



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 9, 2026 – 10:43 PM UTC

PDB ID : 9QJ1 / pdb\_00009qj1  
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *P. aeruginosa*, Q65N mutant soaked with adenosine and probed with rubidium to confirm disruption of a potassium binding site.  
Authors : Malecki, P.H.; Wozniak, K.; Stepniewska, M.; Brzezinski, K.  
Deposited on : 2025-03-18  
Resolution : 2.34 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

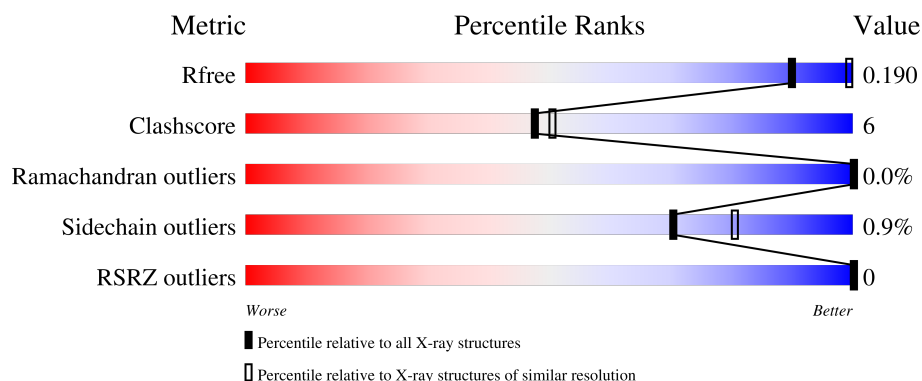
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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  $\geq 3$ , 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	472	
1	B	472	
1	C	472	
1	D	472	

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Mol	Chain	Length	Quality of chain
1	H	472	 88% 9% ..
1	I	472	 86% 11% .
1	J	472	 81% 17% .
1	K	472	 87% 10% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	B	503	-	-	X	-
4	PO4	K	503	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30788 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	461	Total	C	N	O	S	0	3	0
			3571	2250	618	681	22			
1	B	461	Total	C	N	O	S	0	2	0
			3565	2247	617	679	22			
1	C	461	Total	C	N	O	S	0	5	0
			3582	2257	620	683	22			
1	D	461	Total	C	N	O	S	0	2	0
			3565	2247	616	680	22			
1	H	461	Total	C	N	O	S	0	4	0
			3567	2249	617	680	21			
1	I	461	Total	C	N	O	S	0	3	0
			3565	2249	615	680	21			
1	J	461	Total	C	N	O	S	0	5	0
			3585	2262	622	679	22			
1	K	461	Total	C	N	O	S	0	2	0
			3559	2243	616	679	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9I685
A	-1	ASN	-	expression tag	UNP Q9I685
A	0	ALA	-	expression tag	UNP Q9I685
A	65	ASN	GLN	engineered mutation	UNP Q9I685
B	-2	SER	-	expression tag	UNP Q9I685
B	-1	ASN	-	expression tag	UNP Q9I685
B	0	ALA	-	expression tag	UNP Q9I685
B	65	ASN	GLN	engineered mutation	UNP Q9I685
C	-2	SER	-	expression tag	UNP Q9I685
C	-1	ASN	-	expression tag	UNP Q9I685
C	0	ALA	-	expression tag	UNP Q9I685
C	65	ASN	GLN	engineered mutation	UNP Q9I685
D	-2	SER	-	expression tag	UNP Q9I685

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASN	-	expression tag	UNP Q9I685
D	0	ALA	-	expression tag	UNP Q9I685
D	65	ASN	GLN	engineered mutation	UNP Q9I685
H	-2	SER	-	expression tag	UNP Q9I685
H	-1	ASN	-	expression tag	UNP Q9I685
H	0	ALA	-	expression tag	UNP Q9I685
H	65	ASN	GLN	engineered mutation	UNP Q9I685
I	-2	SER	-	expression tag	UNP Q9I685
I	-1	ASN	-	expression tag	UNP Q9I685
I	0	ALA	-	expression tag	UNP Q9I685
I	65	ASN	GLN	engineered mutation	UNP Q9I685
J	-2	SER	-	expression tag	UNP Q9I685
J	-1	ASN	-	expression tag	UNP Q9I685
J	0	ALA	-	expression tag	UNP Q9I685
J	65	ASN	GLN	engineered mutation	UNP Q9I685
K	-2	SER	-	expression tag	UNP Q9I685
K	-1	ASN	-	expression tag	UNP Q9I685
K	0	ALA	-	expression tag	UNP Q9I685
K	65	ASN	GLN	engineered mutation	UNP Q9I685

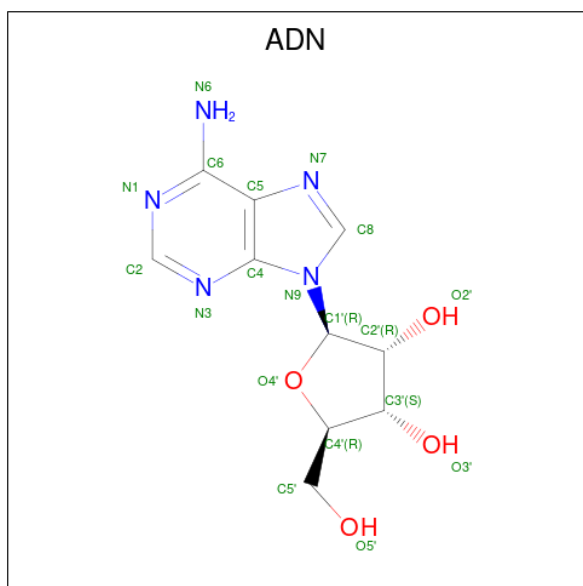
- # NAD
- 
- The image displays the chemical structure of Nicotinamide Adenine Dinucleotide (NAD). The molecule is composed of two nucleotides linked by a pyrophosphate bridge. The top nucleotide consists of a nicotinamide ring (labeled with N1A, N7A, C5A, C4A, N3A, C3A, N3A) attached to a ribose sugar (labeled with C2', C3', C4', C5', C1'). The bottom nucleotide consists of an adenine ring (labeled with N1A, N7A, C5A, C4A, N3A, C3A, N3A) attached to a ribose sugar (labeled with C2', C3', C4', C5', C1'). The two ribose sugars are linked by a pyrophosphate bridge (labeled with P1, P2, O1A, O2A, O3A, O4A, O5A, O6A, O7A, O8A, O9A, O10A, O11A, O12A, O13A, O14A, O15A, O16A, O17A, O18A, O19A, O20A, O21A, O22A, O23A, O24A, O25A, O26A, O27A, O28A, O29A, O30A, O31A, O32A, O33A, O34A, O35A, O36A, O37A, O38A, O39A, O40A, O41A, O42A, O43A, O44A, O45A, O46A, O47A, O48A, O49A, O50A, O51A, O52A, O53A, O54A, O55A, O56A, O57A, O58A, O59A, O60A, O61A, O62A, O63A, O64A, O65A, O66A, O67A, O68A, O69A, O70A, O71A, O72A, O73A, O74A, O75A, O76A, O77A, O78A, O79A, O80A, O81A, O82A, O83A, O84A, O85A, O86A, O87A, O88A, O89A, O90A, O91A, O92A, O93A, O94A, O95A, O96A, O97A, O98A, O99A, O100A, O101A, O102A, O103A, O104A, O105A, O106A, O107A, O108A, O109A, O110A, O111A, O112A, O113A, O114A, O115A, O116A, O117A, O118A, O119A, O120A, O121A, O122A, O123A, O124A, O125A, O126A, O127A, O128A, O129A, O130A, O131A, O132A, O133A, O134A, O135A, O136A, O137A, O138A, O139A, O140A, O141A, O142A, O143A, O144A, O145A, O146A, O147A, O148A, O149A, O150A, O151A, O152A, O153A, O154A, O155A, O156A, O157A, O158A, O159A, O160A, O161A, O162A, O163A, O164A, O165A, O166A, O167A, O168A, O169A, O170A, O171A, O172A, O173A, O174A, O175A, O176A, O177A, O178A, O179A, O180A, O181A, O182A, O183A, O184A, O185A, O186A, O187A, O188A, O189A, O190A, O191A, O192A, O193A, O194A, O195A, O196A, O197A, O198A, O199A, O200A, O201A, O202A, O203A, O204A, O205A, O206A, O207A, O208A, O209A, O210A, O211A, O212A, O213A, O214A, O215A, O216A, O217A, O218A, O219A, O220A, O221A, O222A, O223A, O224A, O225A, O226A, O227A, O228A, O229A, O230A, O231A, O232A, O233A, O234A, O235A, O236A, O237A, O238A, O239A, O240A, O241A, O242A, O243A, O244A, O245A, O246A, O247A, O248A, O249A, O250A, O251A, O252A, O253A, O254A, O255A, O256A, O257A, O258A, O259A, O260A, O261A, O262A, O263A, O264A, O265A, O266A, O267A, O268A, O269A, O270A, O271A, O272A, O273A, O274A, O275A, O276A, O277A, O278A, O279A, O280A, O281A, O282A, O283A, O284A, O285A, O286A, O287A, O288A, O289A, O290A, O291A, O292A, O293A, O294A, O295A, O296A, O297A, O298A, O299A, O300A, O301A, O302A, O303A, O304A, O305A, O306A, O307A, O308A, O309A, O310A, O311A, O312A, O313A, O314A, O315A, O316A, O317A, O318A, O319A, O320A, O321A, O322A, O323A, O324A, O325A, O326A, O327A, O328A, O329A, O330A, O331A, O332A, O333A, O334A, O335A, O336A, O337A, O338A, O339A, O340A, O341A, O342A, O343A, O344A, O345A, O346A, O347A, O348A, O349A, O350A, O351A, O352A, O353A, O354A, O355A, O356A, O357A, O358A, O359A, O360A, O361A, O362A, O363A, O364A, O365A, O366A, O367A, O368A, O369A, O370A, O371A, O372A, O373A, O374A, O375A, O376A, O377A, O378A, O379A, O380A, O381A, O382A, O383A, O384A, O385A, O386A, O387A, O388A, O389A, O390A, O391A, O392A, O393A, O394A, O395A, O396A, O397A, O398A, O399A, O400A, O401A, O402A, O403A, O404A, O405A, O406A, O407A, O408A, O409A, O410A, O411A, O412A, O413A, O414A, O415A, O416A, O417A, O418A, O419A, O420A, O421A, O422A, O423A, O424A, O425A, O426A, O427A, O428A, O429A, O430A, O431A, O432A, O433A, O434A, O435A, O436A, O437A, O438A, O439A, O440A, O441A, O442A, O443A, O444A, O445A, O446A, O447A, O448A, O449A, O450A, O451A, O452A, O453A, O454A, O455A, O456A, O457A, O458A, O459A, O460A, O461A, O462A, O463A, O464A, O465A, O466A, O467A, O468A, O469A, O470A, O471A, O472A, O473A, O474A, O475A, O476A, O477A, O478A, O479A, O480A, O481A, O482A, O483A, O484A, O485A, O486A, O487A, O488A, O489A, O490A, O491A, O492A, O493A, O494A, O495A, O496A, O497A, O498A, O499A, O500A, O501A, O502A, O503A, O504A, O505A, O506A, O507A, O508A, O509A, O510A, O511A, O512A, O513A, O514A, O515A, O516A, O517A, O518A, O519A, O520A, O521A, O522A, O523A, O524A, O525A, O526A, O527A, O528A, O529A, O530A, O531A, O532A, O533A, O534A, O535A, O536A, O537A, O538A, O539A, O540A, O541A, O542A, O543A, O544A, O545A, O546A, O547A, O548A, O549A, O550A, O551A, O552A, O553A, O554A, O555A, O556A, O557A, O558A, O559A, O560A, O561A, O562A, O563A, O564A, O565A, O566A, O567A, O568A, O569A, O570A, O571A, O572A, O573A, O574A, O575A, O576A, O577A, O578A, O579A, O580A, O581A, O582A, O583A, O584A, O585A, O586A, O587A, O588A, O589A, O590A, O591A, O592A, O593A, O594A, O595A, O596A, O597A, O598A, O599A, O600A, O601A, O602A, O603A, O604A, O605A, O606A, O607A, O608A, O609A, O610A, O611A, O612A, O613A, O614A, O615A, O616A, O617A, O618A, O619A, O620A, O621A, O622A, O623A, O624A, O625A, O626A, O627A, O628A, O629A, O630A, O631A, O632A, O633A, O634A, O635A, O636A, O637A, O638A, O639A, O640A, O641A, O642A, O643A, O644A, O645A, O646A, O647A, O648A, O649A, O650A, O651A, O652A, O653A, O654A, O655A, O656A, O657A, O658A, O659A, O660A, O661A, O662A, O663A

