



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:01 am BST

PDB ID : 4PGF
Title : The structure of mono-acetylated SAHH
Authors : Kavran, J.M.; Wang, Y.; Cole, P.A.; Leahy, D.J.
Deposited on : 2014-05-01
Resolution : 2.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

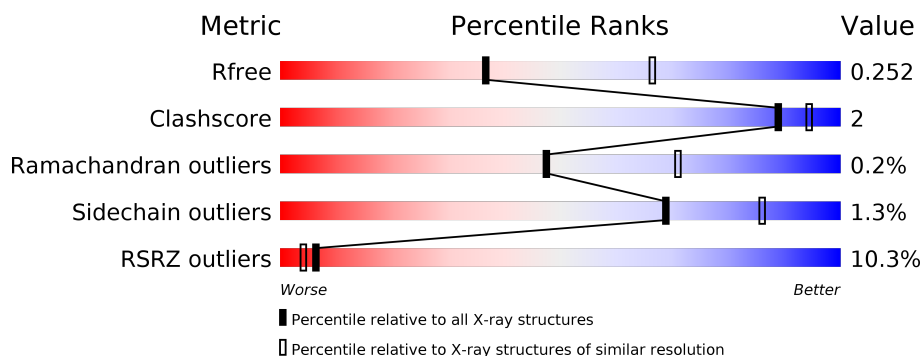
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	432	<div> <div>4%</div> <div>95%</div> <div>5%</div> </div>
1	B	432	<div> <div>17%</div> <div>92%</div> <div>7%</div> </div>

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 13514 atoms, of which 6715 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.

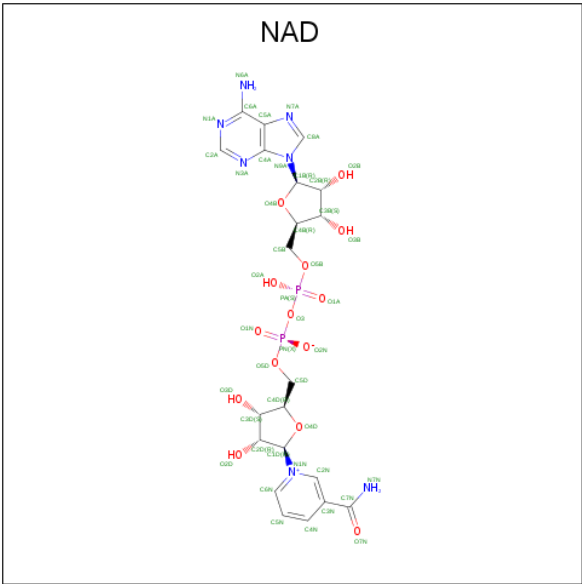
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	430	6671	2116	3335	572	622	26	0	1	0
1	B	428	6615	2102	3302	569	616	26	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

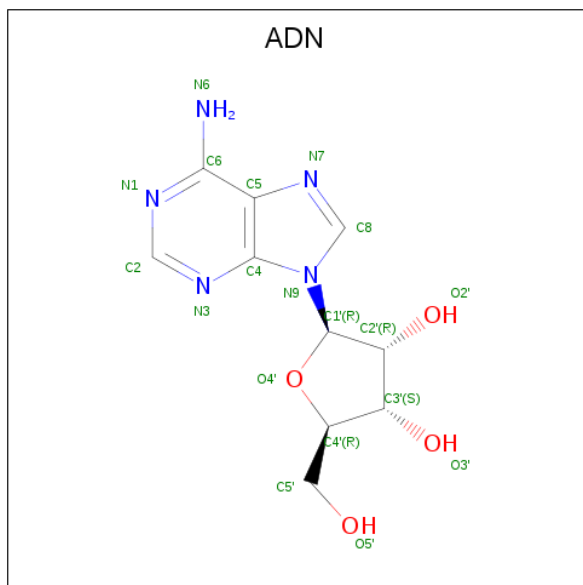
Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ASN	ASP	variant	UNP P23526
A	396	CYS	GLU	engineered mutation	UNP P23526
B	86	ASN	ASP	variant	UNP P23526
B	396	CYS	GLU	engineered mutation	UNP P23526

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			32	10	13	5	4		
3	B	1	Total	C	H	N	O	0	0
			32	10	13	5	4		

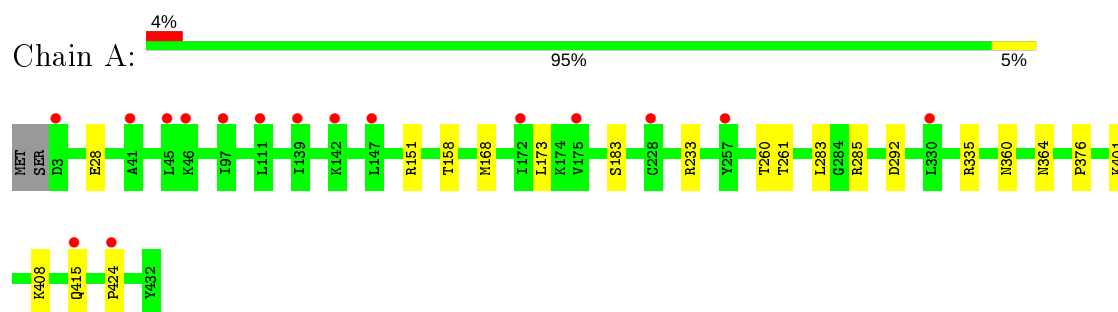
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	11	Total	O	0	0
			11	11		

