



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 09:16 AM BST

PDB ID : 6UK3  
Title : Crystal Structure of S-adenosyl-L-homocysteine hydrolase from *Acanthamoeba castellanii* with bound NAD and Adenosine  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2019-10-04  
Resolution : 1.40 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](mailto: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.

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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 : 2.13  
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) : 2.13

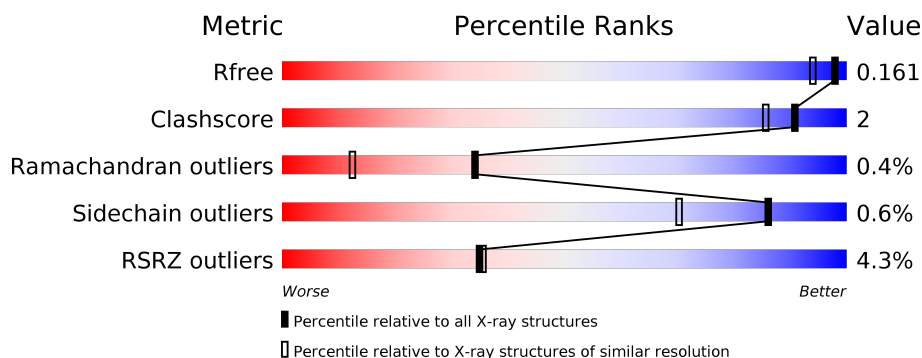
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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  $\geq 3$ , 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	485	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> <div></div> </div> <div>• •</div> </div>
1	B	485	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> <div>•</div> </div>
1	C	485	<div> <div>8%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div></div> </div> <div>• •</div> </div>
1	D	485	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div></div> </div> <div>•</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17784 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 Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	23	0
			3839	2453	652	710	24			
1	B	475	Total	C	N	O	S	0	12	0
			3756	2394	638	700	24			
1	C	475	Total	C	N	O	S	0	12	0
			3753	2392	638	700	23			
1	D	475	Total	C	N	O	S	0	14	0
			3765	2400	640	702	23			

There are 32 discrepancies between the modelled and reference sequences:

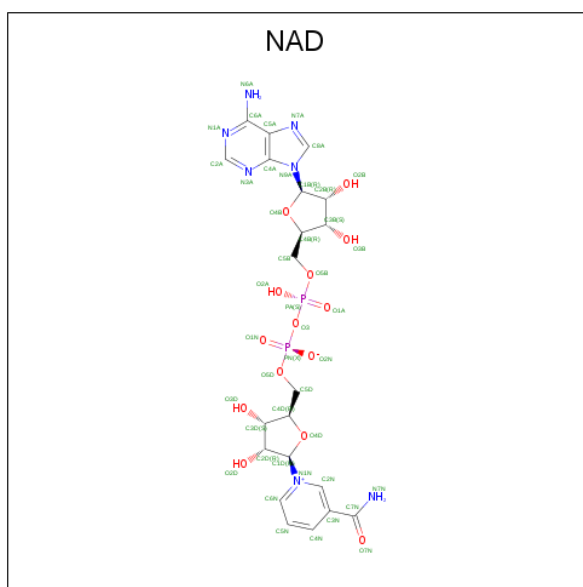
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP L8H6B5
A	-6	ALA	-	expression tag	UNP L8H6B5
A	-5	HIS	-	expression tag	UNP L8H6B5
A	-4	HIS	-	expression tag	UNP L8H6B5
A	-3	HIS	-	expression tag	UNP L8H6B5
A	-2	HIS	-	expression tag	UNP L8H6B5
A	-1	HIS	-	expression tag	UNP L8H6B5
A	0	HIS	-	expression tag	UNP L8H6B5
B	-7	MET	-	initiating methionine	UNP L8H6B5
B	-6	ALA	-	expression tag	UNP L8H6B5
B	-5	HIS	-	expression tag	UNP L8H6B5
B	-4	HIS	-	expression tag	UNP L8H6B5
B	-3	HIS	-	expression tag	UNP L8H6B5
B	-2	HIS	-	expression tag	UNP L8H6B5
B	-1	HIS	-	expression tag	UNP L8H6B5
B	0	HIS	-	expression tag	UNP L8H6B5
C	-7	MET	-	initiating methionine	UNP L8H6B5
C	-6	ALA	-	expression tag	UNP L8H6B5
C	-5	HIS	-	expression tag	UNP L8H6B5
C	-4	HIS	-	expression tag	UNP L8H6B5
C	-3	HIS	-	expression tag	UNP L8H6B5

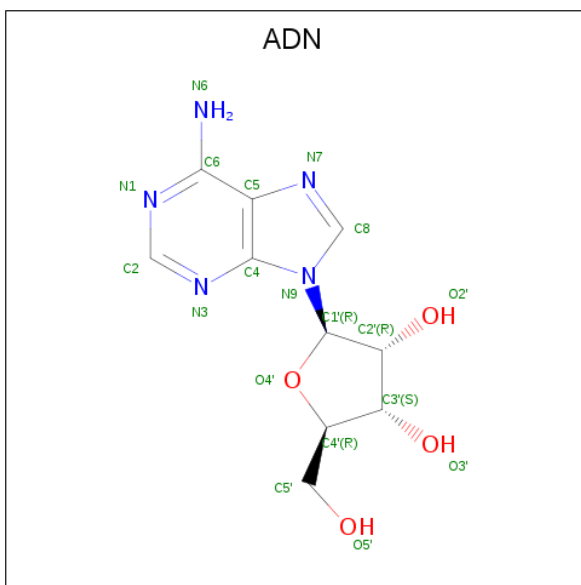
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP L8H6B5
C	-1	HIS	-	expression tag	UNP L8H6B5
C	0	HIS	-	expression tag	UNP L8H6B5
D	-7	MET	-	initiating methionine	UNP L8H6B5
D	-6	ALA	-	expression tag	UNP L8H6B5
D	-5	HIS	-	expression tag	UNP L8H6B5
D	-4	HIS	-	expression tag	UNP L8H6B5
D	-3	HIS	-	expression tag	UNP L8H6B5
D	-2	HIS	-	expression tag	UNP L8H6B5
D	-1	HIS	-	expression tag	UNP L8H6B5
D	0	HIS	-	expression tag	UNP L8H6B5

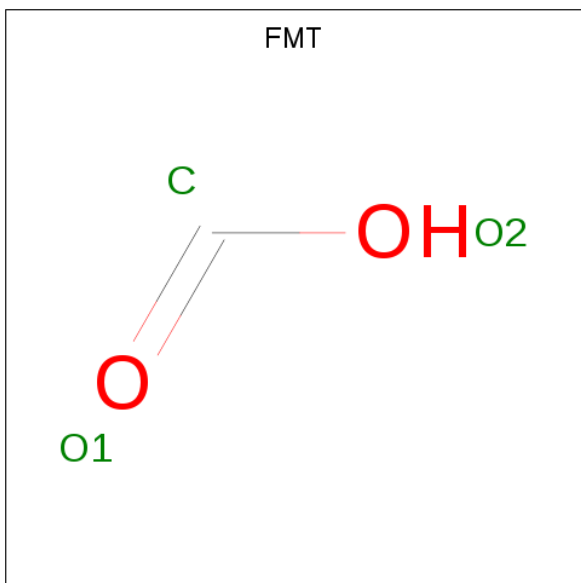
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by author).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	0
			19	10	5	4		
3	C	1	Total	C	N	O	0	0
			19	10	5	4		
3	D	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).