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ADENOSINE (CCD ID: ADN) (formula:  $C_{10}H_{13}N_5O_4$ ).



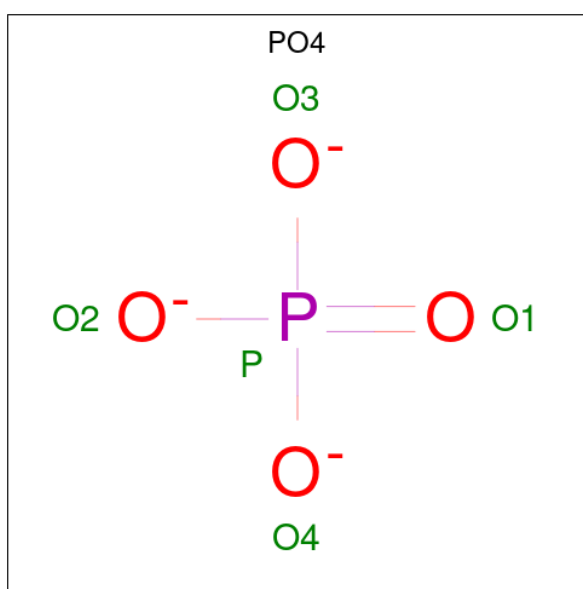
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	1
			19	10	5	4		
3	C	1	Total	C	N	O	0	0
			19	10	5	4		
3	D	1	Total	C	N	O	0	0
			19	10	5	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	1
			19	10	5	4		
3	I	1	Total	C	N	O	0	0
			19	10	5	4		
3	J	1	Total	C	N	O	0	0
			19	10	5	4		
3	K	1	Total	C	N	O	0	1
			19	10	5	4		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		
4	K	1	Total	O	P	0	0
			5	4	1		
4	K	1	Total	O	P	0	0
			5	4	1		
4	K	1	Total	O	P	0	0
			5	4	1		

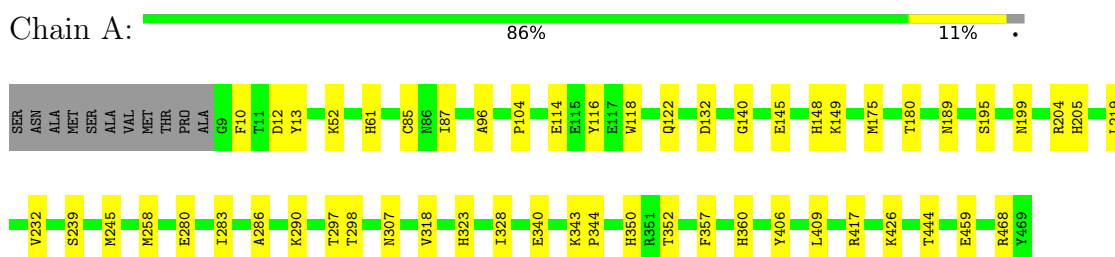
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	217	Total	O	0	3
			217	217		
5	B	219	Total	O	0	1
			219	219		
5	C	201	Total	O	0	0
			201	201		
5	D	231	Total	O	0	1
			231	231		
5	H	178	Total	O	0	3
			178	178		
5	I	202	Total	O	0	1
			202	202		
5	J	214	Total	O	0	1
			214	214		
5	K	193	Total	O	0	2
			193	193		

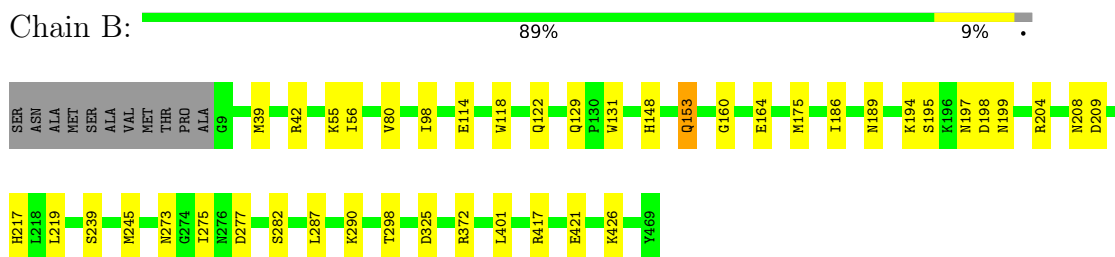
### 3 Residue-property plots

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.

