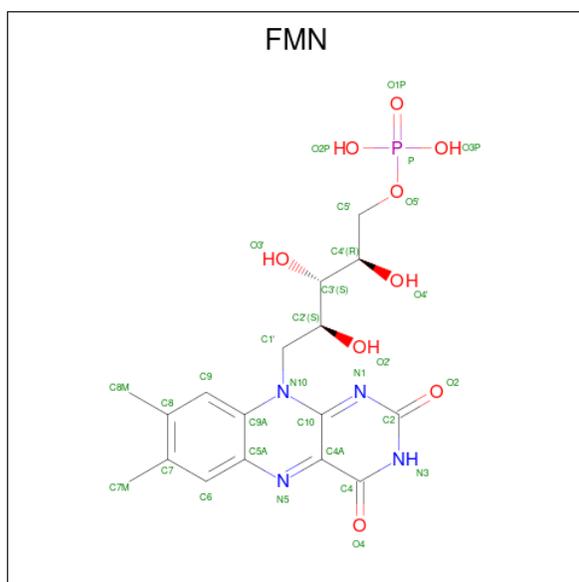
- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

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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		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

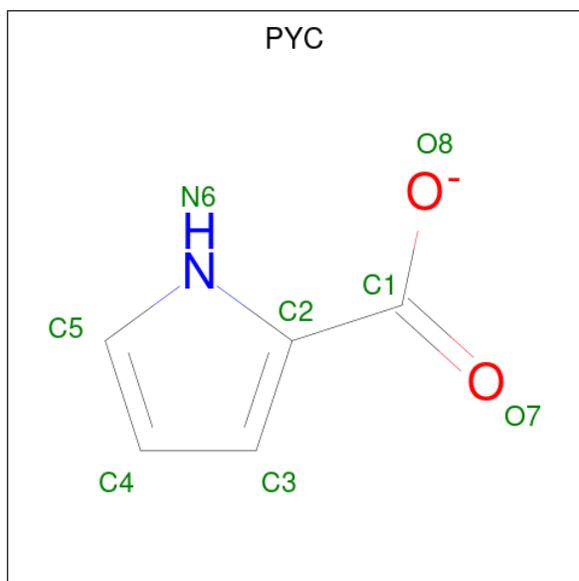
- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).





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

- Molecule 9 is PYRROLE-2-CARBOXYLATE (three-letter code: PYC) (formula: $C_5H_4NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	B	1	8	5	1	2	0	0

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

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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	631	Total 631	O 631	0	0
11	B	189	Total 189	O 189	0	0
11	C	133	Total 133	O 133	0	0
11	D	67	Total 67	O 67	0	0

A200
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

● Molecule 4: SARCOSINE OXIDASE DELTA SUBUNIT

Chain D:  87% 5% 8%

H1
I4
R12
F63
E77
F78
K79
L91
ASP
SER
THR
GLU
GLY
GLY
THR
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	198.80Å 198.80Å 196.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.31 – 2.20 61.31 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.31-2.20) 100.0 (61.31-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.18 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.161 , 0.206 0.161 , 0.206	Depositor DCC
R_{free} test set	5799 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13736	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, NAD, FMN, SO4, PYC, ZN

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	1.04	5/7361 (0.1%)	0.93	19/10017 (0.2%)
2	B	1.01	2/3189 (0.1%)	0.91	6/4340 (0.1%)
3	C	1.11	3/1461 (0.2%)	1.00	6/1998 (0.3%)
4	D	1.03	1/772 (0.1%)	0.88	1/1040 (0.1%)
All	All	1.04	11/12783 (0.1%)	0.93	32/17395 (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	A	0	1
3	C	0	1
All	All	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	477	HIS	CB-CG	9.30	1.66	1.50
1	A	477	HIS	CA-CB	8.05	1.71	1.53
1	A	477	HIS	CA-C	6.84	1.70	1.52
4	D	53	PHE	CE1-CZ	6.38	1.49	1.37
1	A	249	ALA	CA-CB	-5.99	1.39	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	387	ARG	NE-CZ-NH1	-14.34	113.13	120.30
1	A	15	ARG	NE-CZ-NH2	-12.63	113.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	819	ARG	NE-CZ-NH2	-12.61	113.99	120.30
1	A	819	ARG	NE-CZ-NH1	10.36	125.48	120.30
3	C	176	ARG	NE-CZ-NH2	-8.83	115.88	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	SER	Peptide
3	C	199	VAL	Peptide

