wwPDB X-ray Structure Validation Summary Report (i)

Aug 17, 2023 – 04:10 PM JST

PDB ID	:	7YA4
Title	:	Formate dehydrogenase from Novosphingobium sp. AP12 with NAD and Azide
Authors	:	Kim, S.; Kim, K.-J.
Deposited on	:	2022-06-27
Resolution	:	1.80 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:

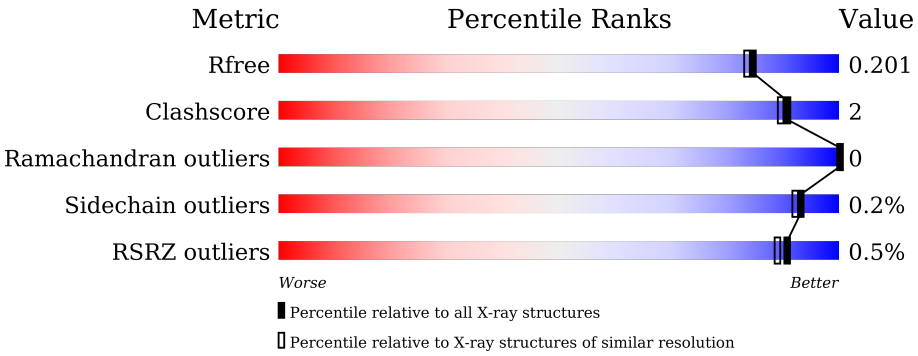
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	392	90% 8% •
1	B	392	92% 6% •
1	C	392	93% • •
1	D	392	% 93% • 5%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ACT	D	402	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 24648 atoms, of which 11752 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 Formate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	H	N	O	S	159	0	0
			5928	1892	2946	515	559	16			
1	B	384	Total	C	H	N	O	S	158	0	0
			5928	1892	2946	515	559	16			
1	C	375	Total	C	H	N	O	S	155	0	0
			5797	1850	2879	506	546	16			
1	D	374	Total	C	H	N	O	S	155	0	0
			5790	1848	2876	505	545	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	LEU	-	expression tag	UNP J2HCX1
A	386	GLU	-	expression tag	UNP J2HCX1
A	387	HIS	-	expression tag	UNP J2HCX1
A	388	HIS	-	expression tag	UNP J2HCX1
A	389	HIS	-	expression tag	UNP J2HCX1
A	390	HIS	-	expression tag	UNP J2HCX1
A	391	HIS	-	expression tag	UNP J2HCX1
A	392	HIS	-	expression tag	UNP J2HCX1
B	385	LEU	-	expression tag	UNP J2HCX1
B	386	GLU	-	expression tag	UNP J2HCX1
B	387	HIS	-	expression tag	UNP J2HCX1
B	388	HIS	-	expression tag	UNP J2HCX1
B	389	HIS	-	expression tag	UNP J2HCX1
B	390	HIS	-	expression tag	UNP J2HCX1
B	391	HIS	-	expression tag	UNP J2HCX1
B	392	HIS	-	expression tag	UNP J2HCX1
C	385	LEU	-	expression tag	UNP J2HCX1
C	386	GLU	-	expression tag	UNP J2HCX1
C	387	HIS	-	expression tag	UNP J2HCX1
C	388	HIS	-	expression tag	UNP J2HCX1
C	389	HIS	-	expression tag	UNP J2HCX1

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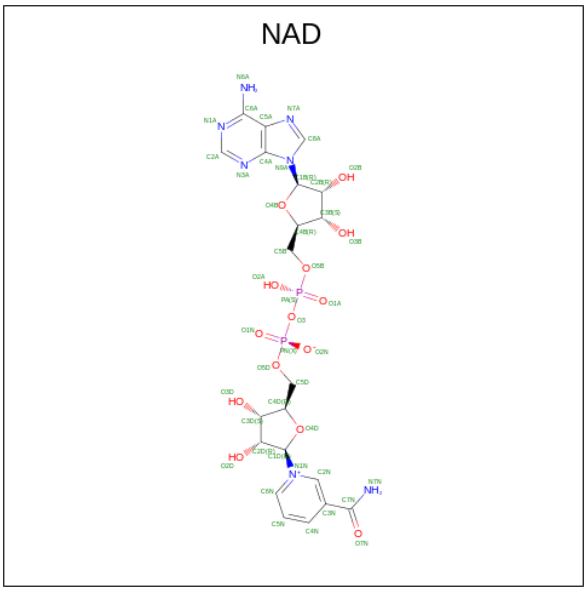
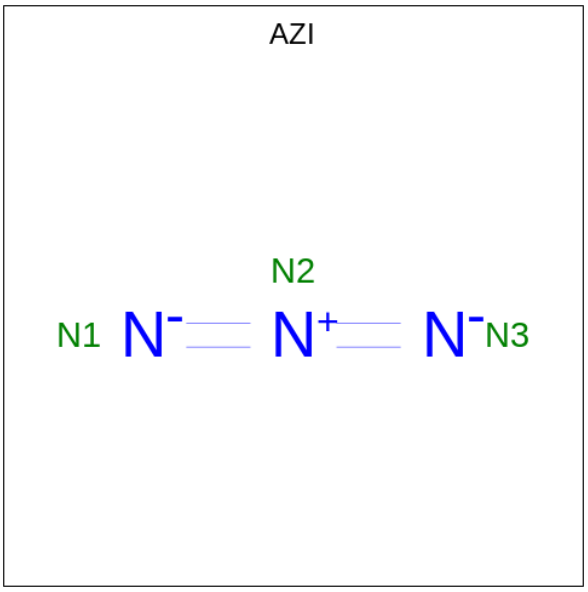
Chain	Residue	Modelled	Actual	Comment	Reference
C	390	HIS	-	expression tag	UNP J2HCX1
C	391	HIS	-	expression tag	UNP J2HCX1
C	392	HIS	-	expression tag	UNP J2HCX1
D	385	LEU	-	expression tag	UNP J2HCX1
D	386	GLU	-	expression tag	UNP J2HCX1
D	387	HIS	-	expression tag	UNP J2HCX1
D	388	HIS	-	expression tag	UNP J2HCX1
D	389	HIS	-	expression tag	UNP J2HCX1
D	390	HIS	-	expression tag	UNP J2HCX1
D	391	HIS	-	expression tag	UNP J2HCX1
D	392	HIS	-	expression tag	UNP J2HCX1