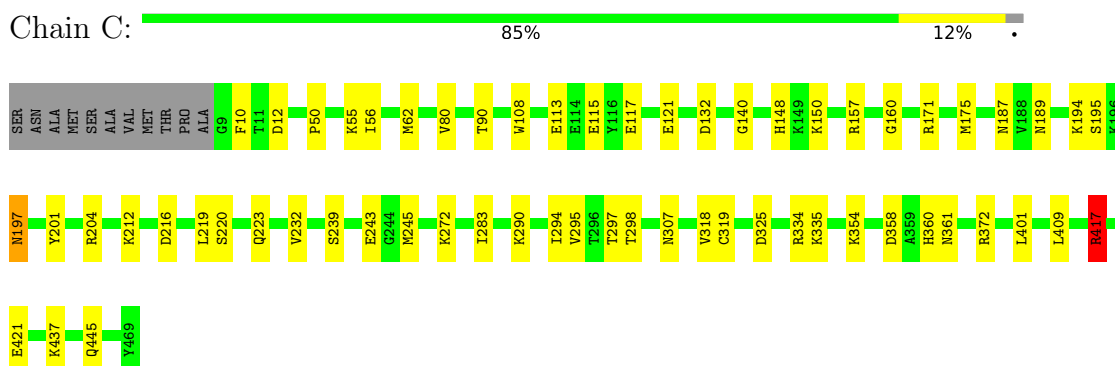
- Molecule 1: Adenosylhomocysteinase



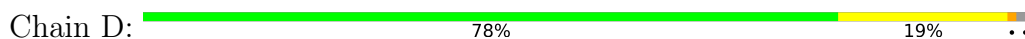
- Molecule 1: Adenosylhomocysteinase

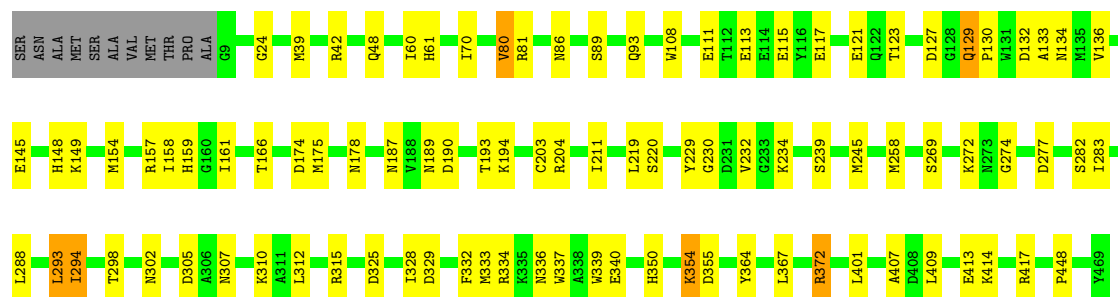


- Molecule 1: Adenosylhomocysteinase



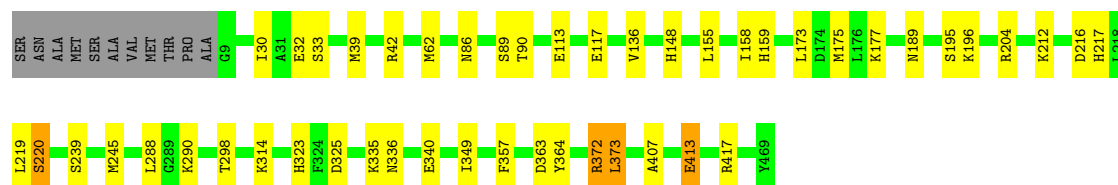
- Molecule 1: Adenosylhomocysteinase





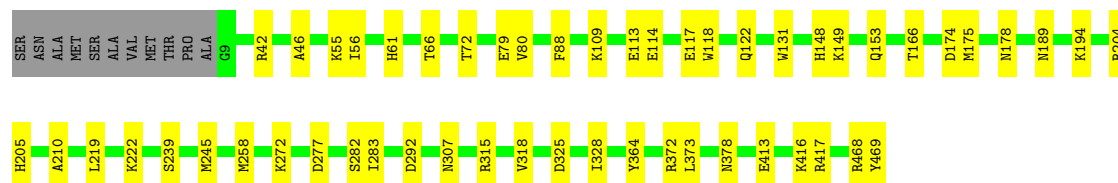
• Molecule 1: Adenosylhomocysteinase

Chain H: 88% 9% ..



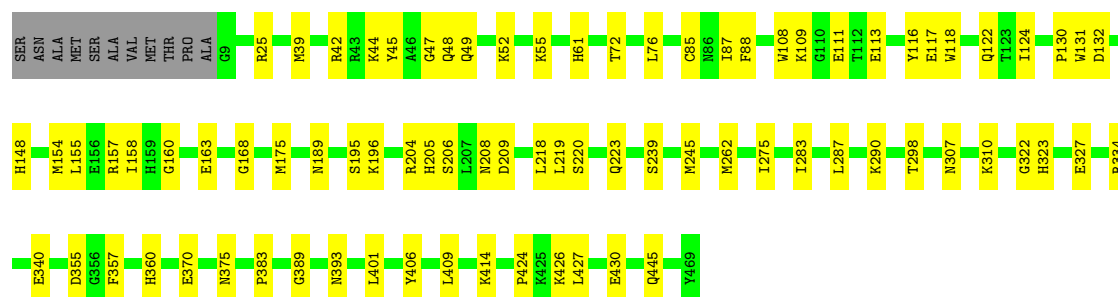
• Molecule 1: Adenosylhomocysteinase

Chain I: 86% 11% .



• Molecule 1: Adenosylhomocysteinase

Chain J: 81% 17% .



• Molecule 1: Adenosylhomocysteinase

Chain K: 87% 10% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.63Å 211.30Å 111.46Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.34 48.59 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.59-2.34) 98.8 (48.59-2.34)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419+SVN	Depositor
R, $R_{free}$	0.183 , 0.209 0.174 , 0.190	Depositor DCC
$R_{free}$ test set	1025 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 26.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.259 for l,-k,h	Xtriage
Reported twinning fraction	0.710 for -l,-k,-h	Depositor
Outliers	0 of 204943 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	30788	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, PO4, ADN

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	0.46	0/3637	0.71	0/4917
1	B	0.46	0/3631	0.70	0/4909
1	C	0.46	0/3654	0.69	1/4940 (0.0%)
1	D	0.57	0/3631	0.81	1/4909 (0.0%)
1	H	0.44	0/3636	0.69	0/4917
1	I	0.45	0/3637	0.70	0/4918
1	J	0.44	0/3660	0.69	0/4945
1	K	0.47	0/3628	0.72	0/4906
All	All	0.47	0/29114	0.71	2/39361 (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	K	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	417	ARG	CB-CG-CD	5.24	123.36	111.30
1	D	80	VAL	N-CA-C	5.21	116.18	107.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	372	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3571	0	3576	37	0
1	B	3565	0	3572	35	0
1	C	3582	0	3590	38	0
1	D	3565	0	3570	66	0
1	H	3567	0	3575	31	0
1	I	3565	0	3578	33	0
1	J	3585	0	3611	58	0
1	K	3559	0	3567	29	0
2	A	44	0	26	3	0
2	B	44	0	26	3	0
2	C	44	0	26	2	0
2	D	44	0	26	3	0
2	H	44	0	26	2	0
2	I	44	0	26	1	0
2	J	44	0	26	4	0
2	K	44	0	26	3	0
3	A	19	0	13	1	0
3	B	19	0	3	0	0
3	C	19	0	13	1	0
3	D	19	0	13	1	0
3	H	19	0	3	1	0
3	I	19	0	13	1	0
3	J	19	0	13	2	0
3	K	19	0	3	0	0
4	A	10	0	0	0	0
4	B	10	0	0	2	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
4	H	20	0	0	0	0
4	J	5	0	0	1	0
4	K	15	0	0	2	0
5	A	217	0	0	4	0
5	B	219	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	201	0	0	3	0
5	D	231	0	0	5	0
5	H	178	0	0	0	0
5	I	202	0	0	1	0
5	J	214	0	0	7	0
5	K	193	0	0	2	0
All	All	30788	0	28921	325	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 325 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:132:ASP:HA	1:D:157:ARG:NH1	1.65	1.09
1:D:132:ASP:HA	1:D:157:ARG:HH12	1.42	0.80
1:I:189:ASN:HA	1:I:194:LYS:HD2	1.64	0.78
1:D:211:ILE:HD13	1:D:293:LEU:HD11	1.65	0.77
1:A:148:HIS:CG	1:A:175:MET:HE1	2.20	0.76

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	462/472 (98%)	452 (98%)	10 (2%)	0	100	100
1	B	461/472 (98%)	450 (98%)	11 (2%)	0	100	100
1	C	464/472 (98%)	454 (98%)	10 (2%)	0	100	100
1	D	461/472 (98%)	446 (97%)	15 (3%)	0	100	100
1	H	462/472 (98%)	450 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	462/472 (98%)	451 (98%)	11 (2%)	0	100	100
1	J	464/472 (98%)	449 (97%)	15 (3%)	0	100	100
1	K	461/472 (98%)	447 (97%)	13 (3%)	1 (0%)	43	50
All	All	3697/3776 (98%)	3599 (97%)	97 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	197	ASN