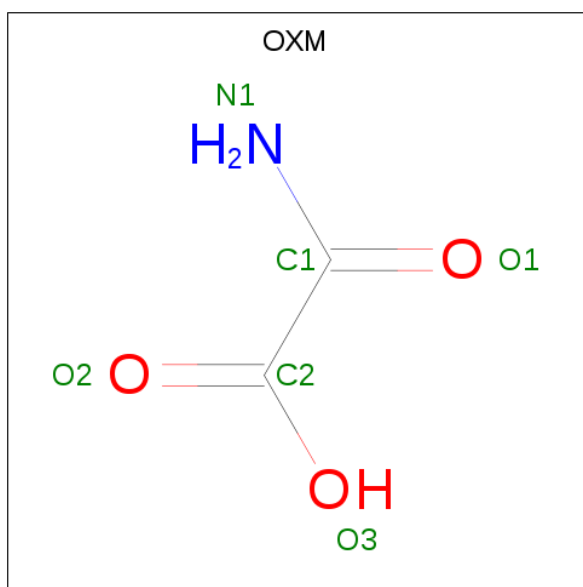


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	A	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0

- Molecule 6 is OXAMIC ACID (three-letter code: OXM) (formula: C<sub>2</sub>H<sub>3</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	658	Total	O	0	18
			675	675		
8	B	563	Total	O	0	8
			570	570		
8	C	570	Total	O	0	6
			575	575		
8	D	538	Total	O	0	5
			542	542		



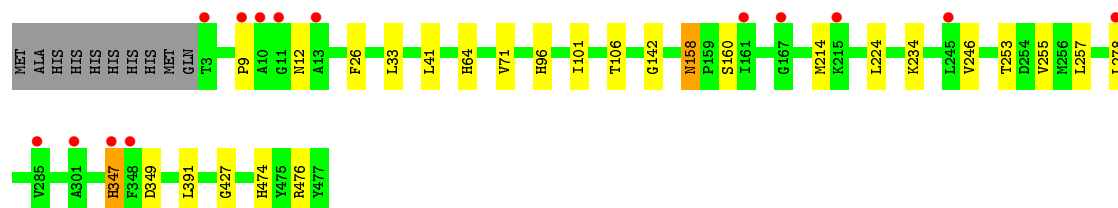
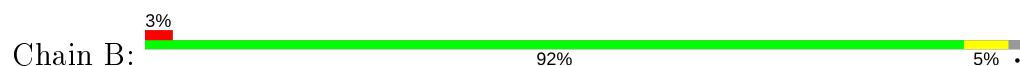
### 3 Residue-property plots [i](#)

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.

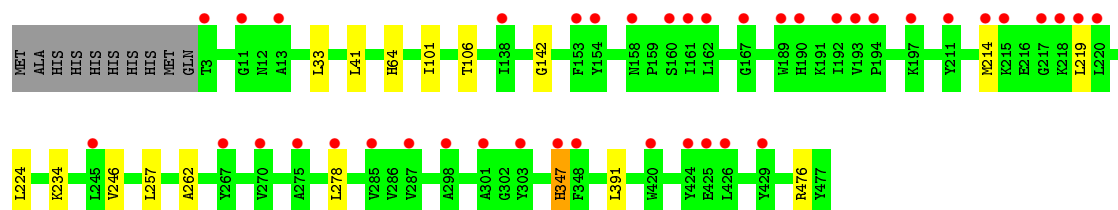
- Molecule 1: Adenosylhomocysteinase



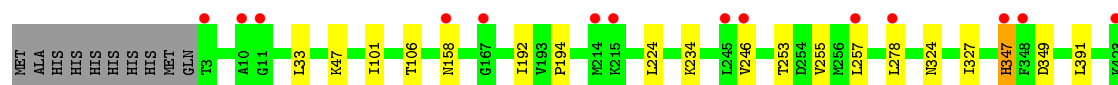
- Molecule 1: Adenosylhomocysteinase

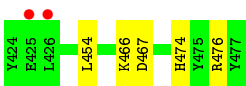


- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.03Å 112.73Å 105.92Å 90.00° 114.72° 90.00°	Depositor
Resolution (Å)	50.00 – 1.40 48.92 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.40) 99.8 (48.92-1.40)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.17rc1_3602	Depositor
R, $R_{free}$	0.130 , 0.161 0.130 , 0.161	Depositor DCC
$R_{free}$ test set	2001 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	17784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAD, K, OXM, ACT, ADN, FMT

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	0.33	0/3976	0.56	0/5375
1	B	0.31	0/3860	0.53	0/5227
1	C	0.31	0/3857	0.54	0/5224
1	D	0.31	0/3875	0.52	0/5249
All	All	0.31	0/15568	0.54	0/21075

There are no bond length outliers.

There are no bond angle outliers.

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	3839	0	3893	9	0
1	B	3756	0	3751	17	0
1	C	3753	0	3744	11	0
1	D	3765	0	3759	16	0
2	A	44	0	26	1	0
2	B	44	0	26	2	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	19	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	0	13	1	0
3	C	19	0	13	1	0
3	D	19	0	13	1	0
4	A	3	0	1	1	0
4	B	9	0	3	2	0
4	C	6	0	2	1	0
4	D	9	0	3	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	0	2	0	0
7	B	8	0	6	0	0
7	C	4	0	3	0	0
7	D	8	0	6	0	0
8	A	675	0	0	1	0
8	B	570	0	0	0	0
8	C	575	0	0	0	0
8	D	542	0	0	3	0
All	All	17784	0	15329	53	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 (53) 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:347[B]:HIS:HA	1:D:391:LEU:HD21	1.58	0.84
1:A:347[B]:HIS:HA	1:A:391:LEU:HD21	1.61	0.82
1:C:347[B]:HIS:HA	1:C:391:LEU:HD21	1.60	0.82
1:B:347[B]:HIS:HA	1:B:391:LEU:HD21	1.60	0.80
1:B:33:LEU:HD23	4:C:503:FMT:H	1.68	0.74
1:A:214[A]:MET:SD	8:A:977:HOH:O	2.54	0.66
2:A:501:NAD:C4N	3:A:502:ADN:H3'	2.27	0.65
2:B:501:NAD:C4N	3:B:502:ADN:H3'	2.27	0.65
2:C:501:NAD:C4N	3:C:502:ADN:H3'	2.27	0.65
2:D:501:NAD:C4N	3:D:502:ADN:H3'	2.28	0.64
1:A:476:ARG:HB2	1:C:234[B]:LYS:HE3	1.85	0.58
1:D:194:PRO:HB2	4:D:506:FMT:H	1.86	0.58
1:A:246:VAL:HG23	1:A:257[A]:LEU:HD11	1.86	0.58
1:B:234[A]:LYS:HE3	1:D:476:ARG:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:508:FMT:H	1:C:33:LEU:HD23	1.87	0.56
1:D:246:VAL:HG11	8:D:911[B]:HOH:O	2.06	0.55
1:B:476:ARG:HB2	1:D:234[B]:LYS:HE3	1.88	0.55
1:A:234[A]:LYS:HE3	1:C:476:ARG:HB2	1.89	0.54
1:D:257[A]:LEU:HD13	1:D:278[A]:LEU:HD23	1.91	0.52
1:C:101:ILE:HG22	1:C:106:THR:HB	1.92	0.51
1:B:257[A]:LEU:HD13	1:B:278[A]:LEU:HD23	1.94	0.49
1:A:33:LEU:HD23	4:D:503:FMT:H	1.93	0.49
1:C:246:VAL:HG23	1:C:257[A]:LEU:HD11	1.95	0.48
1:D:467:ASP:OD1	8:D:601:HOH:O	2.20	0.48
1:D:474[B]:HIS:CD2	1:D:474[B]:HIS:H	2.33	0.46
1:B:142:GLY:HA3	1:B:347[B]:HIS:NE2	2.32	0.45
1:B:9:PRO:O	1:B:12:ASN:HB2	2.16	0.45
1:B:41[B]:LEU:HD23	1:B:71:VAL:HG12	1.99	0.45
1:D:347[B]:HIS:CA	1:D:391:LEU:HD21	2.37	0.45
1:B:246:VAL:HG23	1:B:257[A]:LEU:HD11	1.99	0.44
1:C:262:ALA:HB1	1:C:278[B]:LEU:HD23	1.99	0.44
1:B:253:THR:HB	1:B:255[B]:VAL:HG13	2.00	0.44
1:D:454:LEU:O	1:D:466:LYS:HE2	2.17	0.43
1:B:158:ASN:ND2	1:B:160:SER:OG	2.49	0.43
1:B:26:PHE:CE2	4:B:506:FMT:H	2.53	0.43
1:D:324:ASN:HB3	1:D:327:ILE:HD11	2.01	0.43
1:A:347[B]:HIS:CA	1:A:391:LEU:HD21	2.41	0.43
4:A:503:FMT:H	1:D:33:LEU:HD23	2.01	0.43
1:B:474[A]:HIS:H	1:B:474[A]:HIS:CD2	2.36	0.43
1:D:101:ILE:HG22	1:D:106:THR:HB	2.02	0.42
1:D:246:VAL:HG23	1:D:257[A]:LEU:HD11	2.02	0.42
1:D:253:THR:HB	1:D:255[B]:VAL:HG13	2.01	0.42
1:B:101:ILE:HG22	1:B:106:THR:HB	2.02	0.42
1:B:347[A]:HIS:HB3	2:B:501:NAD:O3D	2.20	0.42
1:C:347[B]:HIS:CA	1:C:391:LEU:HD21	2.41	0.42
1:C:142:GLY:HA3	1:C:347[B]:HIS:NE2	2.36	0.41
1:A:474[A]:HIS:CD2	1:A:474[A]:HIS:H	2.37	0.41
1:B:347[B]:HIS:CA	1:B:391:LEU:HD21	2.40	0.41
1:D:47:LYS:NZ	8:D:603:HOH:O	2.31	0.41
1:B:214[B]:MET:SD	1:B:427:GLY:HA2	2.61	0.41
1:C:41[B]:LEU:HA	1:C:41[B]:LEU:HD12	1.84	0.40
1:C:214:MET:HE2	1:C:219:LEU:HB3	2.03	0.40
1:A:142:GLY:HA3	1:A:347[B]:HIS:NE2	2.37	0.40