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



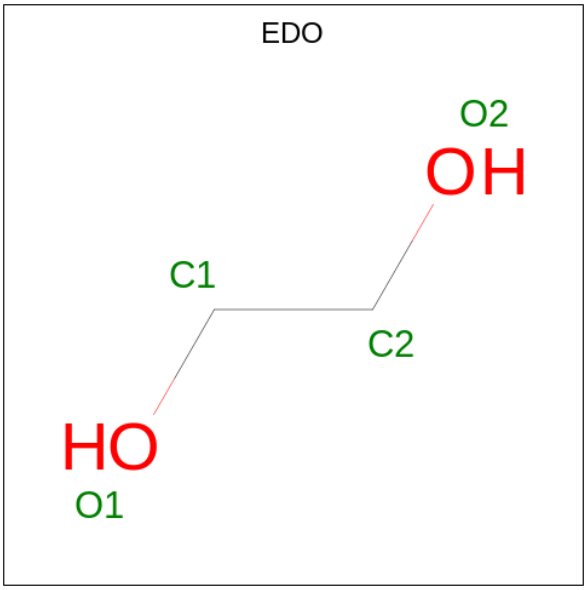
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	6	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	6	0
			70	21	26	7	14	2		

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 3 3	0	0
3	B	1	Total N 3 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 10 2 6 2	1	0
4	A	1	Total C H O 10 2 6 2	1	0

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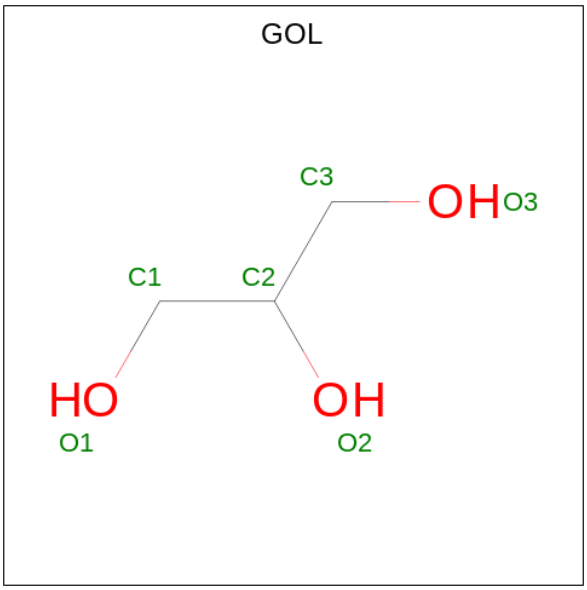
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C H O 10 2 6 2	1	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

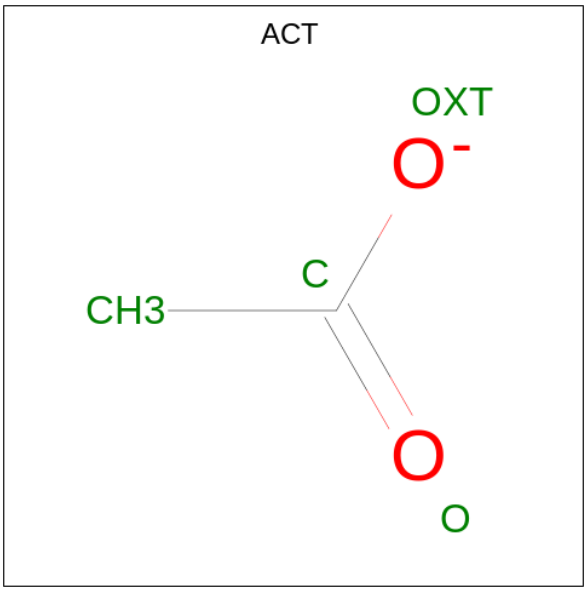
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 14 3 8 3	2	0
6	B	1	Total C H O 14 3 8 3	2	0
6	C	1	Total C H O 14 3 8 3	2	0
6	D	1	Total C H O 14 3 8 3	2	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C H O 7 2 3 2	0	0

- Molecule 8 is water.