### 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	380/385 (99%)	379 (100%)	1 (0%)	86	91
1	B	379/385 (98%)	376 (99%)	3 (1%)	73	82
1	C	382/385 (99%)	379 (99%)	3 (1%)	73	82
1	D	379/385 (98%)	369 (97%)	10 (3%)	40	53
1	H	380/385 (99%)	375 (99%)	5 (1%)	61	73
1	I	380/385 (99%)	377 (99%)	3 (1%)	73	82
1	J	382/385 (99%)	382 (100%)	0	100	100
1	K	379/385 (98%)	376 (99%)	3 (1%)	73	82
All	All	3041/3080 (99%)	3013 (99%)	28 (1%)	70	80

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	354	LYS
1	K	372	ARG
1	H	220[A]	SER
1	I	258	MET
1	D	372	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	153	GLN
1	J	345	GLN
1	K	336	ASN
1	K	122	GLN
1	C	197	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

30 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	A	502	-	21,21,21	0.49	0	31,31,31	0.74	0
2	NAD	B	501	-	46,48,48	0.35	0	64,73,73	0.35	0
2	NAD	J	501	-	46,48,48	0.37	0	64,73,73	0.37	0
4	PO4	B	503	-	4,4,4	1.44	1 (25%)	6,6,6	1.16	1 (16%)
4	PO4	H	506	-	4,4,4	1.51	1 (25%)	6,6,6	0.55	0
4	PO4	B	504	-	4,4,4	1.40	1 (25%)	6,6,6	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	D	501	-	46,48,48	0.37	0	64,73,73	0.35	0
4	PO4	A	504	-	4,4,4	1.44	1 (25%)	6,6,6	0.38	0
3	ADN	I	502	-	21,21,21	0.71	0	31,31,31	0.70	0
4	PO4	H	504	-	4,4,4	1.38	1 (25%)	6,6,6	1.78	2 (33%)
2	NAD	A	501	-	46,48,48	0.35	0	64,73,73	0.33	0
4	PO4	H	503	-	4,4,4	1.33	1 (25%)	6,6,6	0.80	0
2	NAD	C	501	-	46,48,48	0.36	0	64,73,73	0.35	0
3	ADN	J	502	-	21,21,21	0.51	0	31,31,31	0.73	0
4	PO4	K	504	-	4,4,4	1.48	1 (25%)	6,6,6	0.42	0
4	PO4	K	503	-	4,4,4	1.39	1 (25%)	6,6,6	0.73	0
2	NAD	K	501	-	46,48,48	0.35	0	64,73,73	0.34	0
4	PO4	J	503	-	4,4,4	1.26	1 (25%)	6,6,6	0.67	0
3	ADN	D	502	-	21,21,21	0.62	0	31,31,31	0.92	2 (6%)
3	ADN	C	502	-	21,21,21	0.48	0	31,31,31	0.66	0
4	PO4	A	503	-	4,4,4	1.03	0	6,6,6	0.71	0
4	PO4	D	503	-	4,4,4	1.10	0	6,6,6	1.35	1 (16%)
4	PO4	C	503	-	4,4,4	0.71	0	6,6,6	0.45	0
2	NAD	H	501	-	46,48,48	0.36	0	64,73,73	0.34	0
4	PO4	K	505	-	4,4,4	1.54	1 (25%)	6,6,6	0.51	0
4	PO4	H	505	-	4,4,4	1.35	1 (25%)	6,6,6	0.81	0
2	NAD	I	501	-	46,48,48	0.36	0	64,73,73	0.37	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	501	-	-	13/30/62/62	0/5/5/5
2	NAD	K	501	-	-	14/30/62/62	0/5/5/5
3	ADN	A	502	-	-	1/6/22/22	0/3/3/3
2	NAD	B	501	-	-	14/30/62/62	0/5/5/5
2	NAD	J	501	-	-	14/30/62/62	0/5/5/5
2	NAD	C	501	-	-	14/30/62/62	0/5/5/5
2	NAD	H	501	-	-	13/30/62/62	0/5/5/5
3	ADN	D	502	-	-	2/6/22/22	0/3/3/3
3	ADN	J	502	-	-	2/6/22/22	0/3/3/3
3	ADN	C	502	-	-	2/6/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	501	-	-	17/30/62/62	0/5/5/5
3	ADN	I	502	-	-	2/6/22/22	0/3/3/3
2	NAD	I	501	-	-	13/30/62/62	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	505	PO4	P-O1	2.81	1.57	1.50
4	H	506	PO4	P-O1	2.80	1.57	1.50
4	B	503	PO4	P-O1	2.70	1.56	1.50
4	A	504	PO4	P-O1	2.69	1.56	1.50
4	H	504	PO4	P-O1	2.62	1.56	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	504	PO4	O3-P-O2	3.44	118.62	107.91
4	D	503	PO4	O3-P-O2	2.59	115.98	107.91
3	D	502	ADN	C4-N9-C1'	-2.42	120.98	126.63
3	D	502	ADN	C1'-N9-C8	2.37	132.35	127.09
4	B	503	PO4	O3-P-O2	2.24	114.89	107.91

There are no chirality outliers.

5 of 121 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	C5B-O5B-PA-O3
2	A	501	NAD	PN-O3-PA-O5B
2	A	501	NAD	O4D-C1D-N1N-C2N

There are no ring outliers.

17 monomers are involved in 28 short contacts:

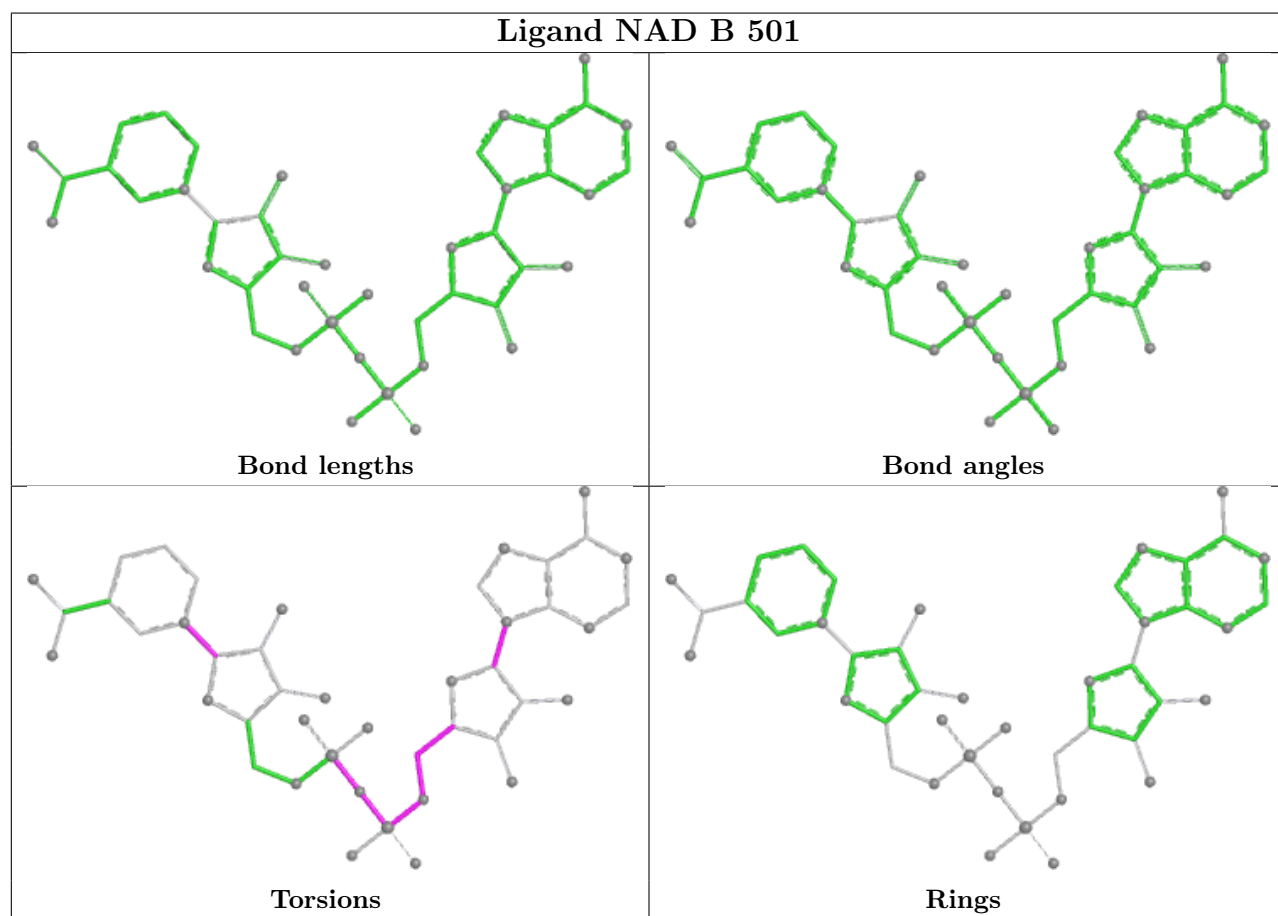
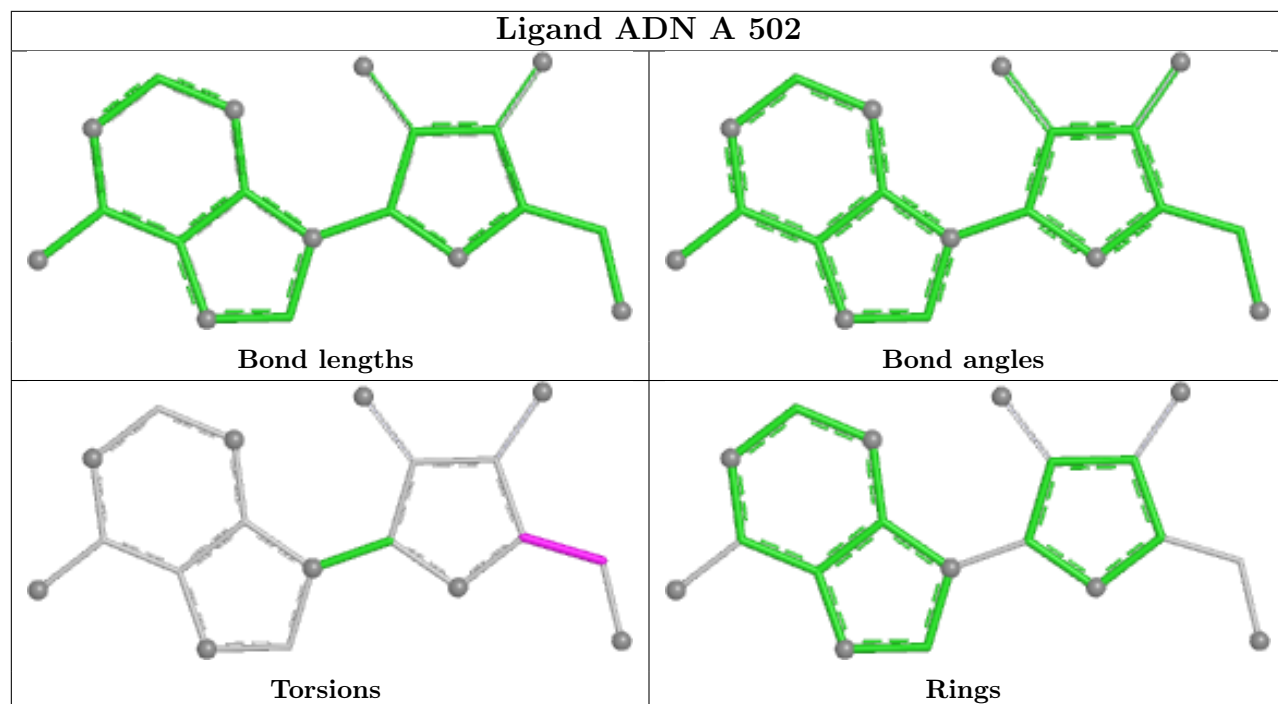
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ADN	1	0
2	B	501	NAD	3	0
2	J	501	NAD	4	0
4	B	503	PO4	2	0