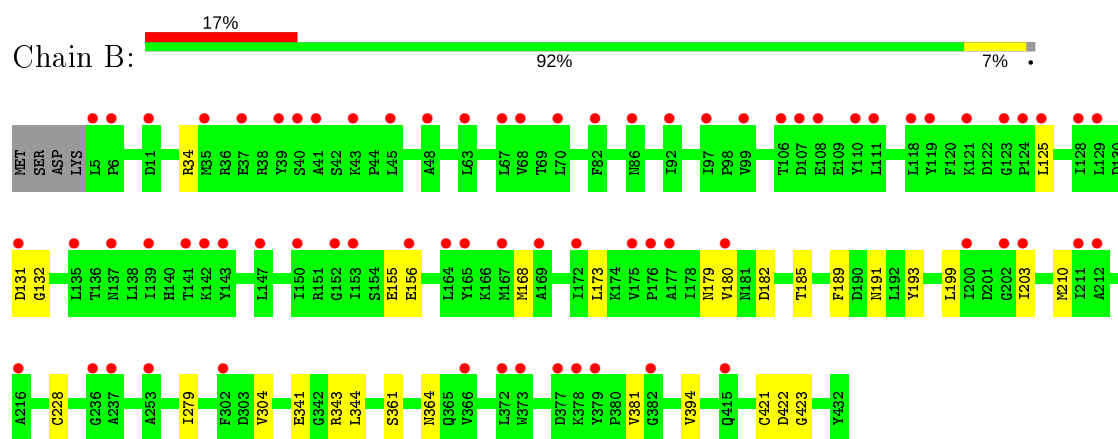
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.60 Å 102.74 Å 175.02 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.00 – 2.59 44.00 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.00-2.59) 99.7 (44.00-2.59)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.58 Å)	Xtriage
Refinement program	PHENIX 1.8.4 _1496	Depositor
R, R_{free}	0.188 , 0.248 0.197 , 0.252	Depositor DCC
R_{free} test set	1377 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13514	wwPDB-VP
Average B, all atoms (Å ²)	73.0	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.*

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: ADN, NAD, ALY

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	0.30	0/3390	0.46	0/4587
1	B	0.28	0/3364	0.45	1/4553 (0.0%)
All	All	0.29	0/6754	0.46	1/9140 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	422	ASP	C-N-CA	8.94	141.07	122.30

There are no chirality outliers.

There are no planarity outliers.

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	3336	3335	3350	9	0
1	B	3313	3302	3327	17	0
2	A	44	26	26	0	0
2	B	44	26	26	0	0
3	A	19	13	13	0	0
3	B	19	13	13	0	0
4	A	13	0	0	1	0
4	B	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6799	6715	6755	26	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.

All (26) 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:132:GLY:N	1:B:155:GLU:OE2	2.29	0.57
1:A:292:ASP:OD2	1:A:335:ARG:NH2	2.41	0.53
1:B:131:ASP:HA	1:B:155:GLU:OE2	2.11	0.50
1:B:168:MET:HE1	1:B:381:VAL:HG12	1.95	0.49
1:B:179:ASN:ND2	1:B:182:ASP:OD2	2.46	0.49
1:A:283:LEU:HD12	1:A:285:ARG:NH1	2.29	0.48
1:A:168:MET:HE2	1:A:173:LEU:HB3	1.96	0.46
1:B:180:VAL:HG13	1:B:364:ASN:HB3	1.96	0.46
1:A:151:ARG:HD3	1:A:376:PRO:HG3	1.98	0.45
1:B:168:MET:HE3	1:B:173:LEU:HD23	1.98	0.45
1:B:279:ILE:HG22	1:B:304:VAL:HB	1.99	0.45
1:A:260:THR:OG1	1:A:261:THR:N	2.48	0.44
1:B:185:THR:HG21	1:B:394:VAL:HG11	2.00	0.43
1:A:28:GLU:OE2	1:A:401:LYS:HE2	2.18	0.43
1:B:131:ASP:HB3	1:B:156:GLU:HB3	2.00	0.43
1:B:156:GLU:OE2	1:B:361:SER:HB3	2.19	0.43
1:A:360:ASN:O	1:A:364:ASN:ND2	2.49	0.43
1:B:199:LEU:HD22	1:B:228:CYS:SG	2.60	0.42
1:A:408:ALY:HE3	1:A:408:ALY:HH31	1.86	0.42
1:B:341:GLU:HB2	1:B:343:ARG:NH1	2.34	0.42
1:A:415:GLN:NE2	4:A:602:HOH:O	2.44	0.41
1:B:199:LEU:HD11	1:B:203:ILE:HD11	2.02	0.41
1:B:185:THR:HG21	1:B:394:VAL:CG1	2.50	0.41
1:B:131:ASP:CB	1:B:156:GLU:HB3	2.51	0.41
1:B:168:MET:HE2	1:B:173:LEU:HB3	2.02	0.40
1:B:189:PHE:HA	1:B:193:TYR:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/432 (99%)	405 (95%)	22 (5%)	1 (0%)	47	71
1	B	425/432 (98%)	402 (95%)	22 (5%)	1 (0%)	47	71
All	All	853/864 (99%)	807 (95%)	44 (5%)	2 (0%)	47	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	PRO
1	B	423	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/355 (100%)	351 (99%)	3 (1%)	81	92
1	B	351/355 (99%)	345 (98%)	6 (2%)	60	81
All	All	705/710 (99%)	696 (99%)	9 (1%)	69	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	THR
1	A	183	SER
1	A	233	ARG
1	B	34	ARG

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Mol	Chain	Res	Type
1	B	125	LEU
1	B	191	ASN
1	B	210	MET
1	B	344	LEU
1	B	421	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	ALY	B	408	1	10,11,12	0.96	1 (10%)	7,12,14	1.58	2 (28%)
1	ALY	A	408	1	10,11,12	0.85	0	7,12,14	1.41	1 (14%)