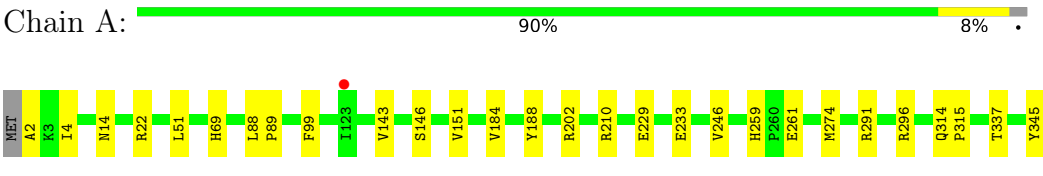
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	282	Total O 282 282	0	0
8	B	252	Total O 252 252	0	0
8	C	229	Total O 229 229	0	0
8	D	202	Total O 202 202	0	0

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.

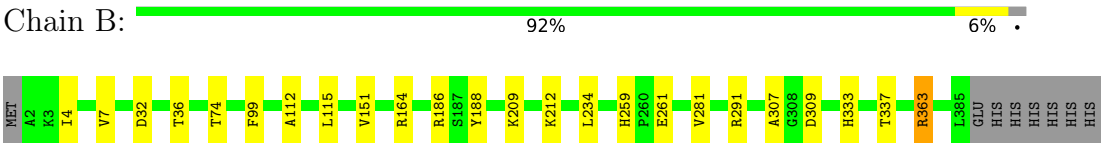
• Molecule 1: Formate dehydrogenase

Chain A:



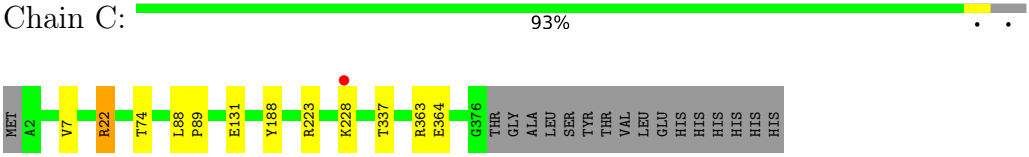
• Molecule 1: Formate dehydrogenase

Chain B:



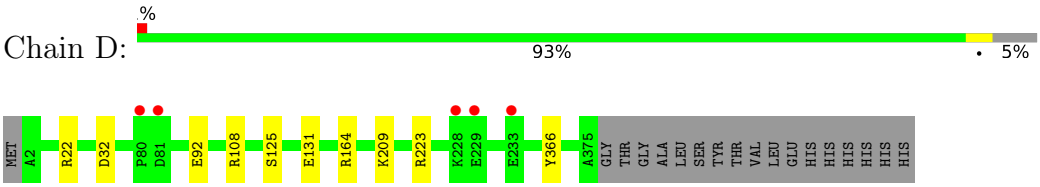
• Molecule 1: Formate dehydrogenase

Chain C:



• Molecule 1: Formate dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.79Å 95.79Å 117.93Å 90.00° 99.28° 90.00°	Depositor
Resolution (Å)	34.14 – 1.80 34.11 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.14-1.80) 95.8 (34.11-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.76 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.155 , 0.191 0.167 , 0.201	Depositor DCC
R_{free} test set	7007 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 42.0	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	0.97	EDS
Total number of atoms	24648	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: EDO, AZI, GOL, NA, ACT, NAD

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	0.52	0/3058	0.79	4/4155 (0.1%)
1	B	0.51	0/3058	0.79	1/4155 (0.0%)
1	C	0.53	1/2993 (0.0%)	0.79	1/4065 (0.0%)
1	D	0.54	2/2989 (0.1%)	0.80	1/4060 (0.0%)
All	All	0.52	3/12098 (0.0%)	0.79	7/16435 (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	2
1	B	0	3
1	C	0	2
1	D	0	2
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	131	GLU	CD-OE1	8.66	1.35	1.25
1	D	92	GLU	CD-OE2	-7.12	1.17	1.25
1	C	131	GLU	CD-OE1	5.98	1.32	1.25

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	186	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	296	ARG	NE-CZ-NH2	-5.83	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	366	TYR	CB-CG-CD1	5.67	124.40	121.00
1	A	366	TYR	CB-CG-CD1	5.46	124.28	121.00
1	A	210	ARG	NE-CZ-NH2	-5.46	117.57	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	ARG	Sidechain
1	A	350	ARG	Sidechain
1	B	164	ARG	Sidechain
1	B	291	ARG	Sidechain
1	B	363	ARG	Sidechain

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	2982	2946	2928	15	0
1	B	2982	2946	2928	15	0
1	C	2918	2879	2861	6	0
1	D	2914	2876	2858	5	0
2	A	44	26	26	1	0
2	B	44	26	26	2	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	8	12	12	1	0
4	C	4	6	6	0	0
5	A	1	0	0	0	0
6	A	6	8	8	0	0
6	B	6	8	8	0	0
6	C	6	8	8	0	0
6	D	6	8	8	1	0
7	D	4	3	3	2	0
8	A	282	0	0	2	0
8	B	252	0	0	0	0
8	C	229	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	202	0	0	2	0
All	All	12896	11752	11680	39	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 2.