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	496/485 (102%)	482 (97%)	11 (2%)	3 (1%)	25	7
1	B	485/485 (100%)	469 (97%)	13 (3%)	3 (1%)	25	7
1	C	485/485 (100%)	471 (97%)	11 (2%)	3 (1%)	25	7
1	D	487/485 (100%)	473 (97%)	12 (2%)	2 (0%)	34	12
All	All	1953/1940 (101%)	1895 (97%)	47 (2%)	11 (1%)	34	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347[A]	HIS
1	A	347[B]	HIS
1	B	347[A]	HIS
1	B	347[B]	HIS
1	C	347[A]	HIS
1	C	347[B]	HIS
1	D	347[A]	HIS
1	D	347[B]	HIS
1	C	64	HIS
1	B	64	HIS
1	A	64	HIS

### 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	417/407 (102%)	416 (100%)	1 (0%)	93	82
1	B	402/407 (99%)	398 (99%)	4 (1%)	76	53
1	C	401/407 (98%)	400 (100%)	1 (0%)	93	82
1	D	403/407 (99%)	399 (99%)	4 (1%)	76	53
All	All	1623/1628 (100%)	1613 (99%)	10 (1%)	86	70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	LEU
1	B	96	HIS
1	B	158	ASN
1	B	224	LEU
1	B	349	ASP
1	C	224	LEU
1	D	158	ASN
1	D	192	ILE
1	D	224	LEU
1	D	349	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	158	ASN
1	D	4	GLN
1	D	158	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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$
7	ACT	B	503	-	1,3,3	6.44	1 (100%)	0,3,3	0.00	-
4	FMT	D	503	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAD	D	501	-	42,48,48	0.54	0	50,73,73	0.81	2 (4%)
3	ADN	B	502	-	18,21,21	0.70	0	18,31,31	0.85	1 (5%)
4	FMT	D	505	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAD	C	501	-	42,48,48	0.56	0	50,73,73	0.84	3 (6%)
4	FMT	C	503	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	506	-	0,2,2	0.00	-	0,1,1	0.00	-
7	ACT	B	504	-	1,3,3	6.68	1 (100%)	0,3,3	0.00	-
4	FMT	B	506	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAD	A	501	-	42,48,48	0.55	0	50,73,73	0.81	2 (4%)
7	ACT	D	504	-	1,3,3	6.37	1 (100%)	0,3,3	0.00	-
2	NAD	B	501	-	42,48,48	0.57	0	50,73,73	0.80	2 (4%)
7	ACT	C	504	-	1,3,3	6.10	1 (100%)	0,3,3	0.00	-
3	ADN	C	502	-	18,21,21	0.64	0	18,31,31	0.88	1 (5%)
4	FMT	C	505	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	505	-	0,2,2	0.00	-	0,1,1	0.00	-
3	ADN	D	502	-	18,21,21	0.66	0	18,31,31	0.87	1 (5%)
7	ACT	D	507	-	1,3,3	6.37	1 (100%)	0,3,3	0.00	-
4	FMT	B	508	-	0,2,2	0.00	-	0,1,1	0.00	-
3	ADN	A	502	-	18,21,21	0.66	0	18,31,31	0.90	1 (5%)
4	FMT	A	503	-	0,2,2	0.00	-	0,1,1	0.00	-
6	OXM	A	505	-	2,5,5	0.58	0	2,6,6	0.88	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	D	501	-	-	5/26/62/62	0/5/5/5
2	NAD	C	501	-	-	5/26/62/62	0/5/5/5
3	ADN	D	502	-	-	1/2/22/22	0/3/3/3
6	OXM	A	505	-	-	0/0/4/4	-
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
2	NAD	B	501	-	-	5/26/62/62	0/5/5/5
3	ADN	A	502	-	-	0/2/22/22	0/3/3/3
3	ADN	C	502	-	-	0/2/22/22	0/3/3/3
3	ADN	B	502	-	-	0/2/22/22	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	504	ACT	CH3-C	6.68	1.57	1.48
7	B	503	ACT	CH3-C	6.44	1.56	1.48
7	D	504	ACT	CH3-C	6.37	1.56	1.48
7	D	507	ACT	CH3-C	6.37	1.56	1.48
7	C	504	ACT	CH3-C	6.10	1.56	1.48

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	C2N-N1N-C1D	-2.58	113.39	119.14
2	A	501	NAD	C2N-N1N-C1D	-2.58	113.39	119.14
3	A	502	ADN	C5-C6-N6	2.47	124.11	120.35
3	C	502	ADN	C5-C6-N6	2.40	124.00	120.35
3	D	502	ADN	C5-C6-N6	2.35	123.92	120.35
2	D	501	NAD	C5A-C6A-N6A	2.28	123.81	120.35
2	A	501	NAD	C5A-C6A-N6A	2.26	123.79	120.35
2	B	501	NAD	C2N-N1N-C1D	-2.25	114.13	119.14
2	D	501	NAD	C2N-N1N-C1D	-2.23	114.17	119.14
3	B	502	ADN	C5-C6-N6	2.20	123.69	120.35
2	B	501	NAD	C5A-C6A-N6A	2.16	123.64	120.35
2	C	501	NAD	C5A-C6A-N6A	2.08	123.51	120.35
2	C	501	NAD	PN-O3-PA	-2.00	125.96	132.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	C	501	NAD	C2D-C1D-N1N-C6N
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
2	D	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	O4B-C4B-C5B-O5B
3	D	502	ADN	C3'-C4'-C5'-O5'

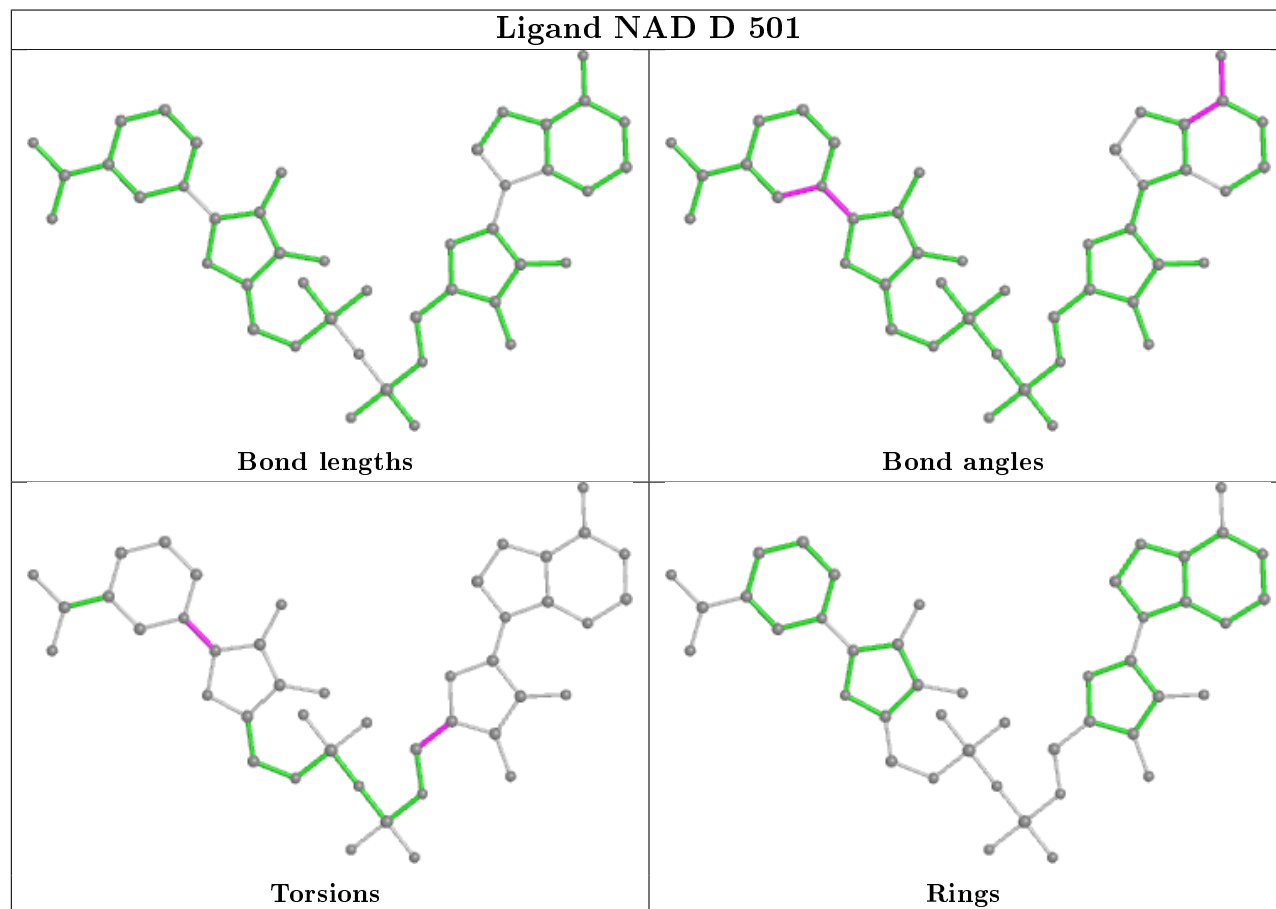
There are no ring outliers.