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
1	ALY	B	408	1	-	3/9/10/12	-
1	ALY	A	408	1	-	3/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	408	ALY	CH-NZ	2.13	1.40	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	ALY	CE-NZ-CH	3.15	127.41	122.56
1	A	408	ALY	CE-NZ-CH	3.13	127.36	122.56
1	B	408	ALY	CH3-CH-NZ	2.14	119.88	116.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	408	ALY	OH-CH-NZ-CE
1	B	408	ALY	CH3-CH-NZ-CE
1	A	408	ALY	OH-CH-NZ-CE
1	A	408	ALY	CH3-CH-NZ-CE
1	B	408	ALY	CG-CD-CE-NZ
1	A	408	ALY	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	408	ALY	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	ADN	B	502	-	18,21,21	0.78	1 (5%)	18,31,31	0.89	0
3	ADN	A	502	-	18,21,21	0.81	1 (5%)	18,31,31	0.91	0
2	NAD	A	501	-	42,48,48	1.58	7 (16%)	50,73,73	1.63	10 (20%)
2	NAD	B	501	-	42,48,48	1.56	5 (11%)	50,73,73	1.69	10 (20%)

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	ADN	B	502	-	-	2/2/22/22	0/3/3/3
3	ADN	A	502	-	-	2/2/22/22	0/3/3/3
2	NAD	A	501	-	-	12/26/62/62	0/5/5/5
2	NAD	B	501	-	-	7/26/62/62	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	PN-O5D	5.14	1.80	1.59
2	A	501	NAD	PN-O5D	4.74	1.78	1.59
2	B	501	NAD	PA-O5B	4.10	1.75	1.59
2	A	501	NAD	PA-O5B	3.99	1.75	1.59
2	A	501	NAD	C7N-N7N	2.67	1.38	1.33
2	B	501	NAD	C7N-N7N	2.59	1.37	1.33
2	A	501	NAD	C2N-N1N	2.51	1.38	1.35
2	B	501	NAD	C2N-N1N	2.34	1.37	1.35
3	A	502	ADN	C2-N3	2.28	1.35	1.32
2	B	501	NAD	O2D-C2D	-2.23	1.37	1.43
2	A	501	NAD	C2A-N3A	2.11	1.35	1.32
2	A	501	NAD	C2A-N1A	2.09	1.37	1.33
3	B	502	ADN	C2-N3	2.07	1.35	1.32
2	A	501	NAD	O2D-C2D	-2.04	1.38	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	PN-O3-PA	-5.58	113.67	132.83
2	A	501	NAD	PN-O3-PA	-4.84	116.22	132.83
2	B	501	NAD	O2A-PA-O1A	3.60	130.02	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAD	O2A-PA-O1A	3.55	129.78	112.24
2	B	501	NAD	O2N-PN-O1N	3.44	129.23	112.24
2	A	501	NAD	O2N-PN-O1N	3.28	128.46	112.24
2	B	501	NAD	C5B-C4B-C3B	-2.81	104.66	115.18
2	A	501	NAD	C5B-C4B-C3B	-2.61	105.39	115.18
2	B	501	NAD	C1B-N9A-C4A	-2.59	122.09	126.64
2	A	501	NAD	O4B-C1B-C2B	-2.59	103.15	106.93
2	A	501	NAD	O2N-PN-O5D	-2.58	95.74	107.75
2	B	501	NAD	O5D-PN-O1N	-2.50	99.28	109.07
2	A	501	NAD	C1B-N9A-C4A	-2.46	122.32	126.64
2	B	501	NAD	O4B-C1B-C2B	-2.45	103.35	106.93
2	A	501	NAD	C3D-C2D-C1D	-2.36	97.43	100.98
2	A	501	NAD	O5D-PN-O1N	-2.35	99.87	109.07
2	B	501	NAD	O2N-PN-O5D	-2.30	97.08	107.75
2	A	501	NAD	PN-O5D-C5D	-2.20	108.80	121.68
2	B	501	NAD	PN-O5D-C5D	-2.12	109.24	121.68
2	B	501	NAD	C3D-C2D-C1D	-2.08	97.84	100.98

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	C5B-O5B-PA-O1A
2	A	501	NAD	C5B-O5B-PA-O2A
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
3	B	502	ADN	C3'-C4'-C5'-O5'
3	A	502	ADN	C3'-C4'-C5'-O5'
2	A	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	C3B-C4B-C5B-O5B
3	B	502	ADN	O4'-C4'-C5'-O5'
3	A	502	ADN	O4'-C4'-C5'-O5'
2	A	501	NAD	O4D-C4D-C5D-O5D
2	A	501	NAD	C5B-O5B-PA-O3
2	B	501	NAD	O4D-C4D-C5D-O5D
2	A	501	NAD	PA-O3-PN-O2N