The worst 5 of 39 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:D:108:ARG:H	7:D:402:ACT:H1	1.50	0.77
1:B:36:THR:HG23	1:B:363:ARG:HH22	1.59	0.67
1:B:36:THR:HG23	1:B:363:ARG:NH2	2.10	0.65
7:D:402:ACT:H2	8:D:668:HOH:O	1.96	0.65
1:B:212:LYS:HD2	1:B:234:LEU:HD23	1.83	0.61

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	382/392 (97%)	375 (98%)	7 (2%)	0	100	100
1	B	382/392 (97%)	372 (97%)	10 (3%)	0	100	100
1	C	373/392 (95%)	362 (97%)	11 (3%)	0	100	100
1	D	372/392 (95%)	359 (96%)	13 (4%)	0	100	100
All	All	1509/1568 (96%)	1468 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	315/323 (98%)	314 (100%)	1 (0%)	92 91
1	B	315/323 (98%)	315 (100%)	0	100 100
1	C	308/323 (95%)	306 (99%)	2 (1%)	86 84
1	D	308/323 (95%)	308 (100%)	0	100 100
All	All	1246/1292 (96%)	1243 (100%)	3 (0%)	93 92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	TYR
1	C	228	LYS
1	C	364	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	255	ASN
1	C	255	ASN
1	C	264	HIS
1	D	224	HIS
1	D	255	ASN

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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	NAD	A	401	-	42,48,48	0.74	1 (2%)	50,73,73	0.87	2 (4%)
2	NAD	B	401	-	42,48,48	0.76	1 (2%)	50,73,73	1.03	2 (4%)
4	EDO	C	402	-	3,3,3	0.23	0	2,2,2	0.39	0
4	EDO	A	403	-	3,3,3	0.18	0	2,2,2	0.19	0
3	AZI	B	402	-	0,2,2	-	-	0,1,1	-	-
4	EDO	A	405	-	3,3,3	0.41	0	2,2,2	0.50	0
6	GOL	A	406	-	5,5,5	0.11	0	5,5,5	0.28	0
3	AZI	A	402	-	0,2,2	-	-	0,1,1	-	-
6	GOL	B	403	-	5,5,5	0.17	0	5,5,5	0.24	0
6	GOL	C	401	-	5,5,5	0.18	0	5,5,5	0.48	0
7	ACT	D	402	-	3,3,3	1.10	0	3,3,3	0.83	0
6	GOL	D	401	-	5,5,5	0.21	0	5,5,5	0.53	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
2	NAD	A	401	-	-	2/26/62/62	0/5/5/5
2	NAD	B	401	-	-	2/26/62/62	0/5/5/5
4	EDO	C	402	-	-	0/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
6	GOL	A	406	-	-	0/4/4/4	-
4	EDO	A	405	-	-	1/1/1/1	-
6	GOL	B	403	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	401	-	-	0/4/4/4	-
6	GOL	D	401	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAD	C2N-N1N	2.62	1.38	1.35
2	A	401	NAD	C8A-N7A	-2.02	1.31	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	NAD	O4B-C1B-C2B	-3.45	101.88	106.93
2	B	401	NAD	C6N-N1N-C2N	-3.20	119.06	121.97
2	A	401	NAD	C5A-C6A-N6A	2.32	123.88	120.35
2	A	401	NAD	C6N-N1N-C2N	-2.28	119.90	121.97

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C6N
6	B	403	GOL	O1-C1-C2-C3
6	D	401	GOL	C1-C2-C3-O3
6	B	403	GOL	O1-C1-C2-O2

There are no ring outliers.