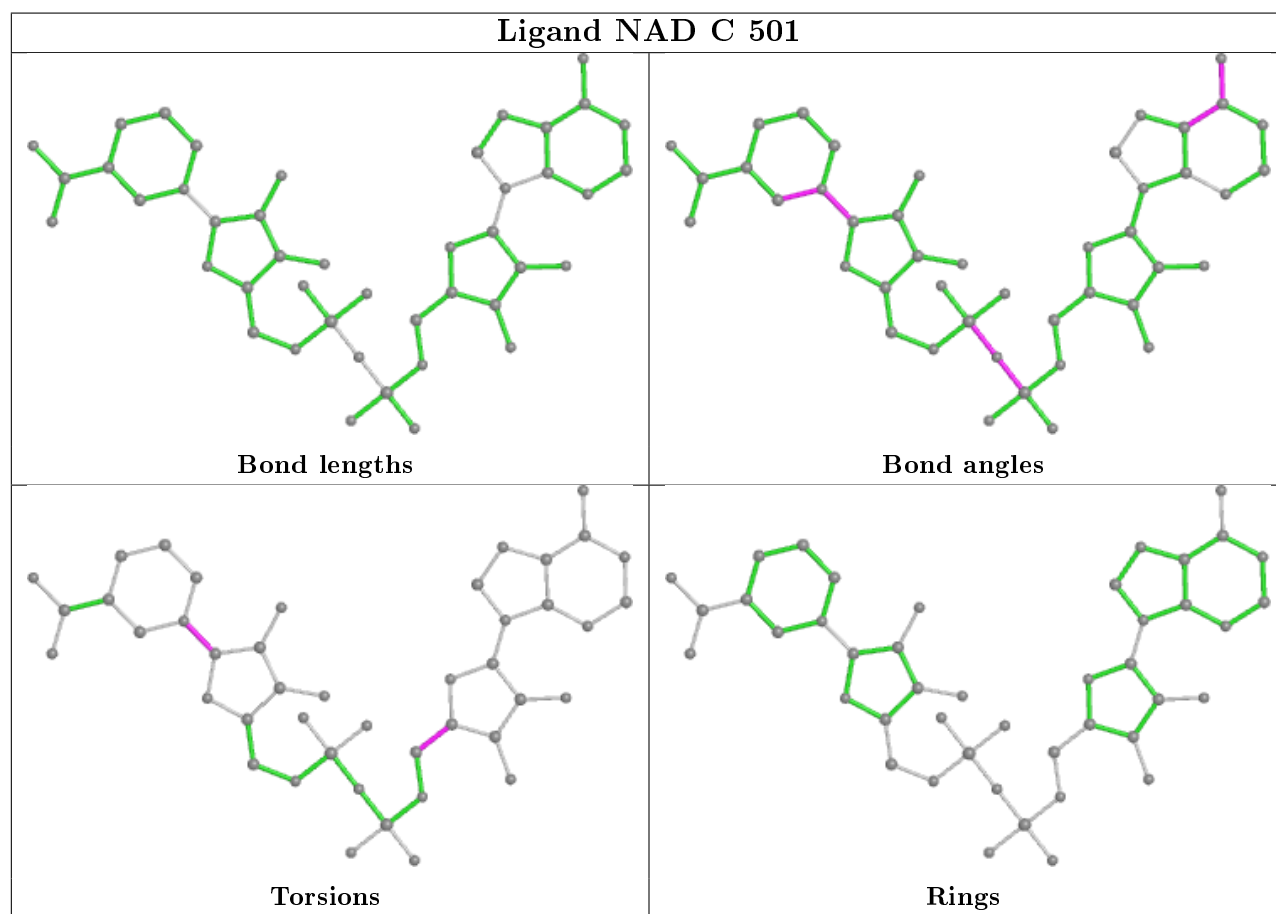
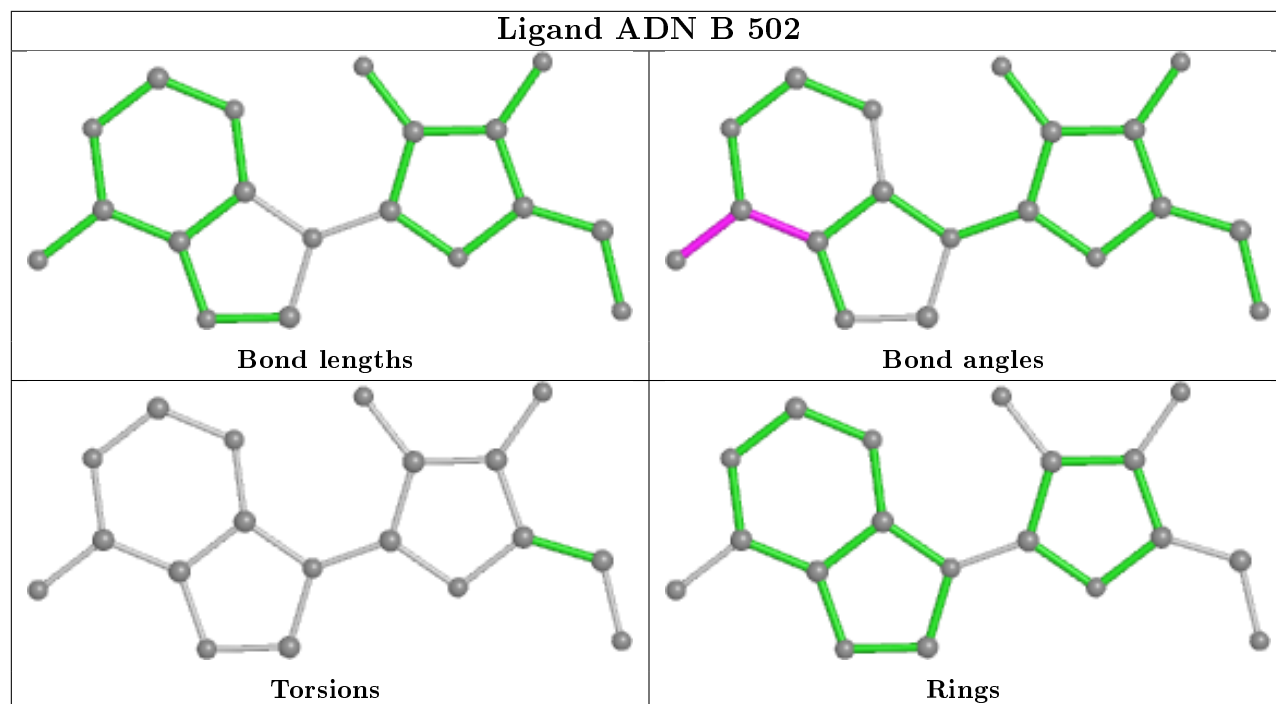
14 monomers are involved in 11 short contacts:

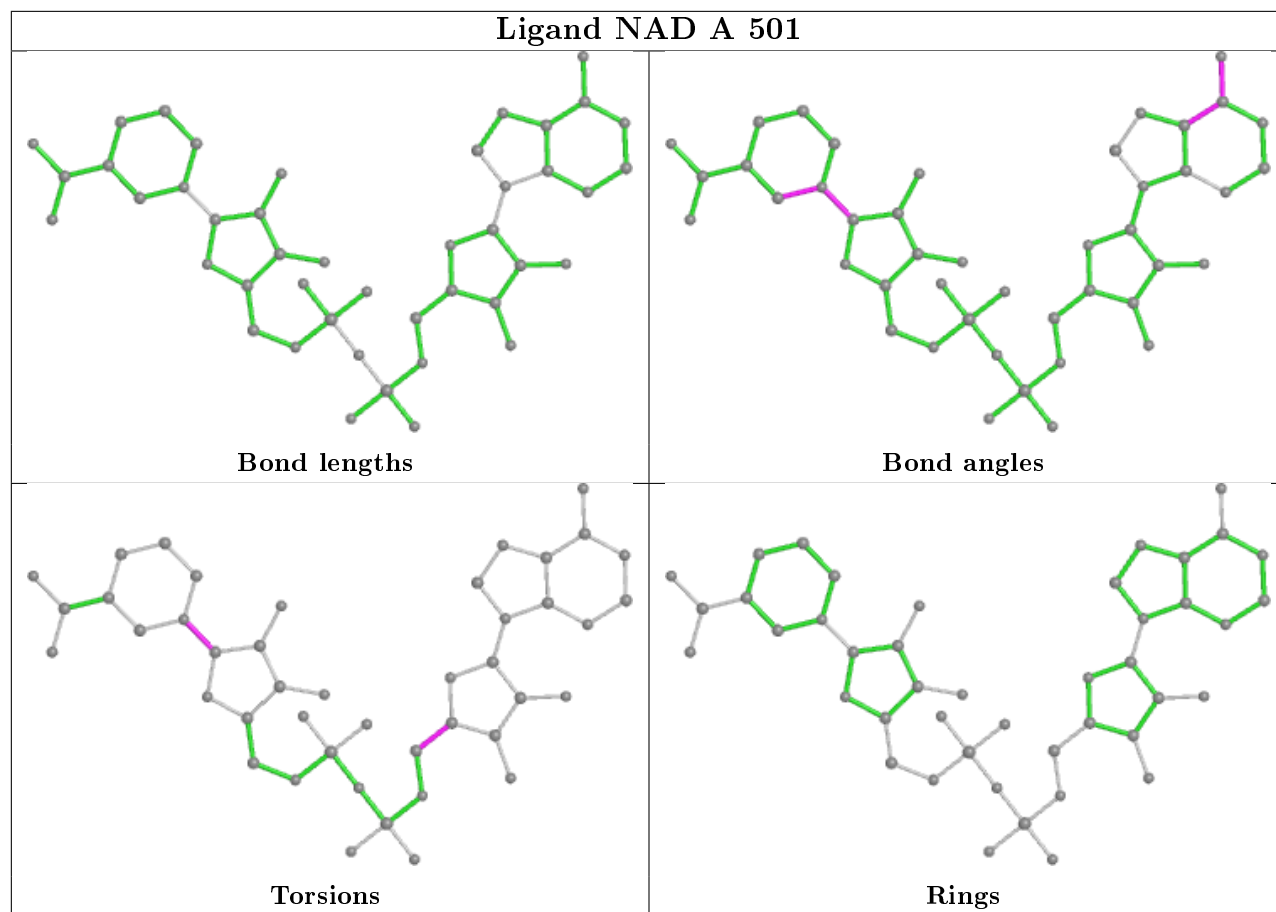
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	FMT	1	0
2	D	501	NAD	1	0
3	B	502	ADN	1	0
2	C	501	NAD	1	0
4	C	503	FMT	1	0
4	D	506	FMT	1	0
4	B	506	FMT	1	0
2	A	501	NAD	1	0
2	B	501	NAD	2	0
3	C	502	ADN	1	0
3	D	502	ADN	1	0
4	B	508	FMT	1	0
3	A	502	ADN	1	0
4	A	503	FMT	1	0

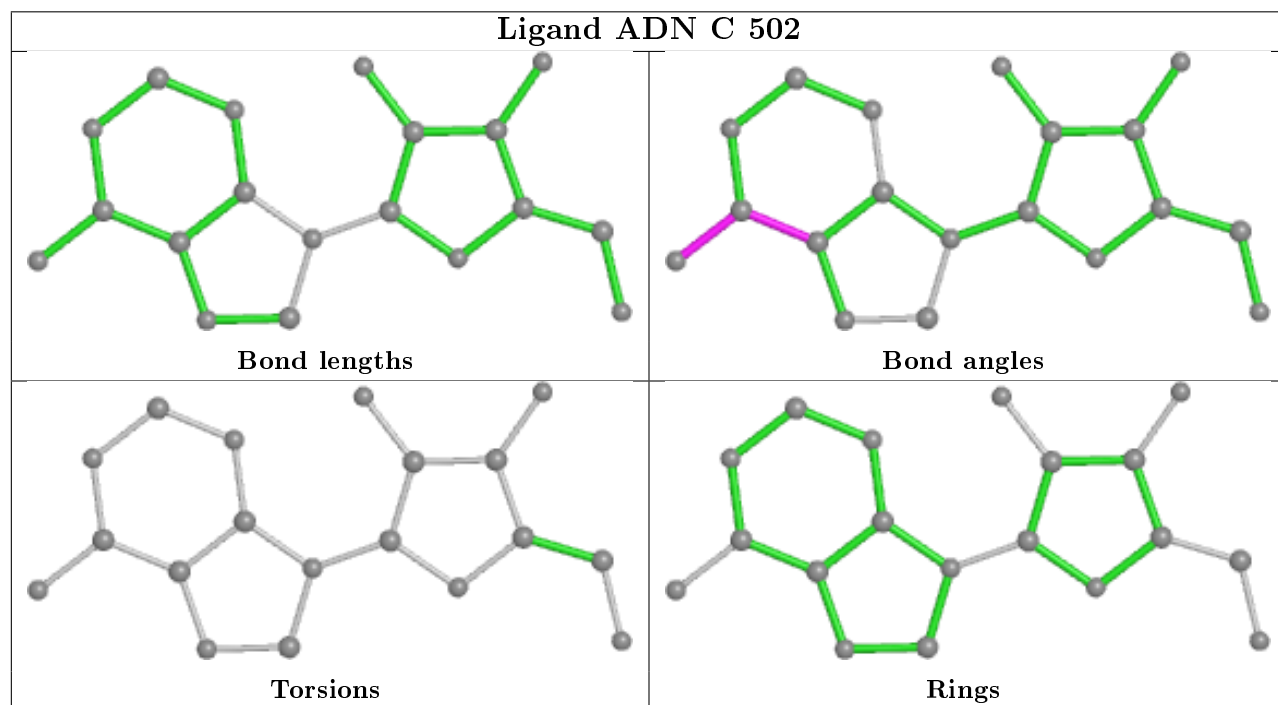
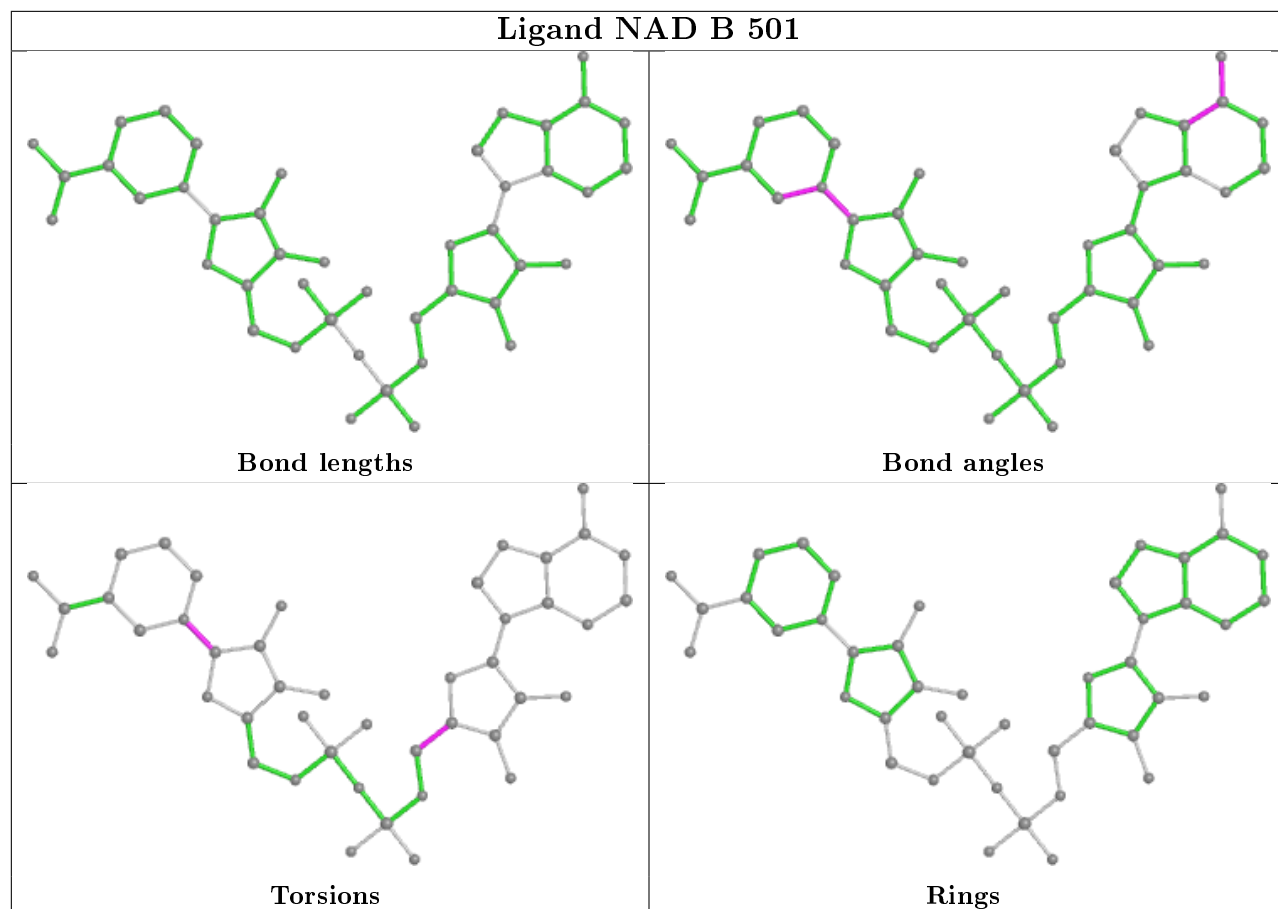
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