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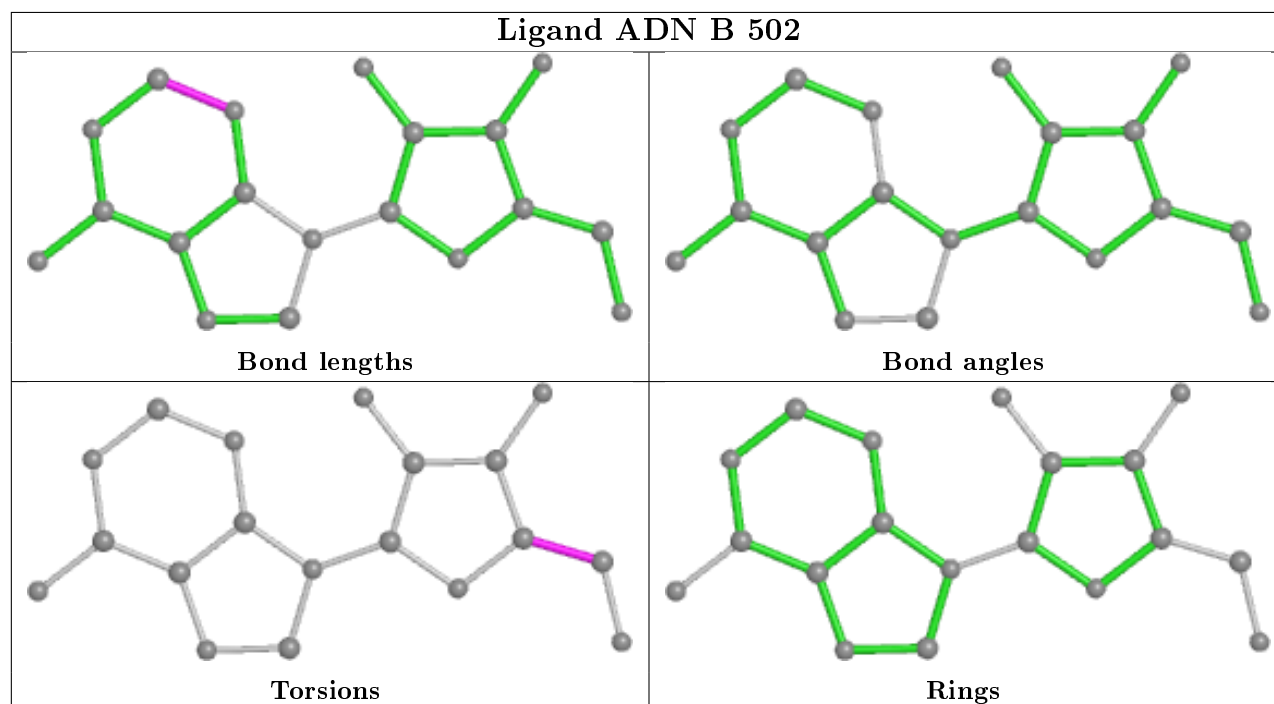
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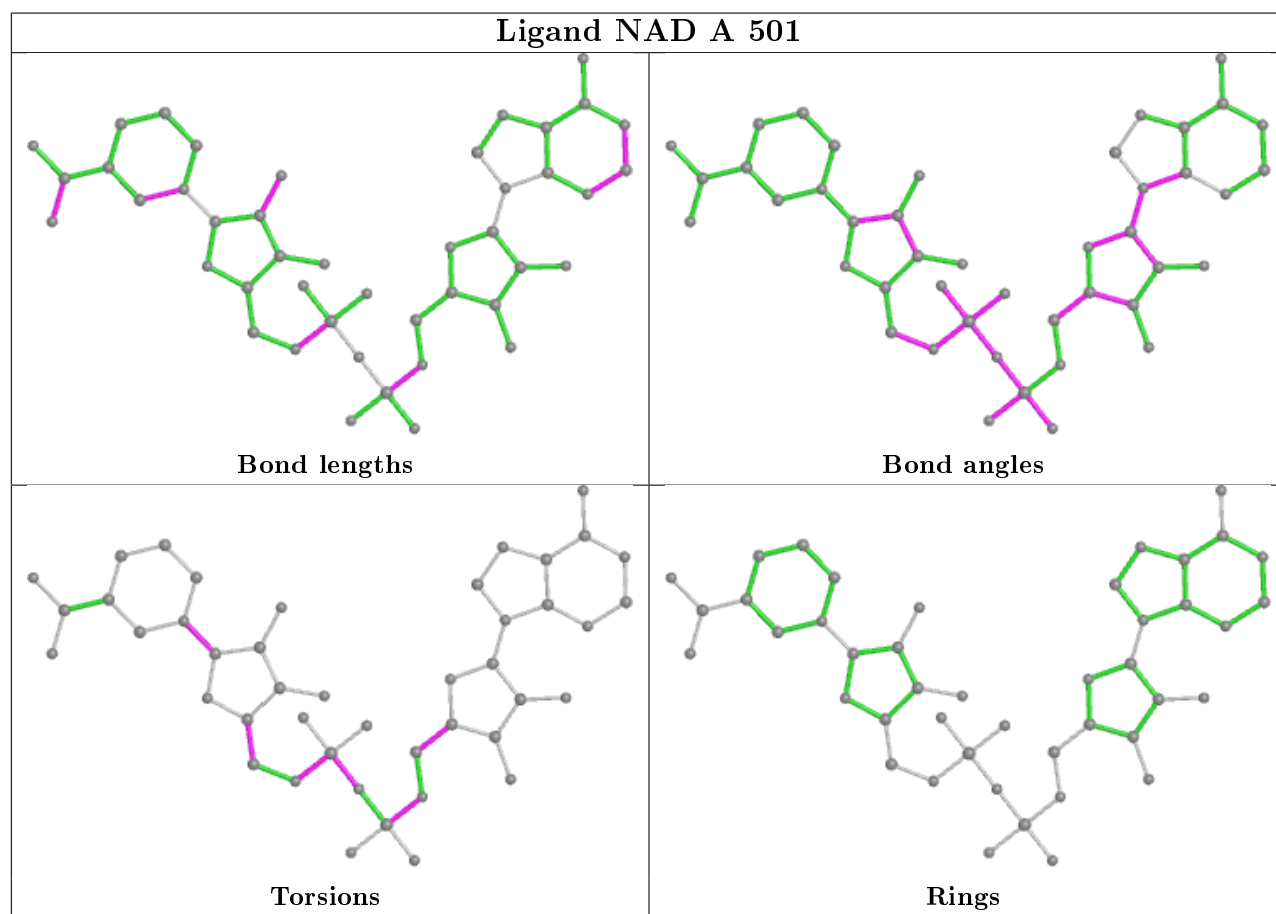
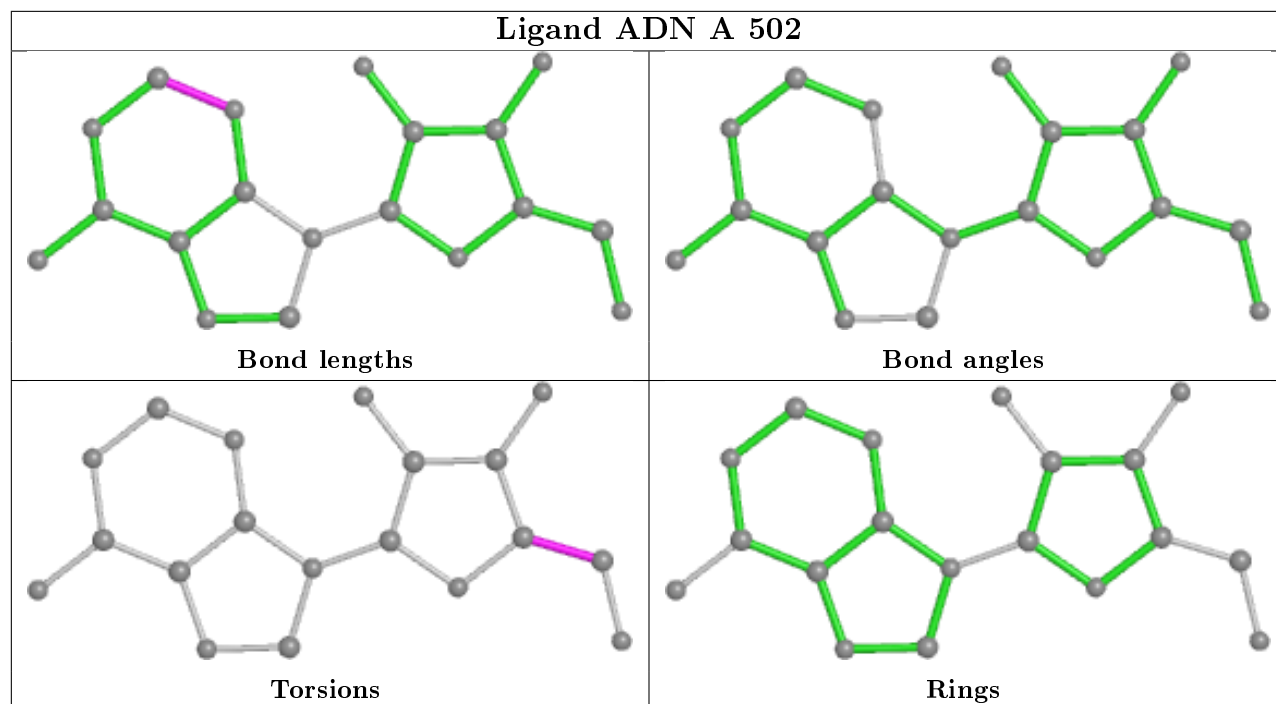
Mol	Chain	Res	Type	Atoms
2	A	501	NAD	C5D-O5D-PN-O1N
2	B	501	NAD	C5D-O5D-PN-O1N
2	B	501	NAD	O4B-C4B-C5B-O5B