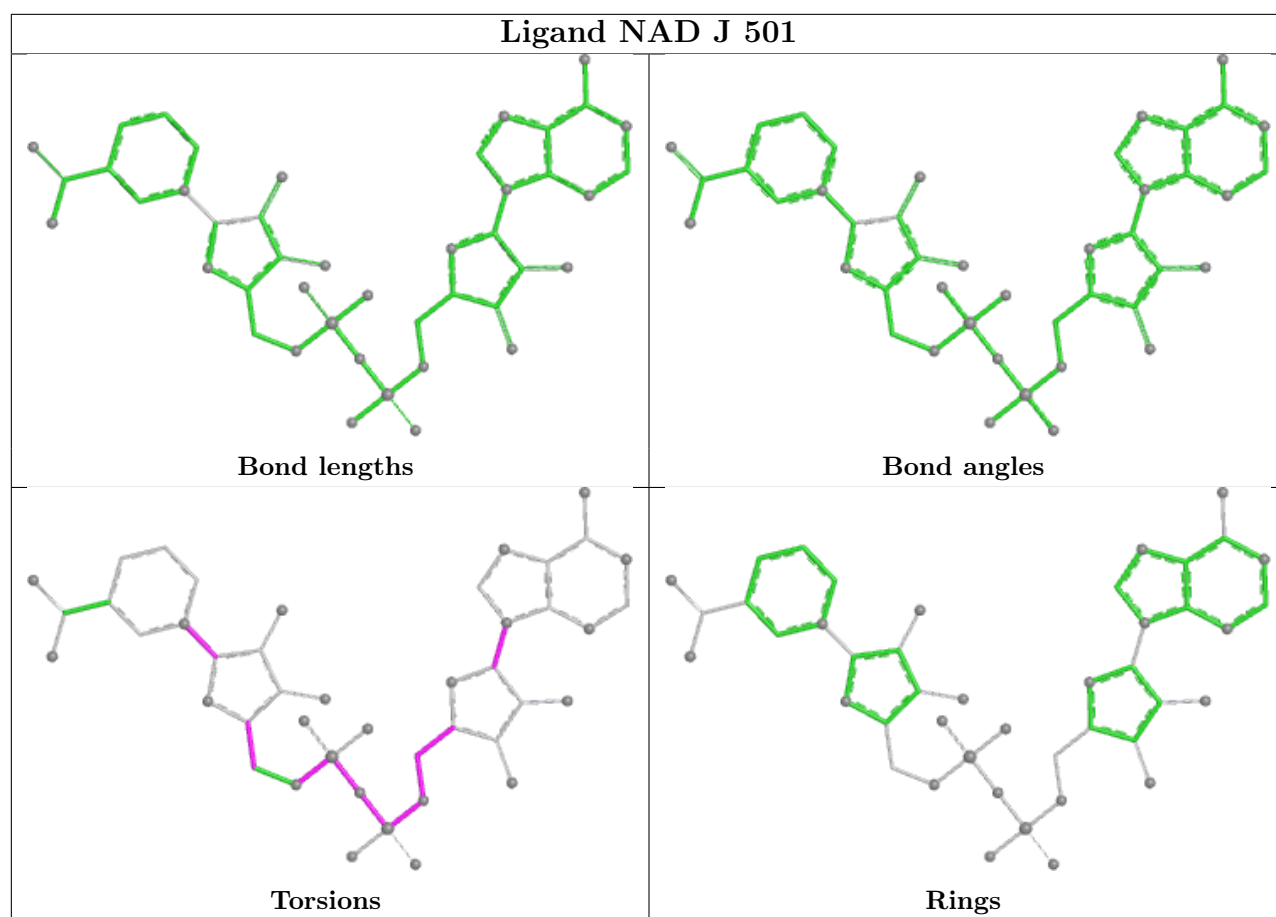
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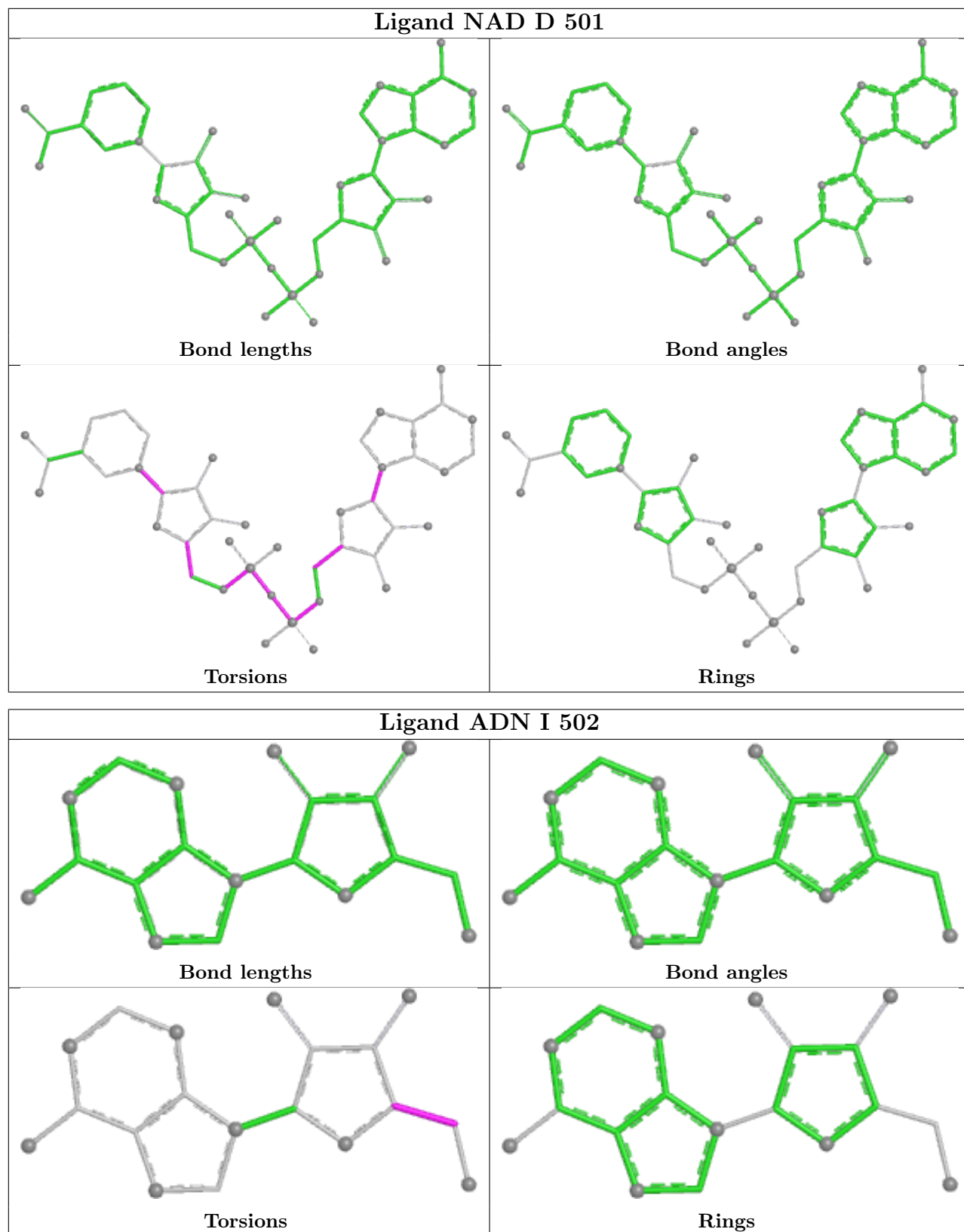
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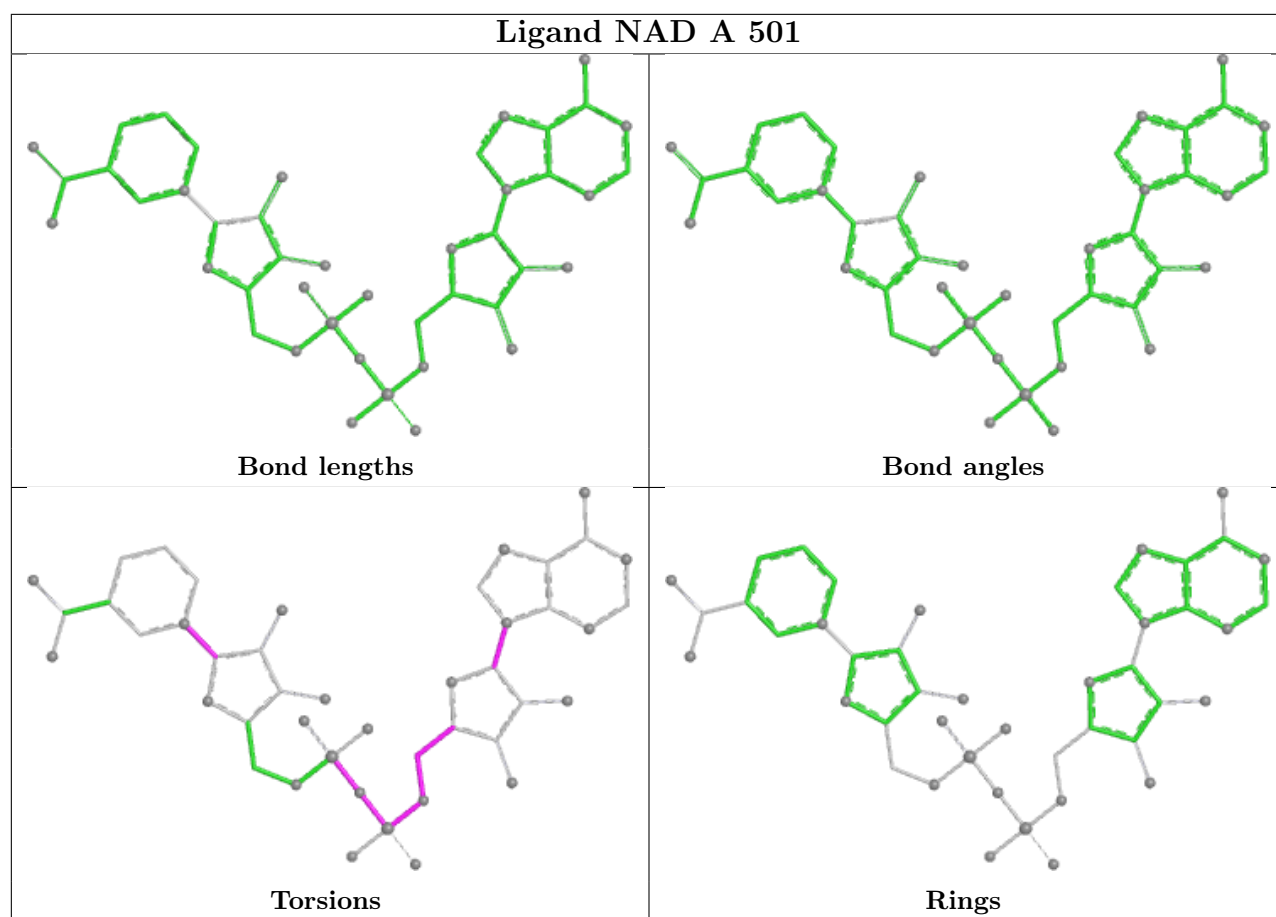
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	NAD	3	0
3	I	502	ADN	1	0
2	A	501	NAD	3	0
2	C	501	NAD	2	0
3	J	502	ADN	2	0
4	K	503	PO4	2	0
2	K	501	NAD	3	0
4	J	503	PO4	1	0
3	D	502	ADN	1	0
3	C	502	ADN	1	0
4	D	503	PO4	1	0
2	H	501	NAD	2	0
2	I	501	NAD	1	0