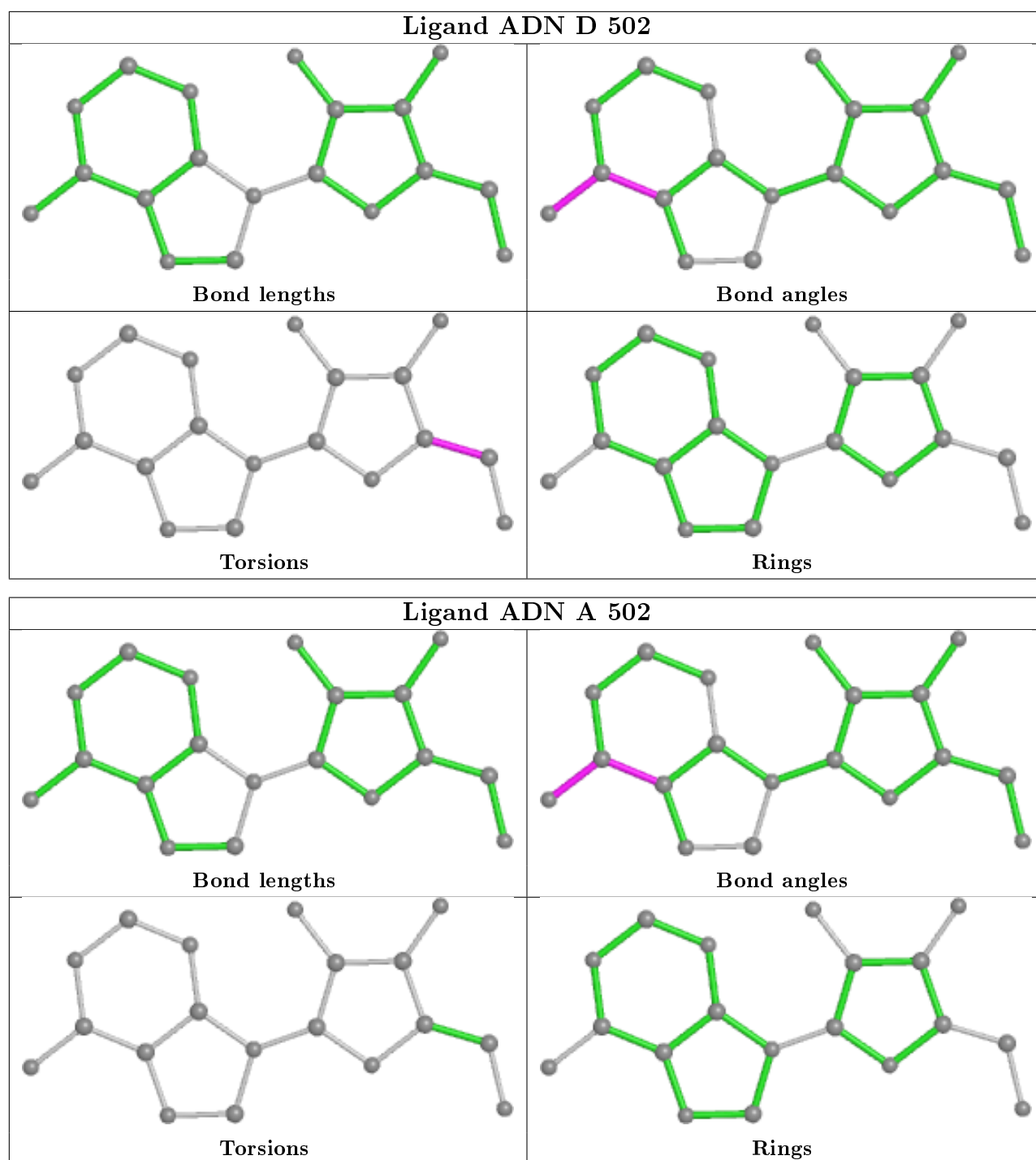
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	475/485 (97%)	0.06	11 (2%) 60 60	11, 16, 28, 58	0
1	B	475/485 (97%)	0.04	14 (2%) 51 50	11, 18, 38, 64	0
1	C	475/485 (97%)	0.52	41 (8%) 10 9	10, 18, 40, 62	0
1	D	475/485 (97%)	0.14	16 (3%) 45 44	11, 19, 39, 55	0
All	All	1900/1940 (97%)	0.19	82 (4%) 35 35	10, 18, 38, 64	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	ALA	7.4
1	C	348[A]	PHE	5.3
1	A	3	THR	5.3
1	D	10	ALA	5.2
1	A	348[A]	PHE	5.0
1	B	11	GLY	4.8
1	D	11	GLY	4.7
1	B	167	GLY	4.6
1	B	348[A]	PHE	4.2
1	D	3	THR	3.8
1	D	348[A]	PHE	3.8
1	D	215	LYS	3.7
1	C	193	VAL	3.4
1	C	426	LEU	3.2
1	C	211	TYR	3.2
1	C	420	TRP	3.2
1	D	423	LYS	3.1
1	C	3	THR	3.1
1	C	161	ILE	3.1
1	B	3	THR	3.1
1	D	257[A]	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	215	LYS	2.8
1	A	10	ALA	2.8
1	C	278[A]	LEU	2.7
1	C	218	LYS	2.7
1	D	278[A]	LEU	2.7
1	D	246	VAL	2.7
1	A	255[A]	VAL	2.6
1	C	189	TRP	2.6
1	C	11	GLY	2.6
1	A	278[A]	LEU	2.6
1	B	301	ALA	2.6
1	C	347[A]	HIS	2.6
1	C	285	VAL	2.5
1	C	153	PHE	2.5
1	B	13	ALA	2.4
1	D	425	GLU	2.4
1	C	197	LYS	2.4
1	B	9	PRO	2.4
1	C	160	SER	2.4
1	C	194	PRO	2.4
1	C	217	GLY	2.4
1	C	192	ILE	2.4
1	D	347[A]	HIS	2.4
1	B	245	LEU	2.4
1	A	257[A]	LEU	2.4
1	D	214	MET	2.4
1	B	347[A]	HIS	2.3
1	A	283	ALA	2.3
1	C	303	TYR	2.3
1	C	138	ILE	2.3
1	A	245	LEU	2.3
1	B	278[A]	LEU	2.3
1	C	220	LEU	2.3
1	D	426	LEU	2.3
1	C	424	TYR	2.3
1	C	287	VAL	2.2
1	C	245	LEU	2.2
1	C	13	ALA	2.2
1	C	301	ALA	2.2
1	A	211	TYR	2.2
1	A	246	VAL	2.2
1	D	167	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	270	VAL	2.2
1	C	298	ALA	2.1
1	C	162	LEU	2.1
1	C	158	ASN	2.1
1	C	154	TYR	2.1
1	B	285	VAL	2.1
1	A	347[A]	HIS	2.1
1	D	245	LEU	2.1
1	B	215	LYS	2.1
1	D	158	ASN	2.1
1	C	275	ALA	2.1
1	C	190	HIS	2.1
1	C	167	GLY	2.1
1	C	219	LEU	2.1
1	B	161	ILE	2.0
1	C	267	TYR	2.0
1	C	429	TYR	2.0
1	C	214	MET	2.0
1	C	425	GLU	2.0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	FMT	B	505	3/3	0.45	0.17	62,62,62,62	0
4	FMT	D	506	3/3	0.67	0.26	111,111,111,111	0
4	FMT	B	506	3/3	0.70	0.32	93,93,93,93	0
7	ACT	D	507	4/4	0.72	0.16	73,73,73,73	0