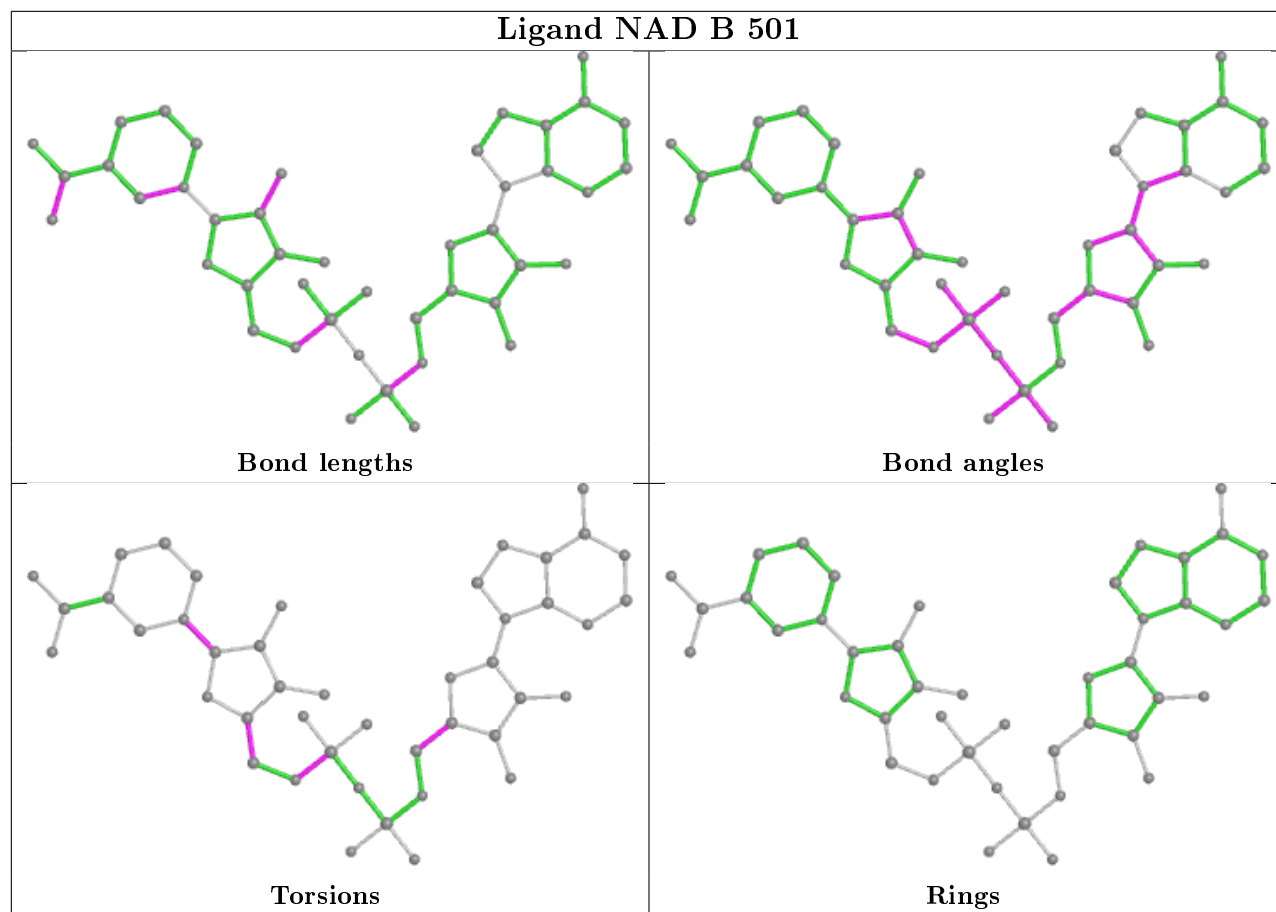
There are no ring outliers.