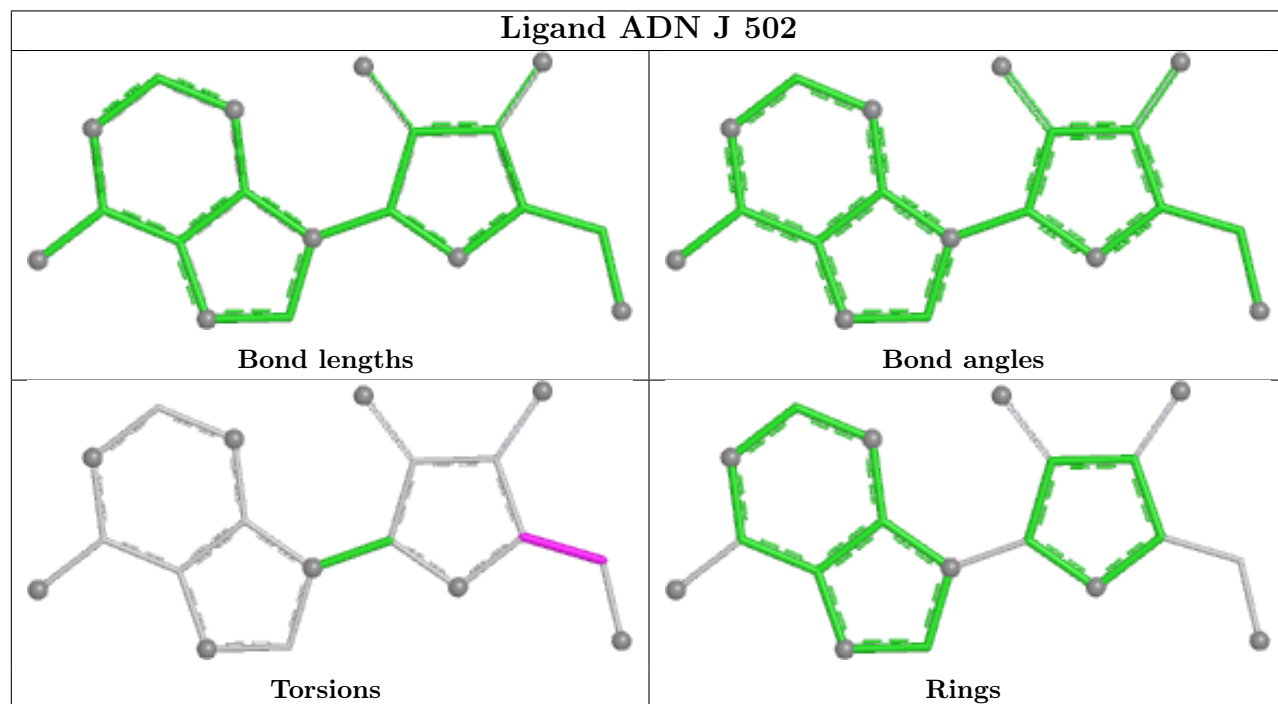
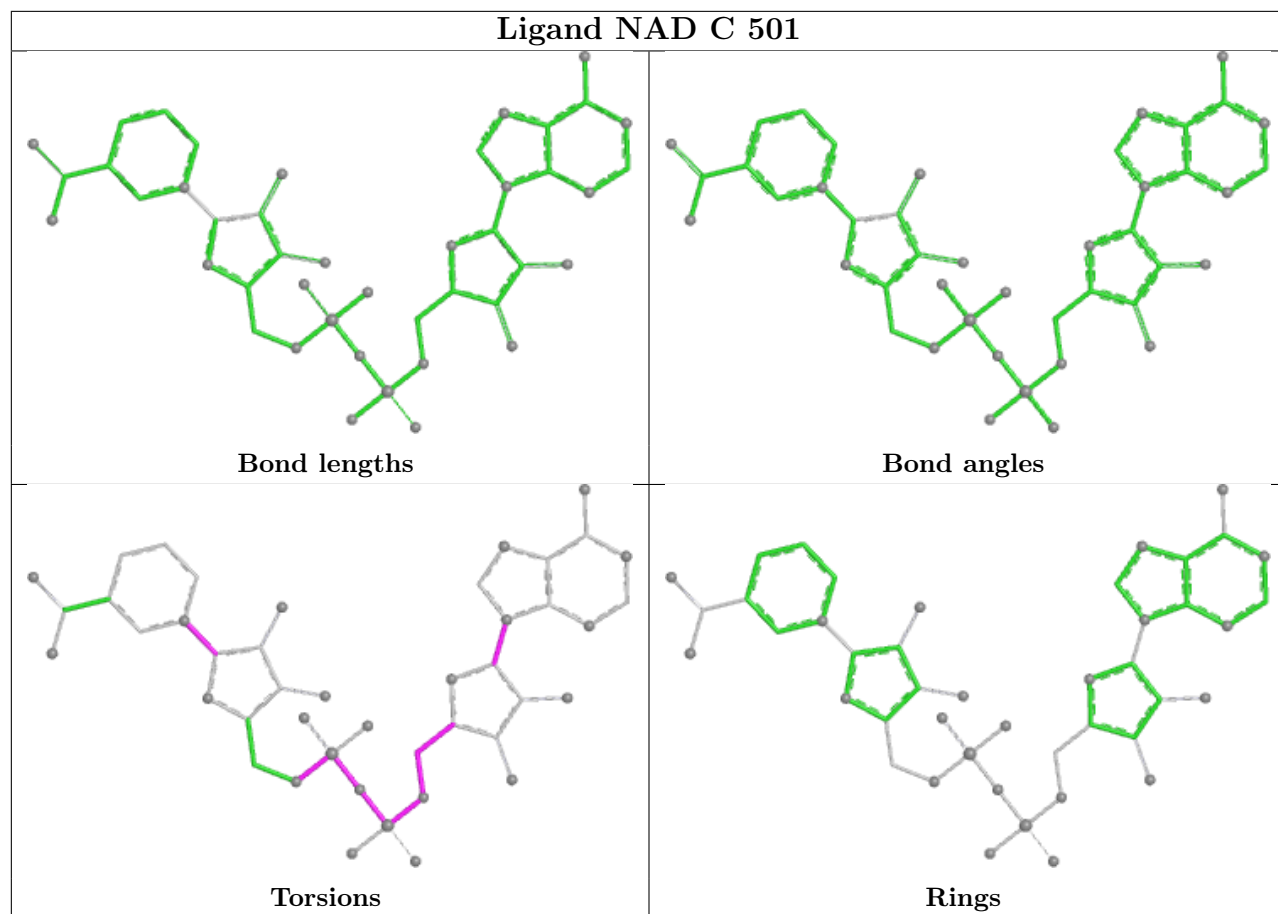
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