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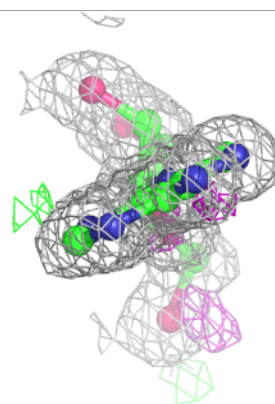
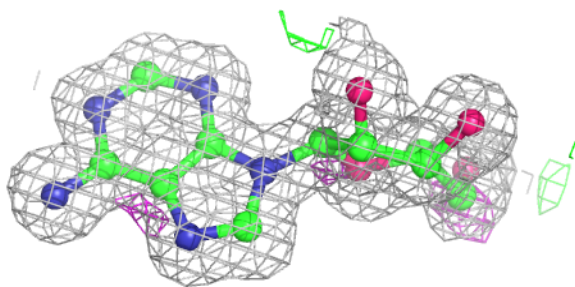
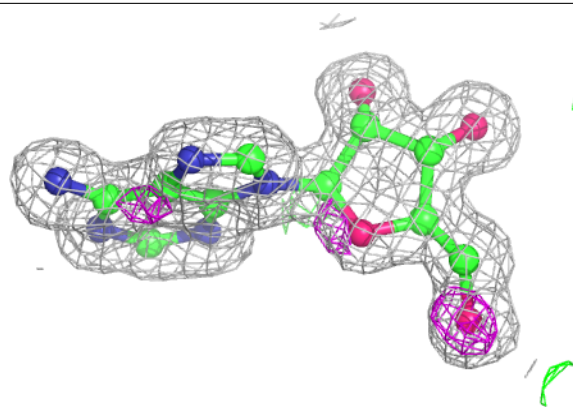
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FMT	C	505	3/3	0.73	0.35	104,104,104,104	0
7	ACT	B	504	4/4	0.74	0.20	46,47,47,48	0
4	FMT	D	505	3/3	0.81	0.21	69,69,70,70	0
7	ACT	B	503	4/4	0.82	0.22	63,63,63,63	0
6	OXM	A	505	6/6	0.82	0.21	51,52,54,54	0
7	ACT	C	504	4/4	0.83	0.15	68,68,68,68	0
7	ACT	D	504	4/4	0.84	0.15	56,57,57,57	0
4	FMT	C	503	3/3	0.93	0.12	38,38,38,38	0
4	FMT	A	503	3/3	0.95	0.12	42,42,42,43	0
4	FMT	B	508	3/3	0.95	0.15	41,41,41,41	0
3	ADN	A	502	19/19	0.96	0.08	10,12,18,19	0
4	FMT	D	503	3/3	0.96	0.17	38,38,38,39	0
3	ADN	C	502	19/19	0.96	0.08	12,13,19,20	0
3	ADN	D	502	19/19	0.97	0.07	13,14,21,21	0
2	NAD	C	501	44/44	0.97	0.09	10,12,13,14	0
3	ADN	B	502	19/19	0.97	0.07	11,13,19,20	0
5	K	C	506	1/1	0.98	0.08	13,13,13,13	1
2	NAD	B	501	44/44	0.98	0.07	12,13,15,17	0
2	NAD	A	501	44/44	0.98	0.08	11,12,14,15	0
2	NAD	D	501	44/44	0.98	0.07	12,13,15,16	0
5	K	A	504	1/1	0.99	0.09	13,13,13,13	1
5	K	B	507	1/1	0.99	0.07	13,13,13,13	1
5	K	D	508	1/1	1.00	0.09	15,15,15,15	1

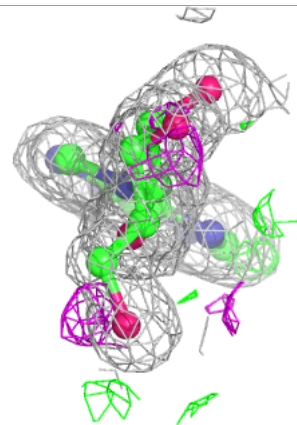
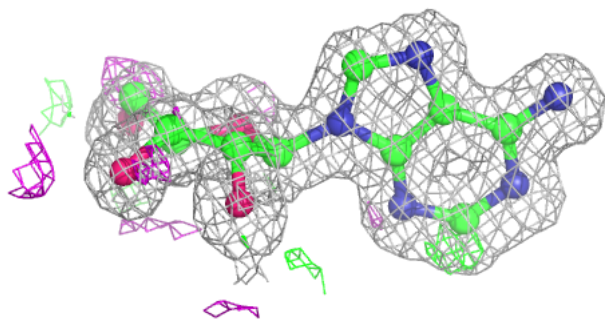
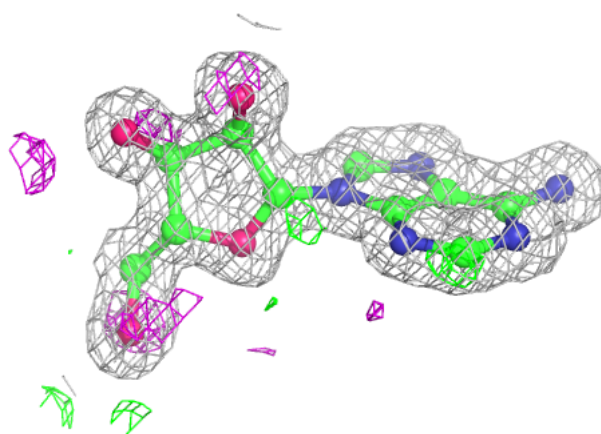
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

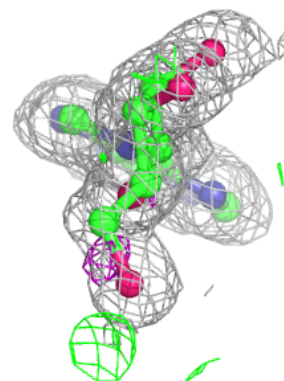
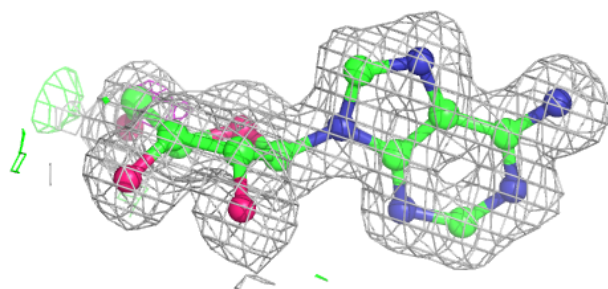
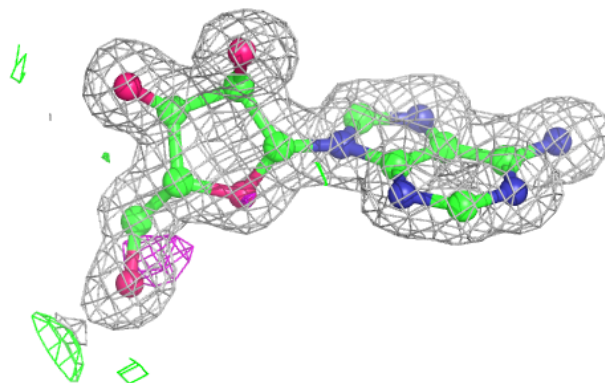
**Electron density around ADN C 502:**