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	7229	0	7104	101	1
2	B	3108	0	3035	54	0
3	C	1433	0	1434	17	0
4	D	749	0	706	3	0
5	A	44	0	26	4	0
6	A	35	0	0	3	0
6	B	15	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	B	53	0	31	4	0
8	B	31	0	18	9	0
9	B	8	0	4	0	0
10	D	1	0	0	0	0
11	A	631	0	0	13	1
11	B	189	0	0	5	0
11	C	133	0	0	2	0
11	D	67	0	0	0	0
All	All	13736	0	12358	173	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 7.

The worst 5 of 173 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	1.71	1.50
1:A:830:ASP:OD1	1:A:909:HIS:CE1	1.88	1.26
1:A:696:ALA:HB3	6:A:2509:SO4:O3	1.41	1.17
2:B:384:ALA:O	2:B:387:ARG:HD3	1.44	1.12
2:B:387:ARG:HH11	2:B:387:ARG:HG3	0.98	1.11

All (2) 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)
1:A:477:HIS:NE2	1:A:477:HIS:NE2[11_555]	1.27	0.93
11:A:1080:HOH:O	11:A:1080:HOH:O[9_555]	1.63	0.57

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%)	941 (98%)	18 (2%)	2 (0%)	47	55
2	B	402/404 (100%)	387 (96%)	15 (4%)	0	100	100
3	C	193/203 (95%)	187 (97%)	6 (3%)	0	100	100
4	D	89/99 (90%)	87 (98%)	2 (2%)	0	100	100
All	All	1645/1670 (98%)	1602 (97%)	41 (2%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	406	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%)	709 (95%)	38 (5%)	24	29
2	B	319/319 (100%)	305 (96%)	14 (4%)	28	35
3	C	143/151 (95%)	134 (94%)	9 (6%)	18	20
4	D	75/81 (93%)	74 (99%)	1 (1%)	69	81
All	All	1284/1298 (99%)	1222 (95%)	62 (5%)	25	32

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	848	LYS
3	C	97	LEU
1	A	918	ARG
3	C	93	GLU
3	C	169	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	816	HIS
3	C	158	ASN
2	B	7	HIS
3	C	182	HIS
2	B	344	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 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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
5	NAD	A	965	-	42,48,48	1.65	5 (11%)	50,73,73	1.60	7 (14%)
7	FAD	B	405	-	53,58,58	1.55	6 (11%)	68,89,89	1.39	12 (17%)
6	SO4	A	2502	-	4,4,4	0.23	0	6,6,6	0.29	0
6	SO4	A	2504	-	4,4,4	0.18	0	6,6,6	0.34	0
6	SO4	A	2507	-	4,4,4	0.18	0	6,6,6	0.46	0
6	SO4	A	2509	-	4,4,4	0.36	0	6,6,6	0.45	0
6	SO4	A	2500	-	4,4,4	0.15	0	6,6,6	0.27	0
6	SO4	D	2503	-	4,4,4	0.16	0	6,6,6	0.19	0
8	FMN	B	406	-	33,33,33	2.07	9 (27%)	48,50,50	2.35	11 (22%)
6	SO4	A	2501	-	4,4,4	0.29	0	6,6,6	0.59	0
6	SO4	C	2508	-	4,4,4	0.60	0	6,6,6	0.28	0
9	PYC	B	801	-	8,8,8	1.39	0	8,10,10	1.44	1 (12%)
6	SO4	B	2510	-	4,4,4	0.44	0	6,6,6	0.65	0
6	SO4	B	2511	-	4,4,4	0.18	0	6,6,6	0.45	0
6	SO4	A	2506	-	4,4,4	0.26	0	6,6,6	0.31	0
6	SO4	B	2505	-	4,4,4	0.16	0	6,6,6	0.25	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
5	NAD	A	965	-	-	5/26/62/62	0/5/5/5
9	PYC	B	801	-	-	0/2/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FMN	B	406	-	-	6/18/18/18	0/3/3/3
7	FAD	B	405	-	-	3/30/50/50	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)
7	B	405	FAD	C4X-N5	7.15	1.44	1.30
5	A	965	NAD	O7N-C7N	6.35	1.36	1.24
8	B	406	FMN	O5'-C5'	-6.24	1.20	1.44
5	A	965	NAD	C2N-N1N	4.82	1.40	1.35
8	B	406	FMN	C4A-N5	3.91	1.38	1.30