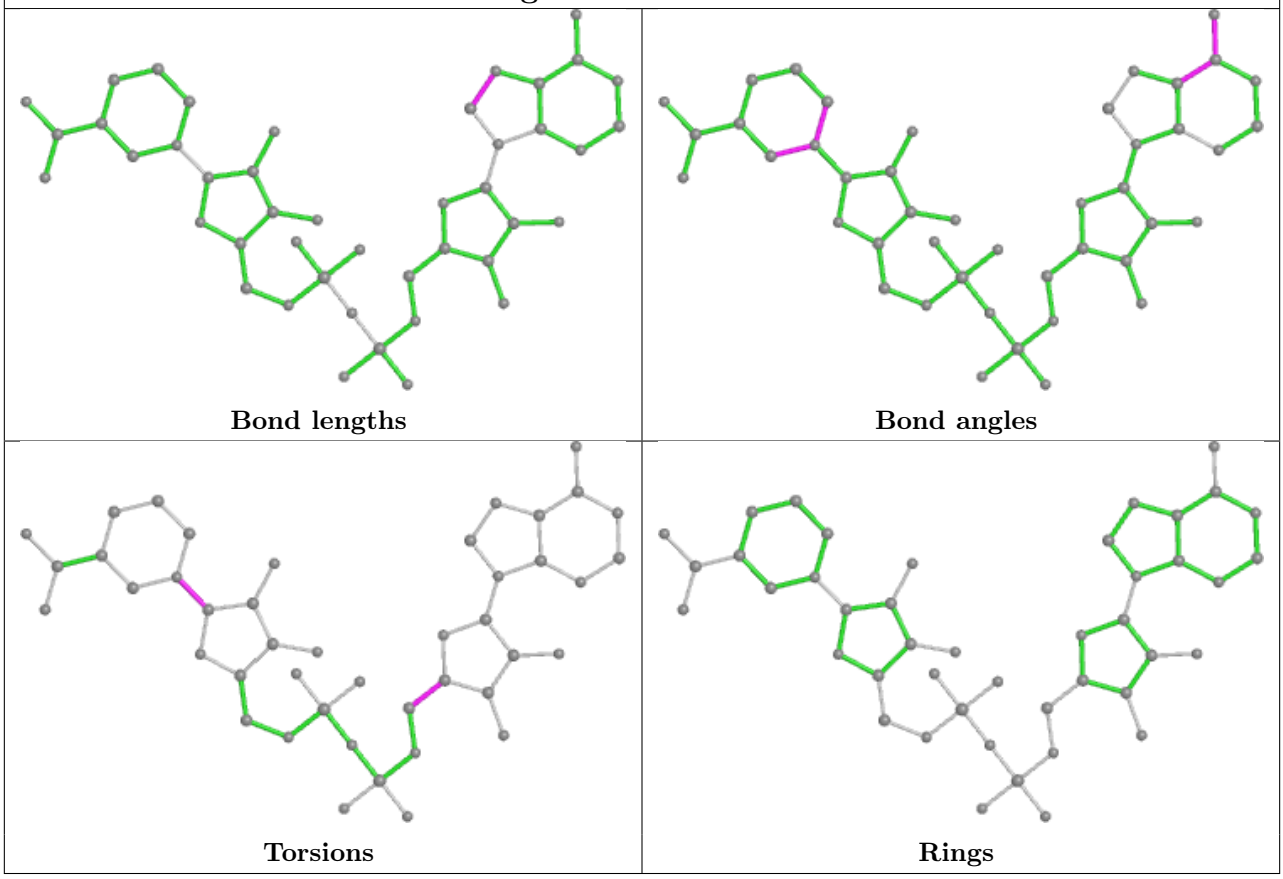
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	1	0
2	B	401	NAD	2	0
4	A	405	EDO	1	0
7	D	402	ACT	2	0
6	D	401	GOL	1	0

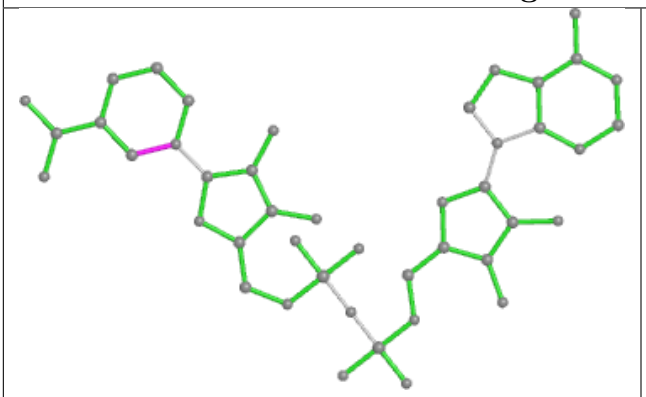
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