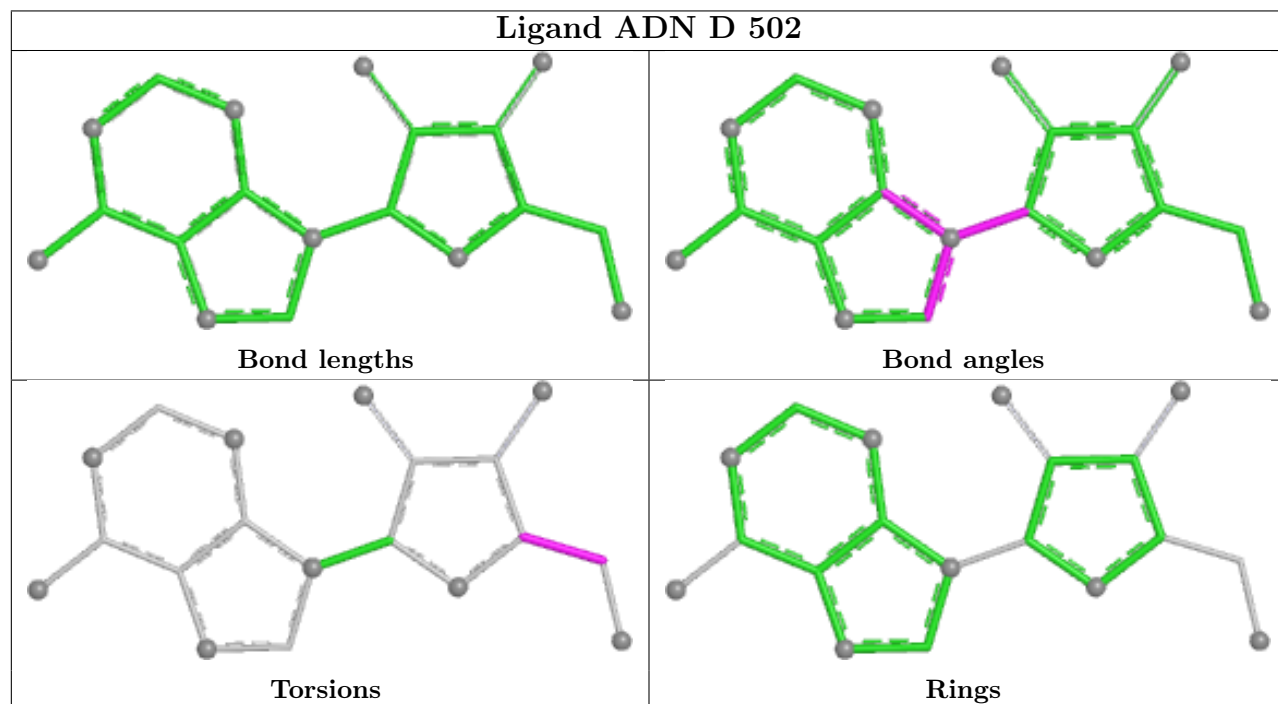
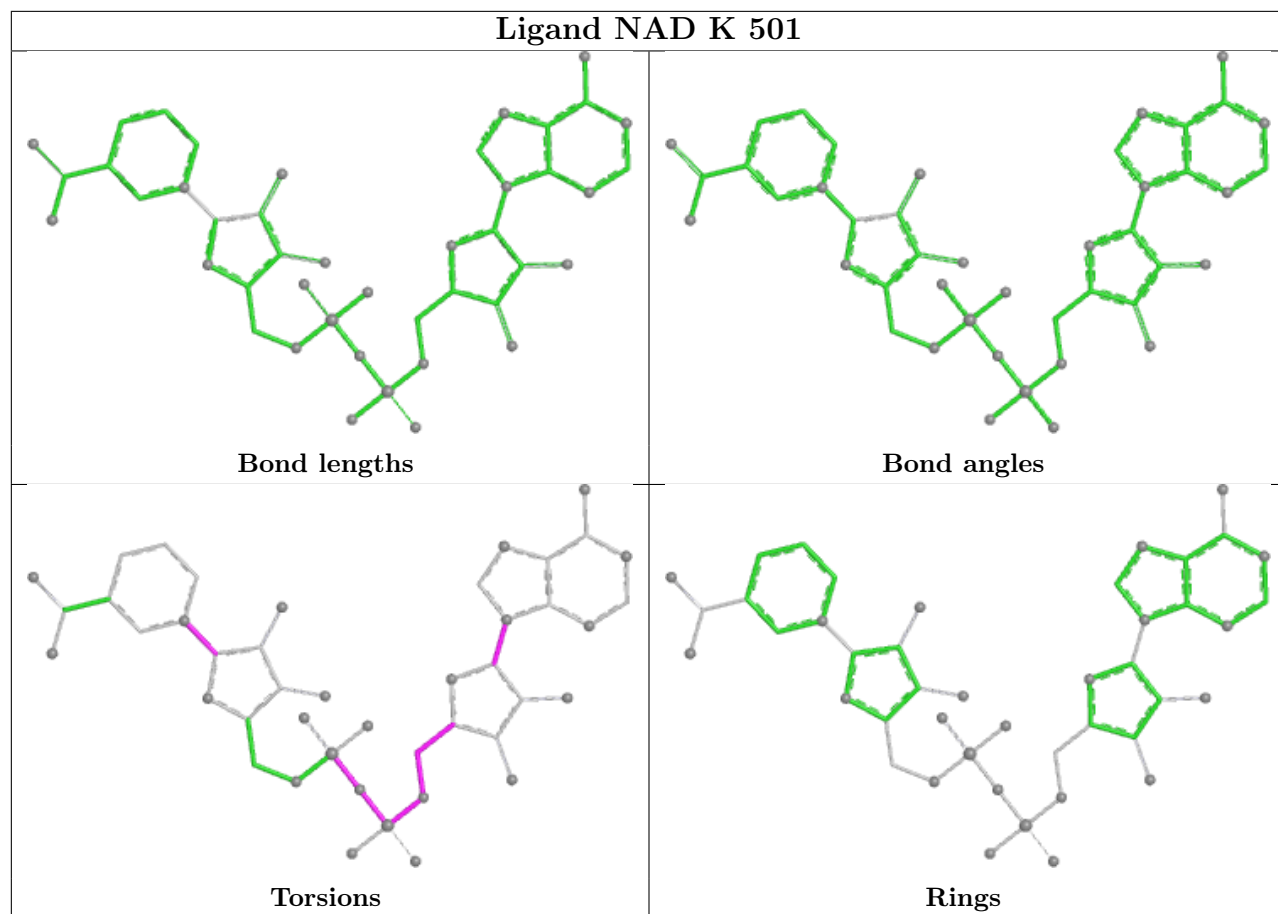