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	406	FMN	C5'-C4'-C3'	-9.29	94.25	112.20
8	B	406	FMN	O4'-C4'-C5'	-6.14	96.13	109.92
5	A	965	NAD	O4B-C1B-C2B	-5.69	98.61	106.93
8	B	406	FMN	O5'-P-O1P	5.21	121.09	106.47
5	A	965	NAD	N3A-C2A-N1A	-4.11	122.25	128.68

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	406	FMN	C1'-C2'-C3'-C4'
8	B	406	FMN	C2'-C3'-C4'-C5'
8	B	406	FMN	C3'-C4'-C5'-O5'
8	B	406	FMN	O4'-C4'-C5'-O5'
8	B	406	FMN	O3'-C3'-C4'-C5'

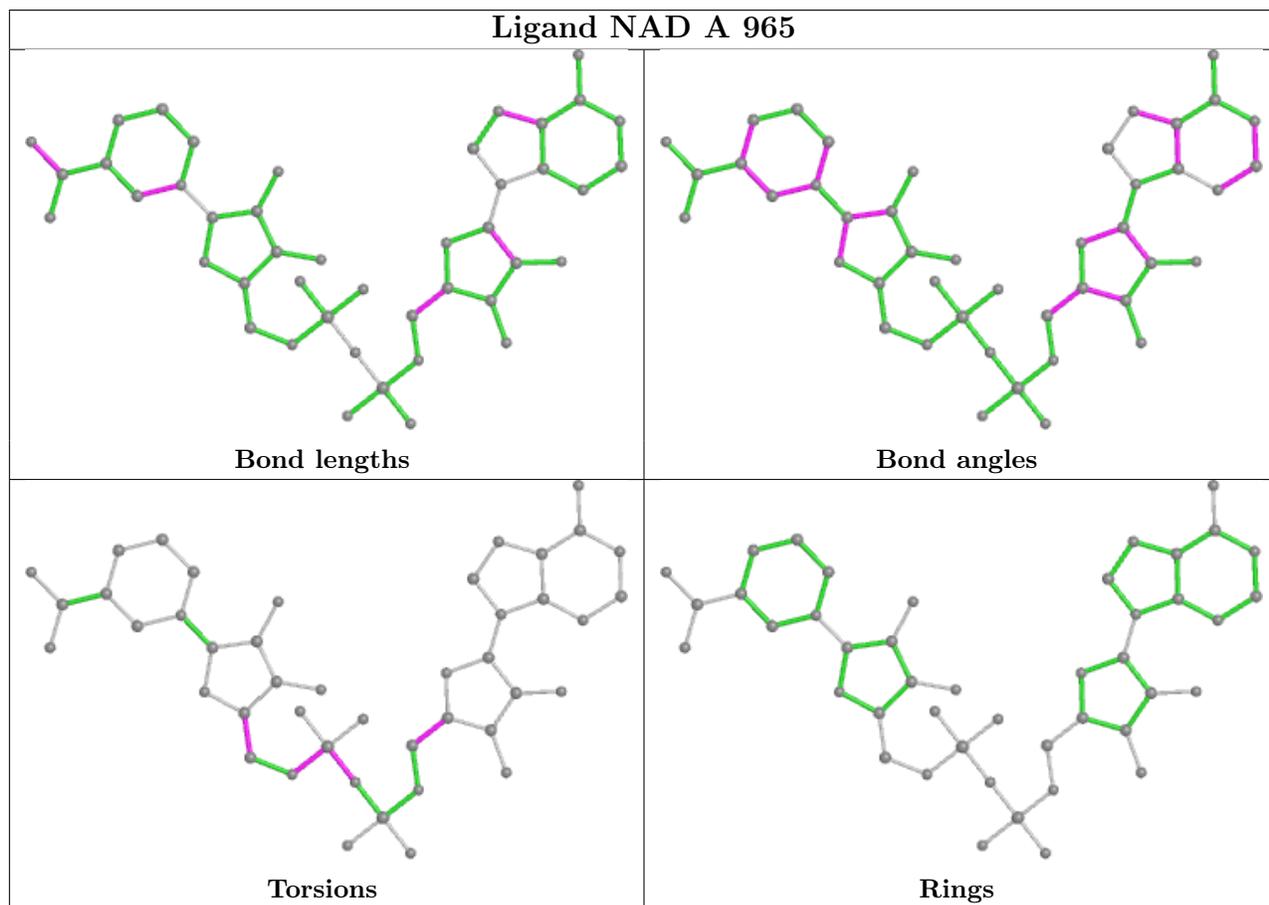
There are no ring outliers.