No monomer is involved in short contacts.

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

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, 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	429/432 (99%)	0.44	16 (3%) 41 34	44, 58, 72, 106	0
1	B	427/432 (98%)	1.00	72 (16%) 1 1	44, 72, 103, 226	0
All	All	856/864 (99%)	0.72	88 (10%) 6 4	44, 61, 100, 226	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	ILE	6.9
1	B	111	LEU	6.3
1	B	378	LYS	5.9
1	B	175	VAL	5.5
1	B	118	LEU	5.2
1	B	379	TYR	5.1
1	B	124	PRO	4.9
1	B	150	ILE	4.8
1	B	86	ASN	4.5
1	B	152	GLY	4.4
1	B	39	TYR	4.2
1	B	372	LEU	4.1
1	B	129	LEU	4.0
1	B	177	ALA	3.9
1	B	97	ILE	3.8
1	B	143	TYR	3.7
1	B	377	ASP	3.6
1	B	373	TRP	3.6
1	B	92	ILE	3.6
1	B	123	GLY	3.6
1	B	121	LYS	3.4
1	B	107	ASP	3.3
1	B	45	LEU	3.3
1	B	99	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	165	TYR	3.2
1	A	172	ILE	3.2
1	B	82	PHE	3.2
1	B	141	THR	3.1
1	B	135	LEU	3.1
1	A	45	LEU	3.1
1	B	40	SER	3.0
1	B	67	LEU	3.0
1	B	366	VAL	2.9
1	B	164	LEU	2.9
1	B	125	LEU	2.8
1	B	110	TYR	2.8
1	B	119	TYR	2.8
1	B	108	GLU	2.7
1	B	415	GLN	2.7
1	B	6	PRO	2.7
1	B	37	GLU	2.7
1	B	131	ASP	2.7
1	B	237	ALA	2.7
1	B	203	ILE	2.7
1	B	142	LYS	2.7
1	B	382	GLY	2.7
1	B	302	PHE	2.6
1	B	236	GLY	2.6
1	B	137	ASN	2.6
1	B	106	THR	2.5
1	B	35	MET	2.5
1	B	212	ALA	2.5
1	B	70	LEU	2.5
1	B	11	ASP	2.5
1	B	128	ILE	2.4
1	B	68	VAL	2.4
1	B	180	VAL	2.4
1	A	3	ASP	2.4
1	A	142	LYS	2.4
1	B	176	PRO	2.4
1	B	48	ALA	2.4
1	B	147	LEU	2.4
1	B	156	GLU	2.3
1	B	202	GLY	2.3
1	B	216	ALA	2.3
1	B	63	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	172	ILE	2.3
1	A	228	CYS	2.3
1	B	169	ALA	2.3
1	B	5	LEU	2.2
1	A	111	LEU	2.2
1	A	147	LEU	2.2
1	B	43	LYS	2.2
1	A	424	PRO	2.2
1	B	200	ILE	2.2
1	A	330	LEU	2.2
1	A	257	TYR	2.1
1	A	41	ALA	2.1
1	A	97	ILE	2.1
1	A	415	GLN	2.1
1	A	175	VAL	2.1
1	B	211	ILE	2.1
1	B	167	MET	2.1
1	A	46	LYS	2.1
1	B	253	ALA	2.1
1	B	139	ILE	2.1
1	B	41	ALA	2.0
1	A	139	ILE	2.0

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

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(Å ²)	Q<0.9
1	ALY	B	408	12/13	0.88	0.32	55,68,79,79	0
1	ALY	A	408	12/13	0.88	0.23	53,73,88,89	0