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

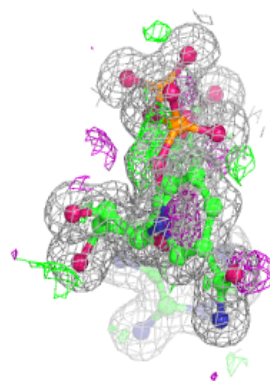
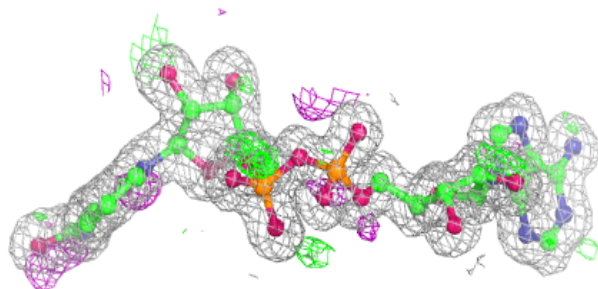
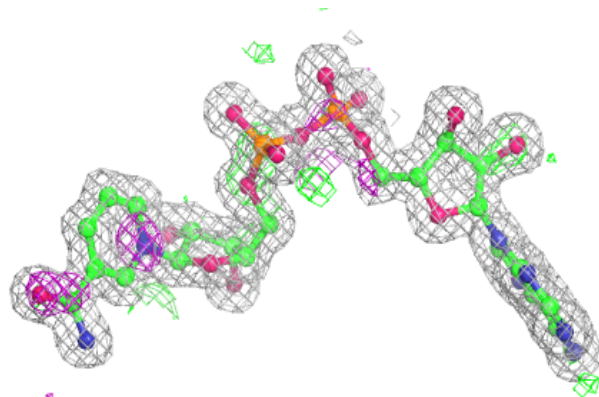


**Electron density around ADN D 502:**

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

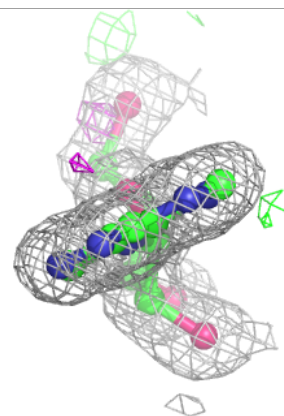
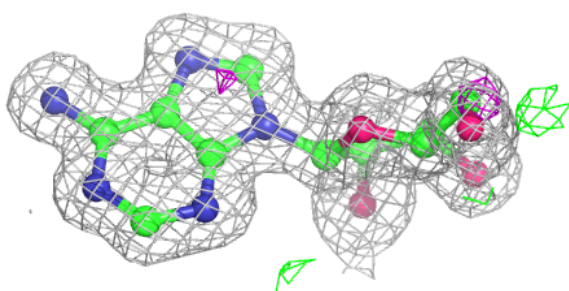
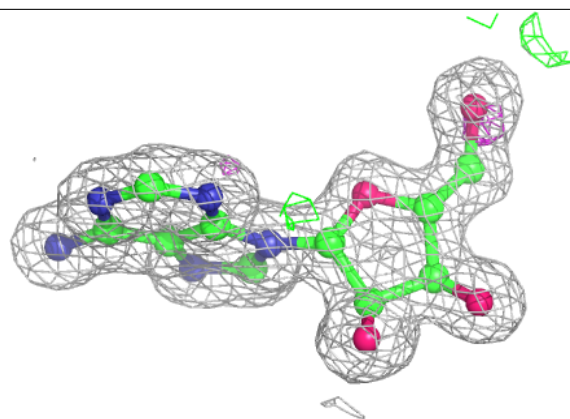
**Electron density around NAD C 501:**

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

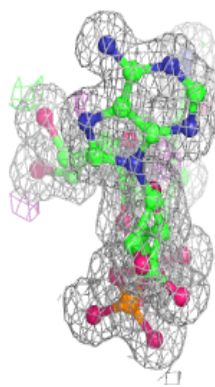
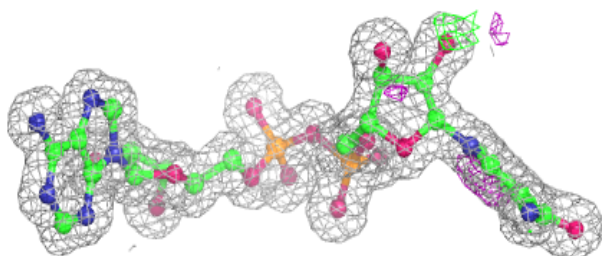
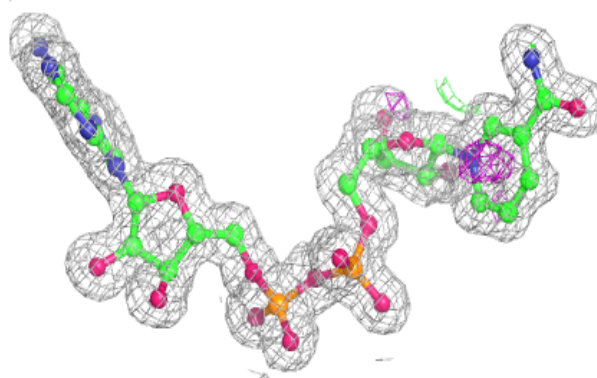


**Electron density around ADN B 502:**

$2mF_o-DF_c$  (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:**

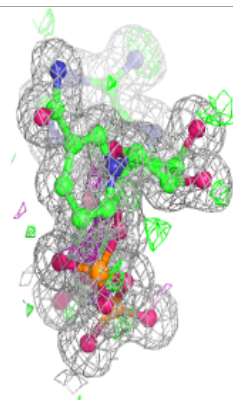
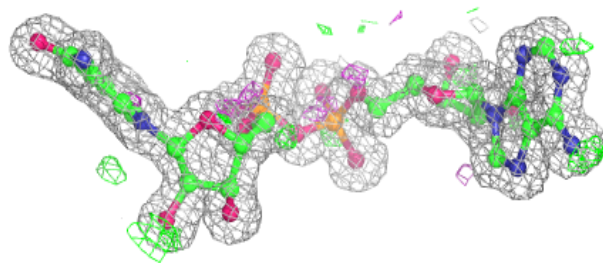
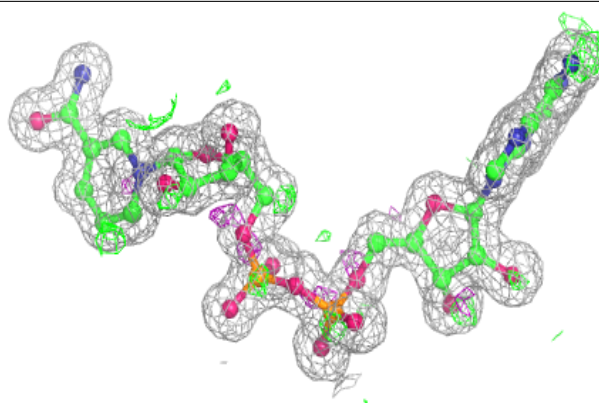
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



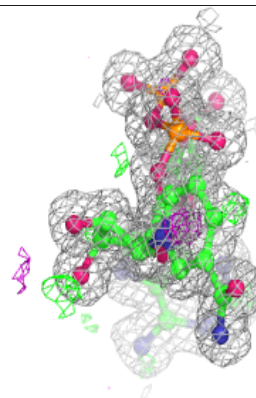
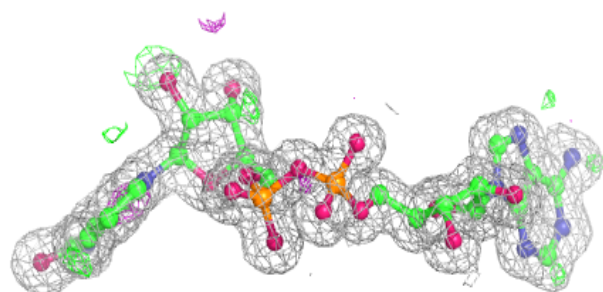
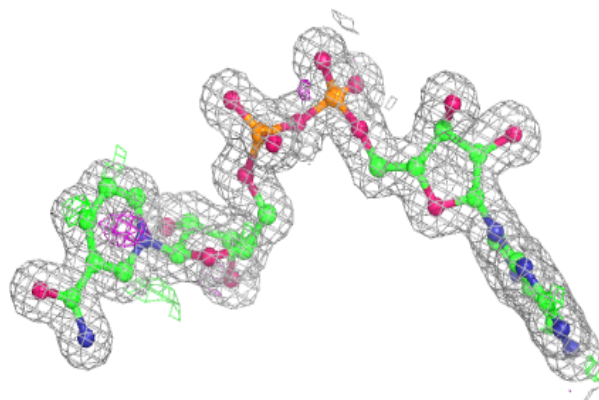


**Electron density around NAD A 501:**

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

**Electron density around NAD D 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

There are no such residues in this entry.