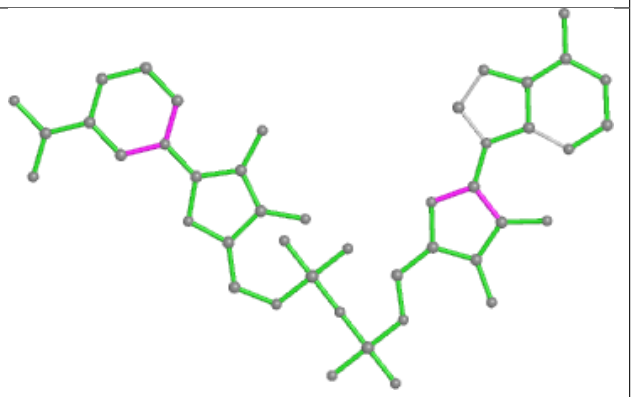
Ligand NAD A 401



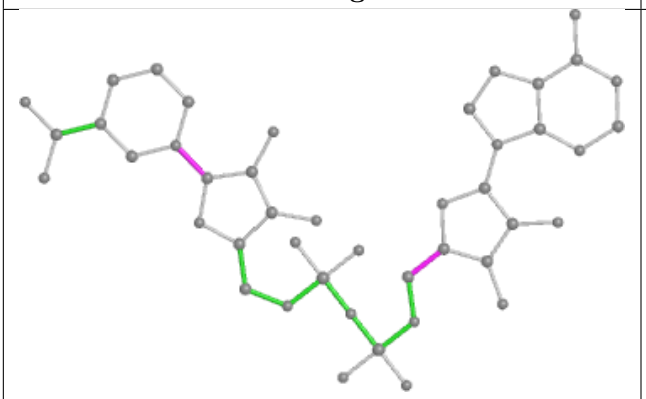
Ligand NAD B 401



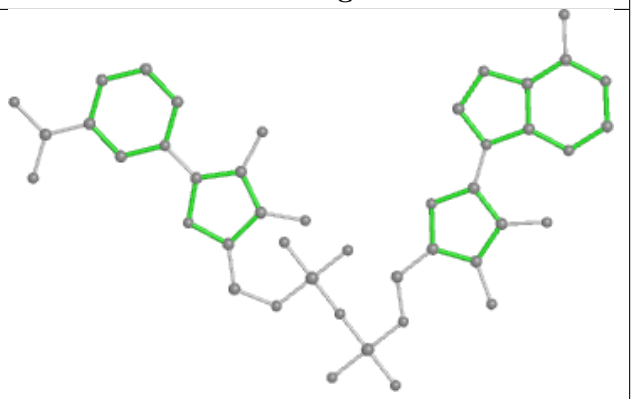
Bond lengths



Bond angles

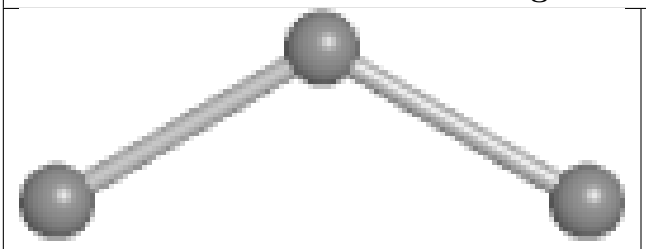


Torsions

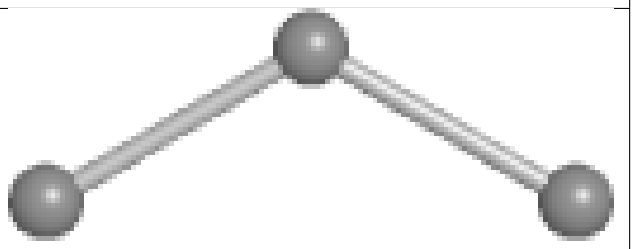


Rings

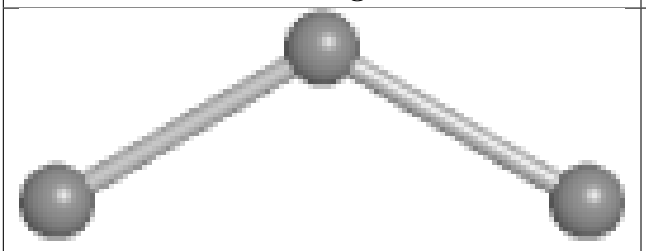
Ligand AZI B 402



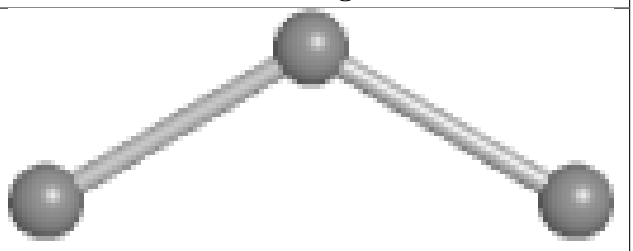
Bond lengths



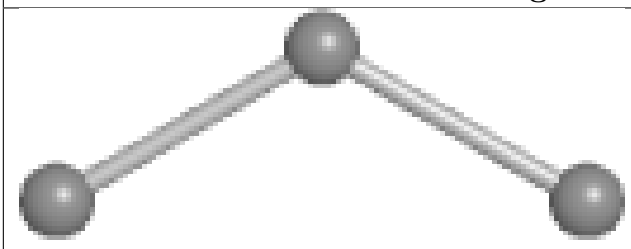
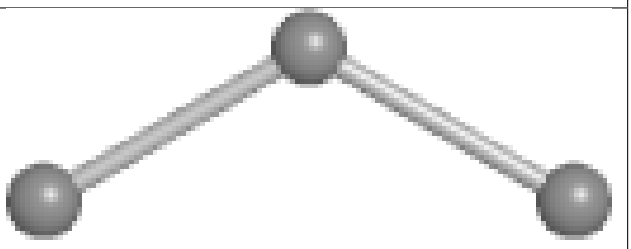
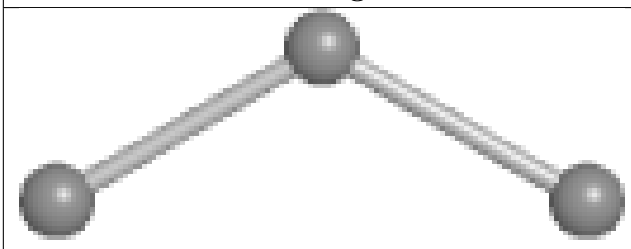
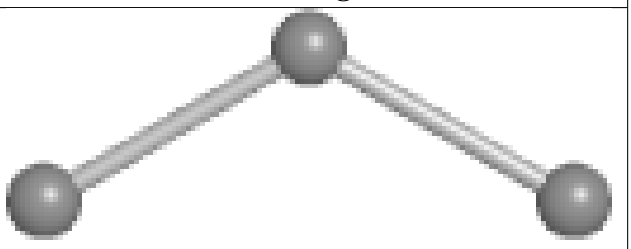
Bond angles