6.3 Carbohydrates ⓘ

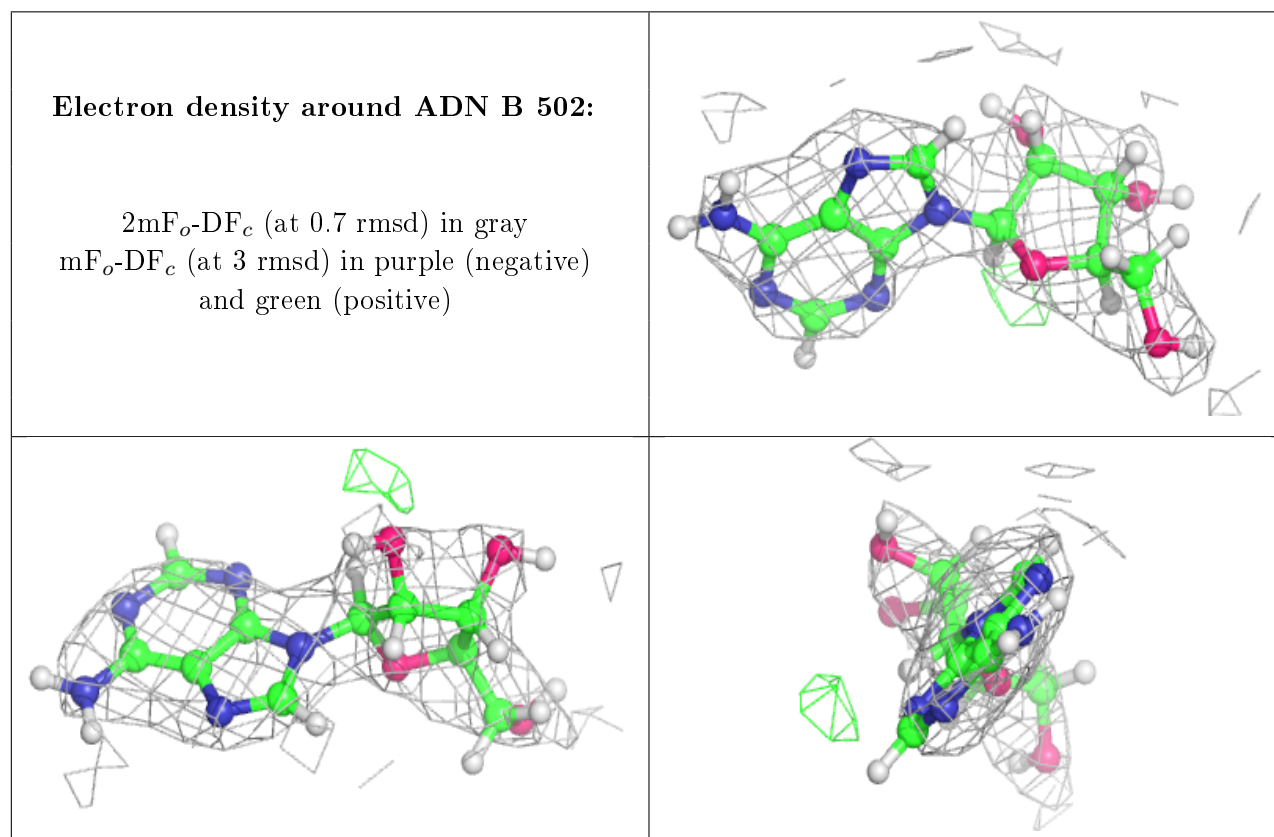
There are no carbohydrates in this entry.

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.

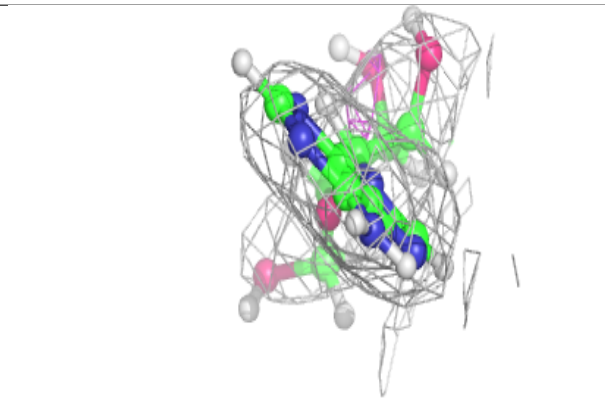
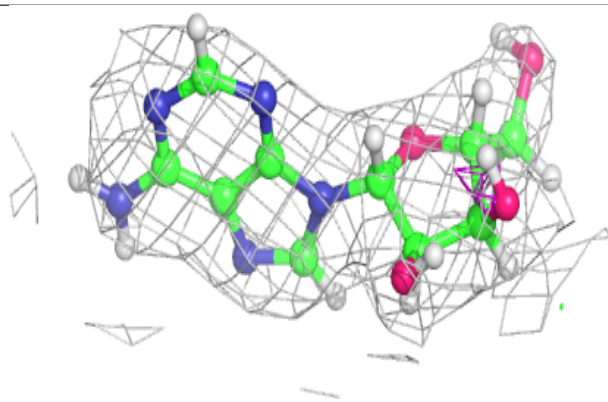
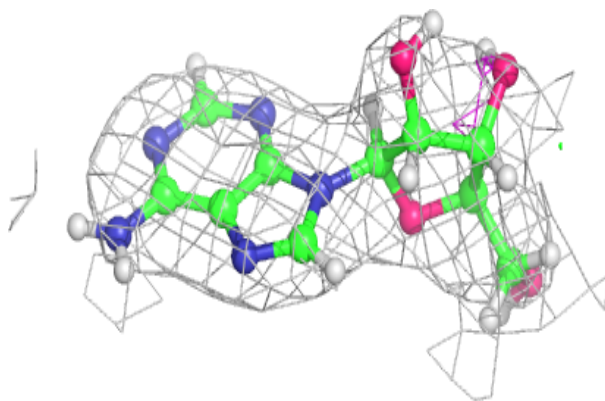
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADN	B	502	19/19	0.92	0.23	71,78,94,96	0
3	ADN	A	502	19/19	0.92	0.20	56,60,72,73	0
2	NAD	B	501	44/44	0.95	0.17	53,66,82,87	0
2	NAD	A	501	44/44	0.97	0.16	47,56,68,70	0

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.