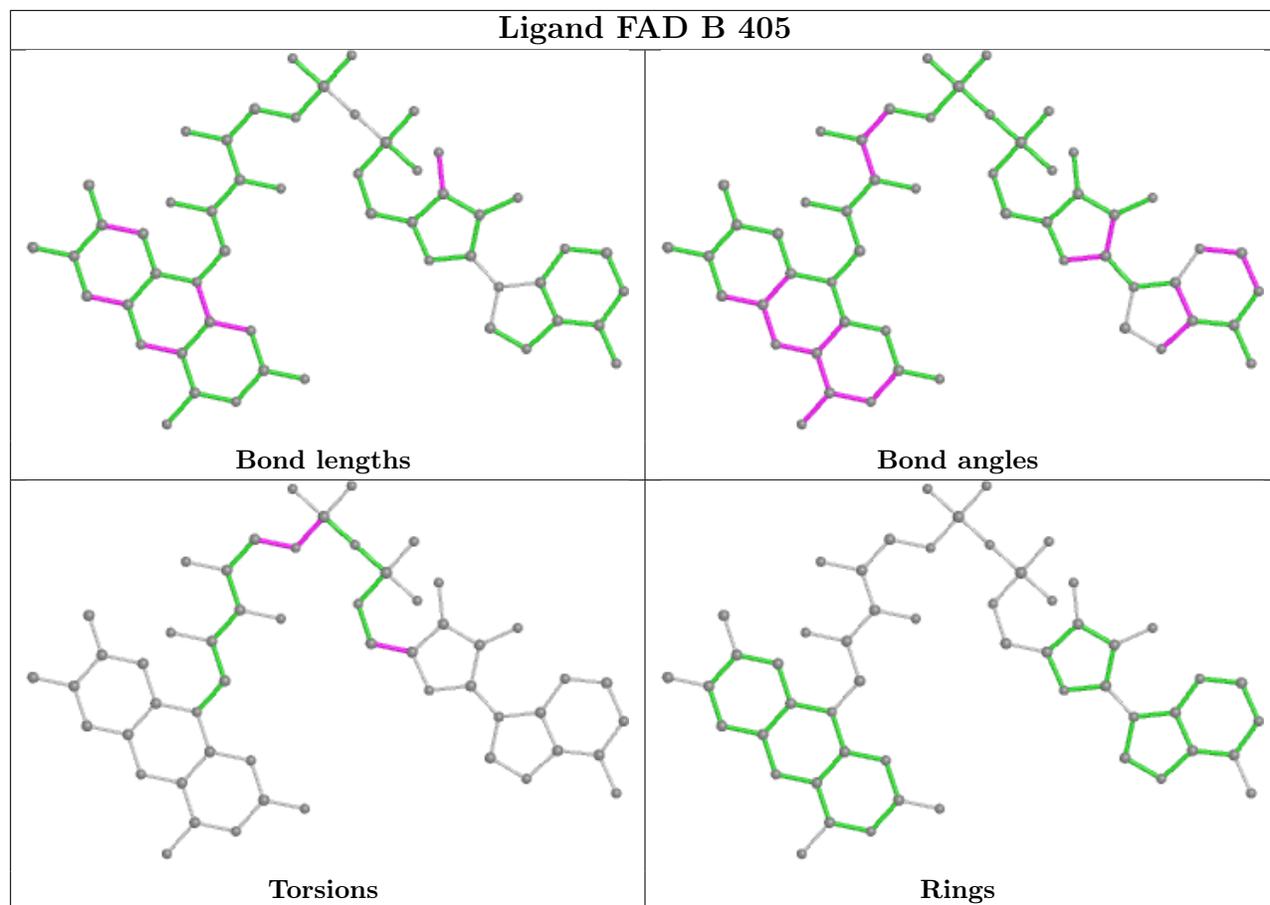
4 monomers are involved in 20 short contacts:

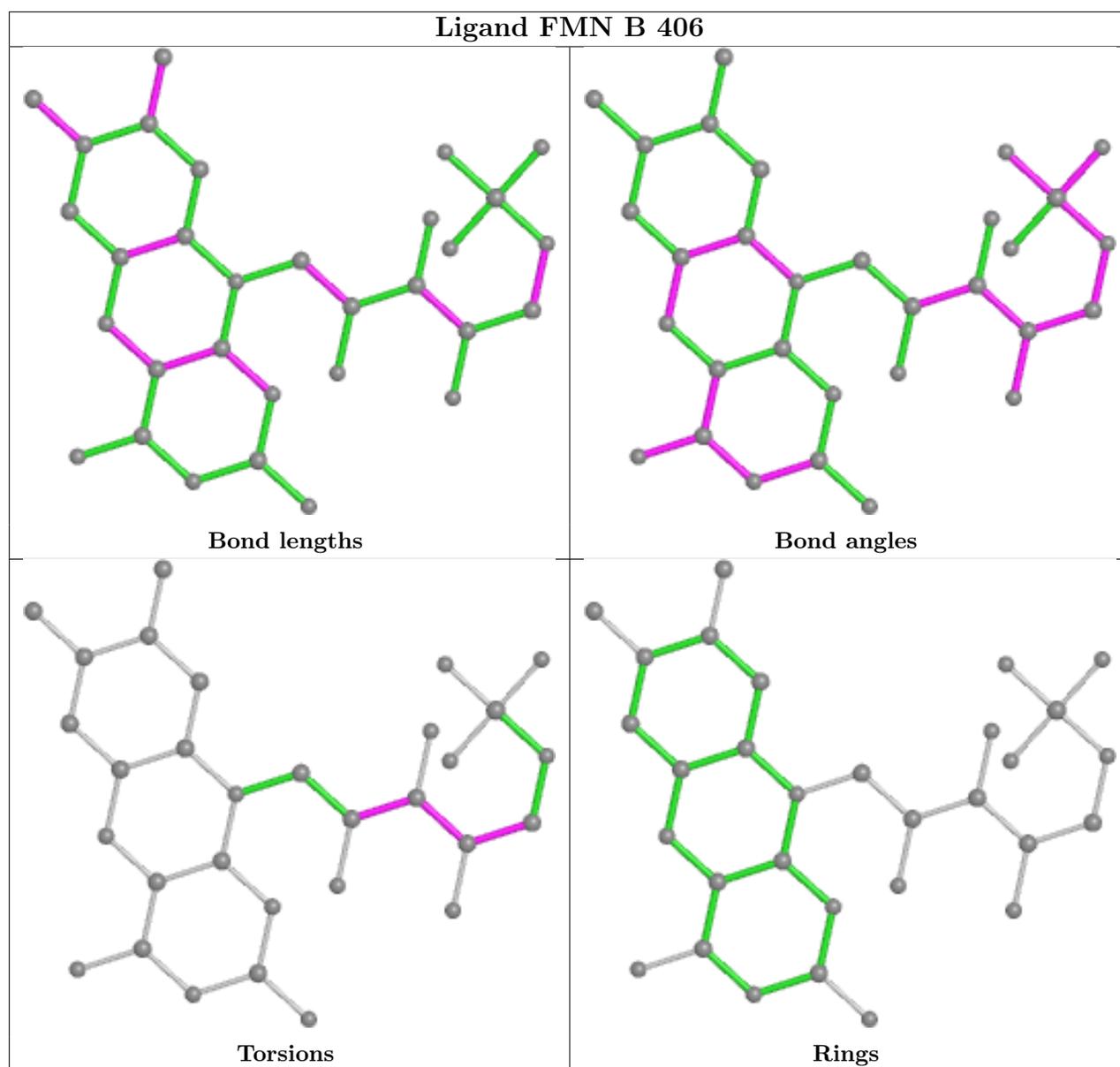
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	965	NAD	4	0
7	B	405	FAD	4	0
6	A	2509	SO4	3	0
8	B	406	FMN	9	0