Torsions



Rings

Ligand AZI A 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	384/392 (97%)	-0.30	1 (0%) 94 92	10, 15, 26, 37	0
1	B	384/392 (97%)	-0.31	0 100 100	11, 17, 29, 44	0
1	C	375/392 (95%)	-0.37	1 (0%) 94 92	11, 17, 32, 49	0
1	D	374/392 (95%)	-0.36	5 (1%) 77 74	10, 18, 32, 49	0
All	All	1517/1568 (96%)	-0.33	7 (0%) 91 89	10, 17, 30, 49	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	81	ASP	3.6
1	D	229	GLU	2.4
1	D	233	GLU	2.3
1	D	80	PRO	2.3
1	A	123	ILE	2.1

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

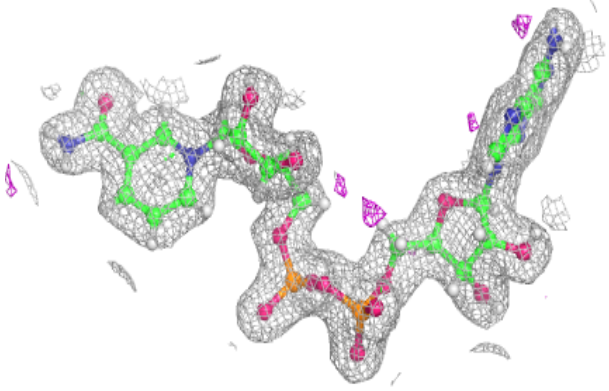
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

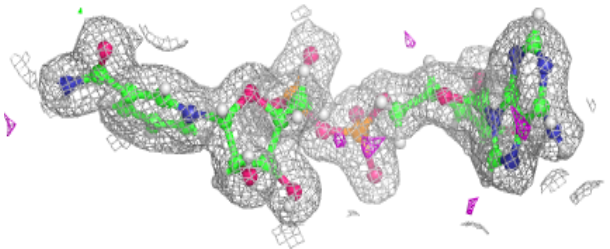
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	403	4/4	0.76	0.13	38,43,46,47	1
7	ACT	D	402	4/4	0.85	0.23	23,25,30,42	0
4	EDO	C	402	4/4	0.91	0.10	24,29,32,32	1
4	EDO	A	405	4/4	0.91	0.12	33,34,38,39	1
6	GOL	A	406	6/6	0.92	0.11	29,33,35,36	2
6	GOL	D	401	6/6	0.93	0.12	27,29,34,35	2
6	GOL	B	403	6/6	0.93	0.15	30,36,39,40	2
6	GOL	C	401	6/6	0.94	0.09	26,27,29,29	2
2	NAD	A	401	44/44	0.97	0.11	7,12,17,20	6
2	NAD	B	401	44/44	0.97	0.10	9,14,16,18	6
3	AZI	B	402	3/3	0.98	0.13	14,14,16,17	0
3	AZI	A	402	3/3	0.99	0.16	12,12,12,14	0
5	NA	A	404	1/1	1.00	0.06	14,14,14,14	0

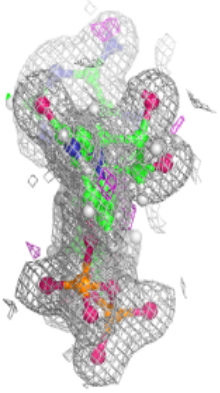
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 401:

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

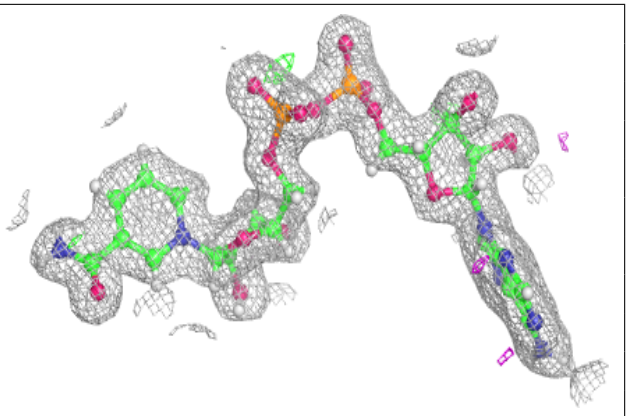


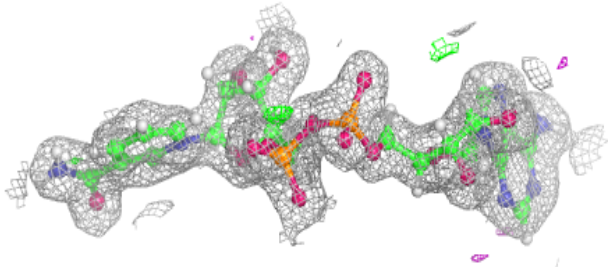


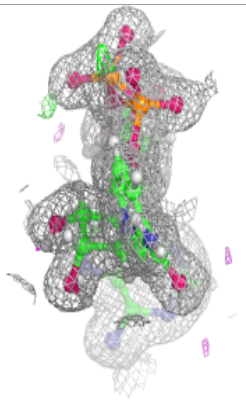


Electron density around NAD B 401:

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

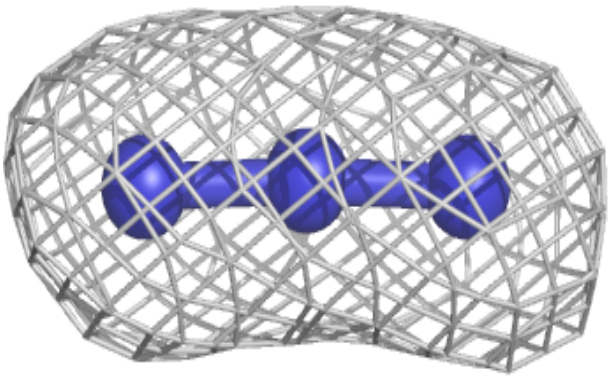


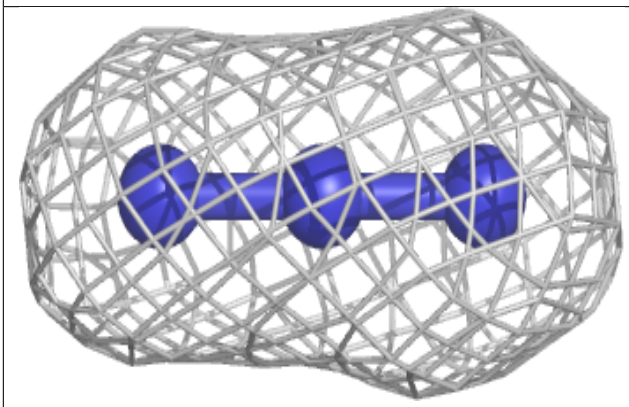


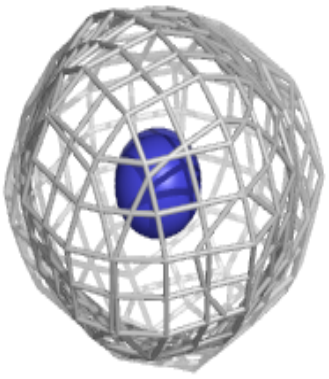


Electron density around AZI B 402:

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

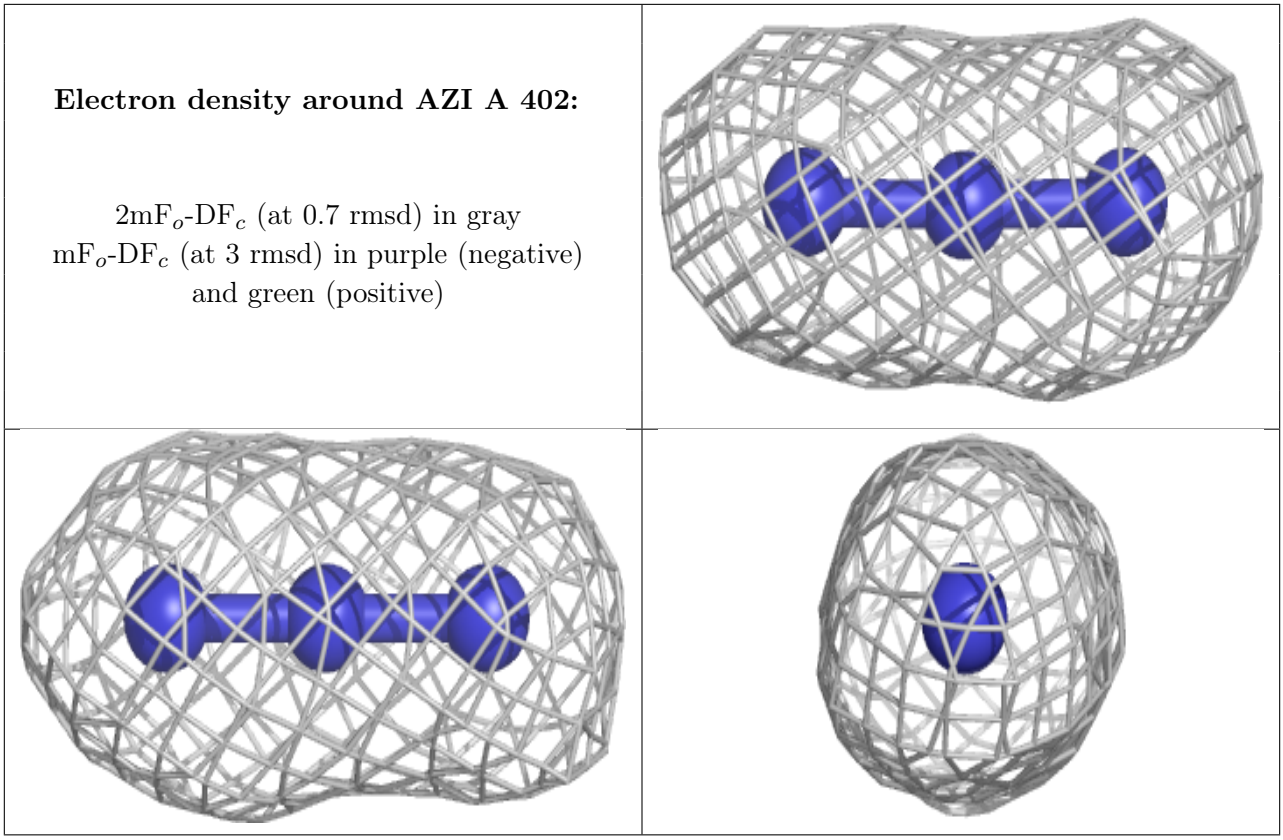






Electron density around AZI A 402:

$2mF_o$-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.