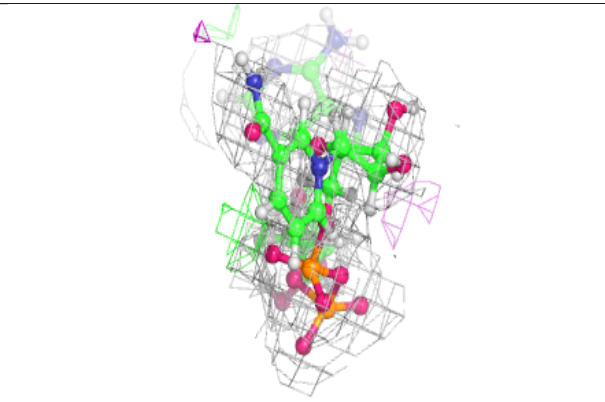
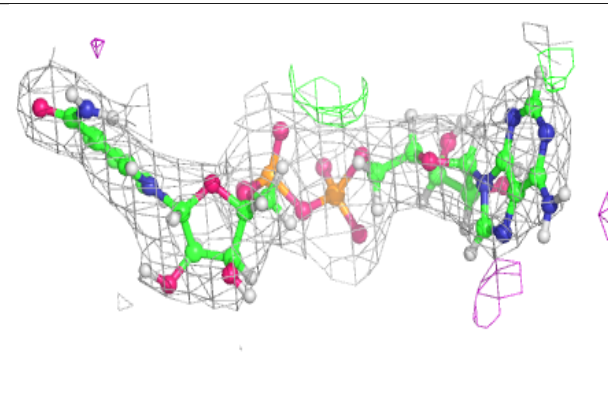
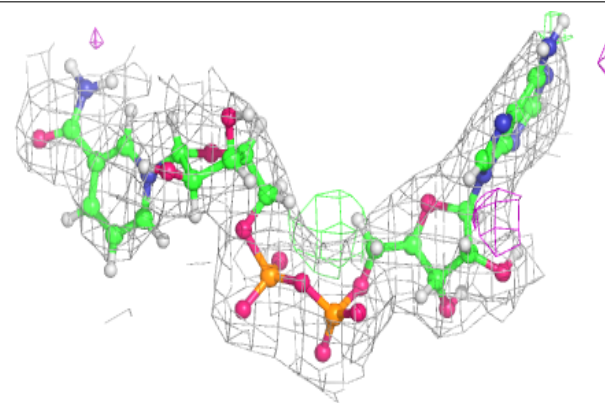


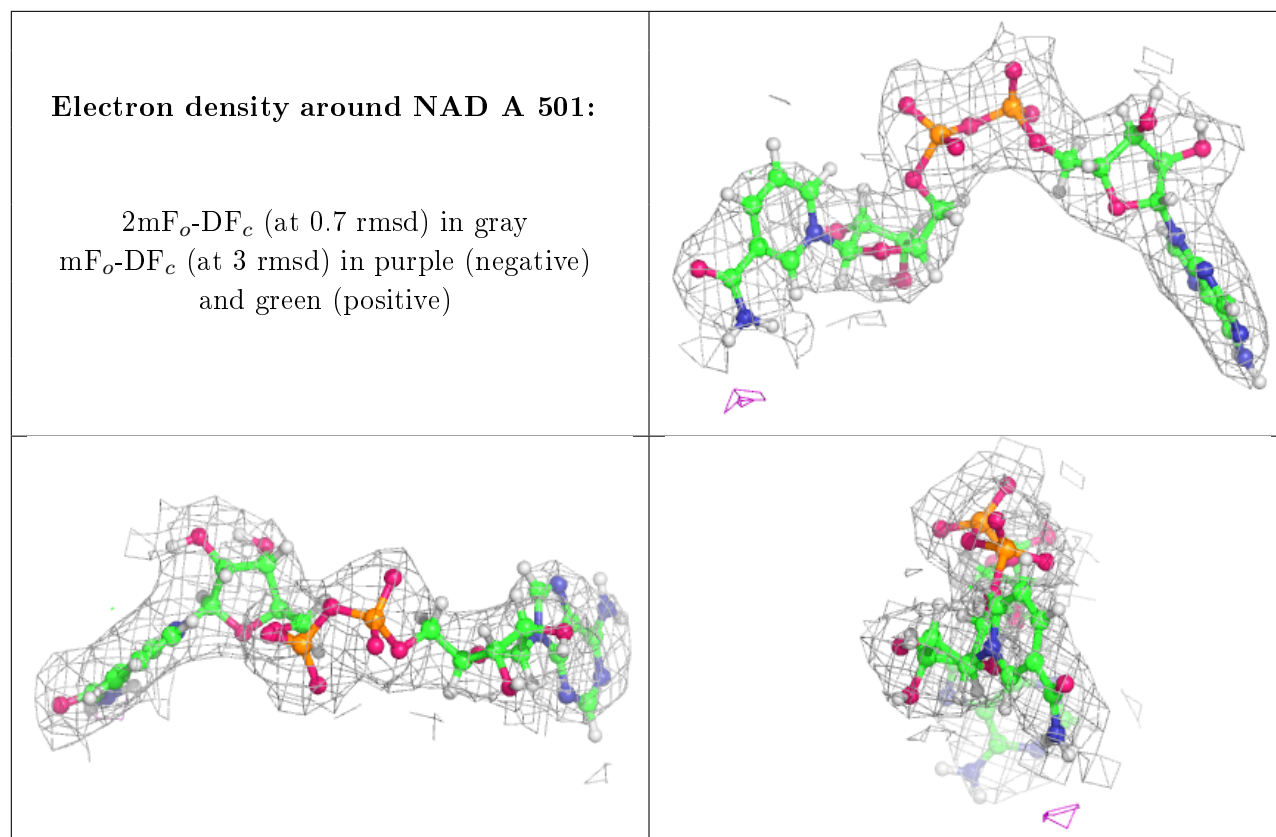
Electron density around ADN A 502:

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

**Electron density around NAD B 501:**

$2mF_o-DF_c$ (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.