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, 95th 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%)	-0.62	5 (0%) 91 90	11, 24, 41, 59	0
2	B	404/404 (100%)	-0.55	5 (1%) 79 77	13, 25, 38, 84	0
3	C	195/203 (96%)	-0.74	0 100 100	14, 22, 42, 49	0
4	D	91/99 (91%)	-0.80	0 100 100	15, 22, 42, 54	0
All	All	1653/1670 (98%)	-0.63	10 (0%) 89 88	11, 24, 41, 84	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	ASP	8.4
2	B	1	ALA	7.5
2	B	3	LEU	7.3
1	A	909	HIS	3.8
1	A	226	PRO	2.8

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](#)

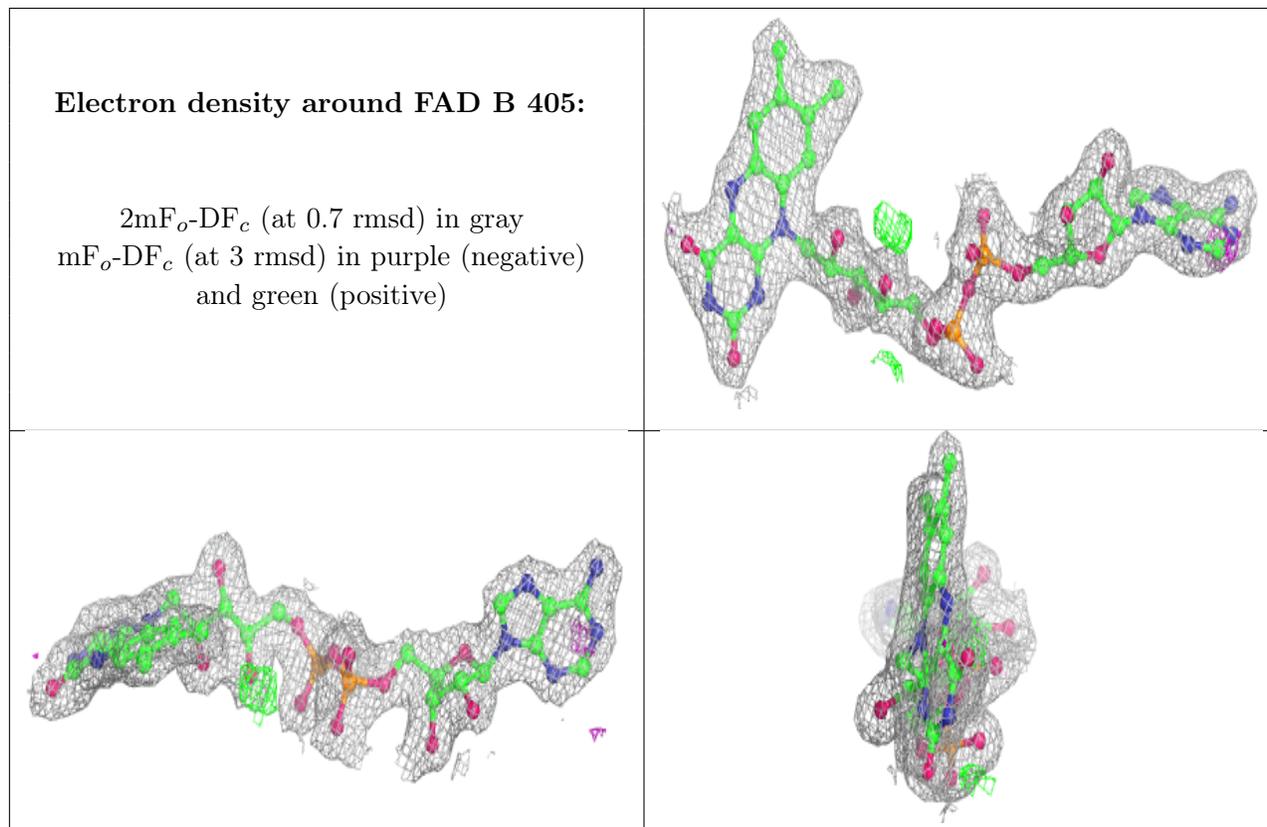
There are no monosaccharides in this entry.

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, 95th 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.

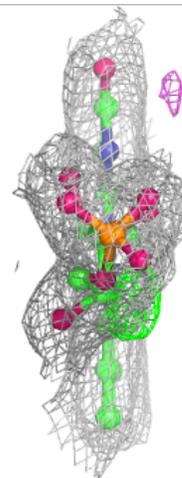
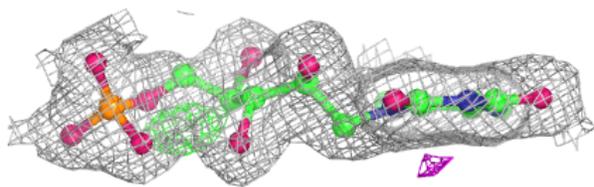
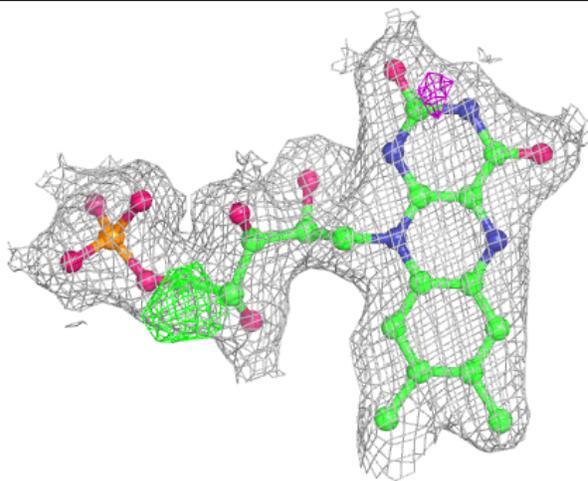
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	B	2511	5/5	0.90	0.11	73,73,75,76	0
6	SO4	A	2506	5/5	0.93	0.27	65,65,67,68	0
6	SO4	B	2510	5/5	0.94	0.23	52,53,57,57	0
6	SO4	D	2503	5/5	0.94	0.13	82,82,83,83	0
6	SO4	A	2502	5/5	0.95	0.29	76,76,77,78	0
6	SO4	A	2507	5/5	0.96	0.20	59,60,62,64	0
9	PYC	B	801	8/8	0.96	0.14	44,44,46,48	0
6	SO4	A	2501	5/5	0.97	0.12	46,47,50,51	0
7	FAD	B	405	53/53	0.97	0.10	11,22,27,28	0
6	SO4	B	2505	5/5	0.97	0.20	56,57,58,60	0
8	FMN	B	406	31/31	0.98	0.09	11,15,19,23	0
6	SO4	A	2509	5/5	0.98	0.13	44,46,49,52	0
6	SO4	A	2500	5/5	0.99	0.13	65,66,67,68	0
6	SO4	C	2508	5/5	0.99	0.13	30,33,35,35	0
5	NAD	A	965	44/44	0.99	0.09	8,14,19,25	0
6	SO4	A	2504	5/5	1.00	0.08	29,30,35,37	0
10	ZN	D	100	1/1	1.00	0.08	19,19,19,19	0

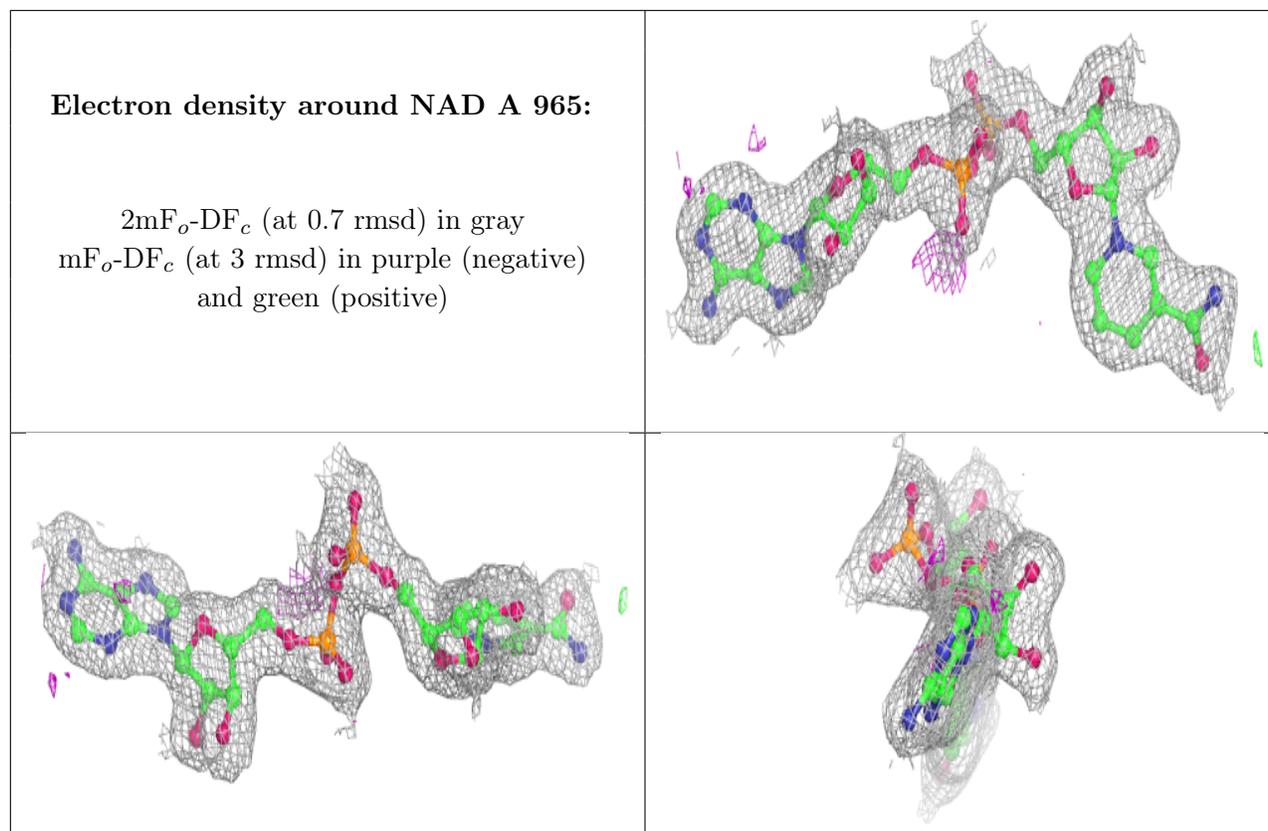
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.