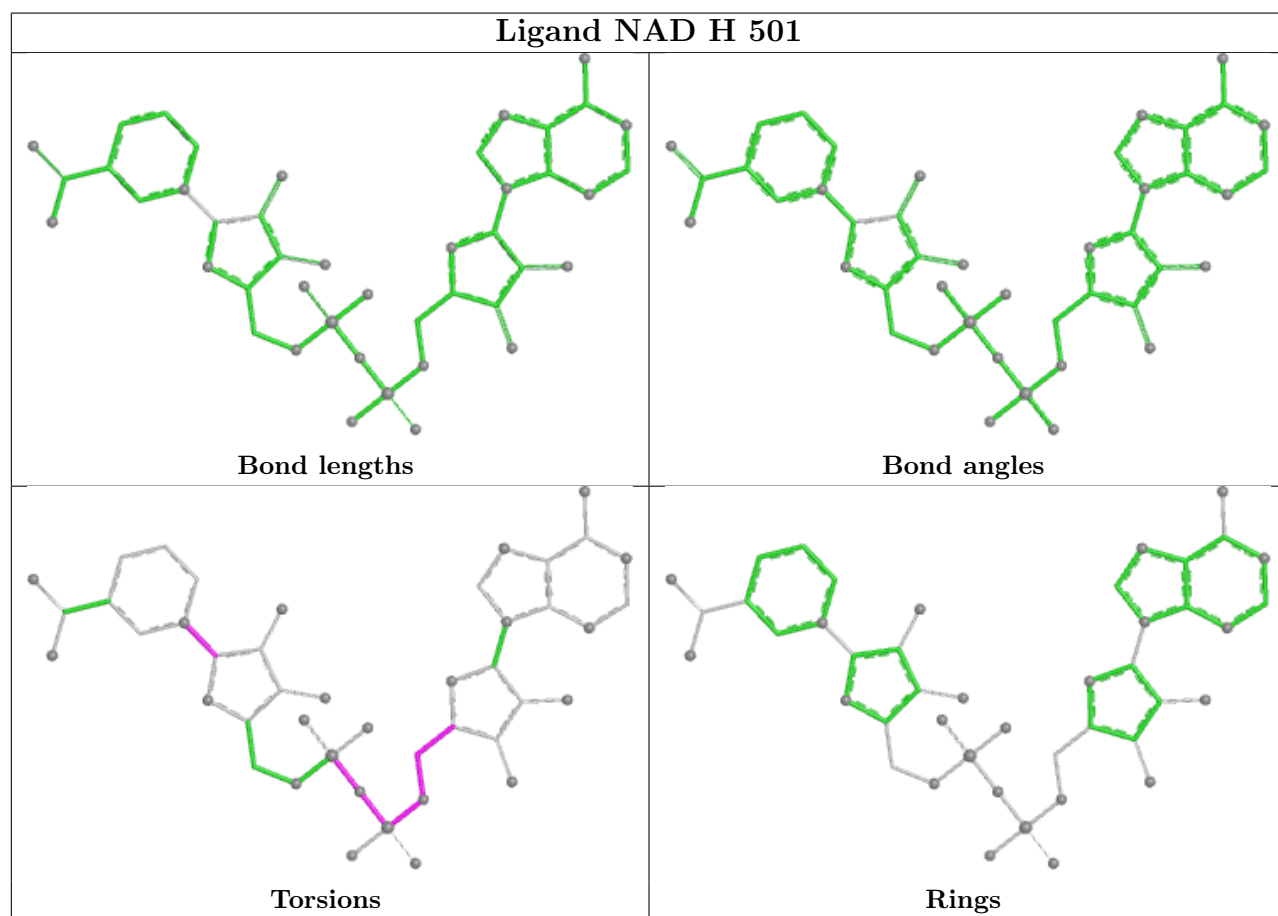
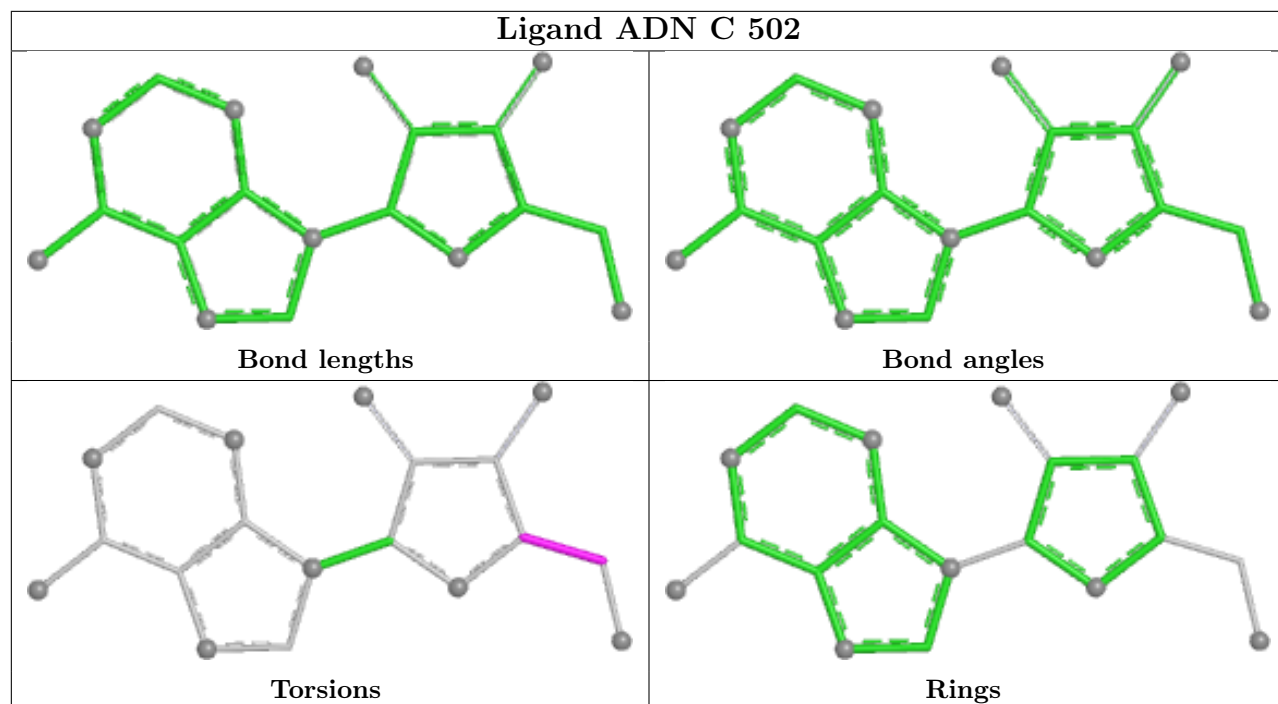


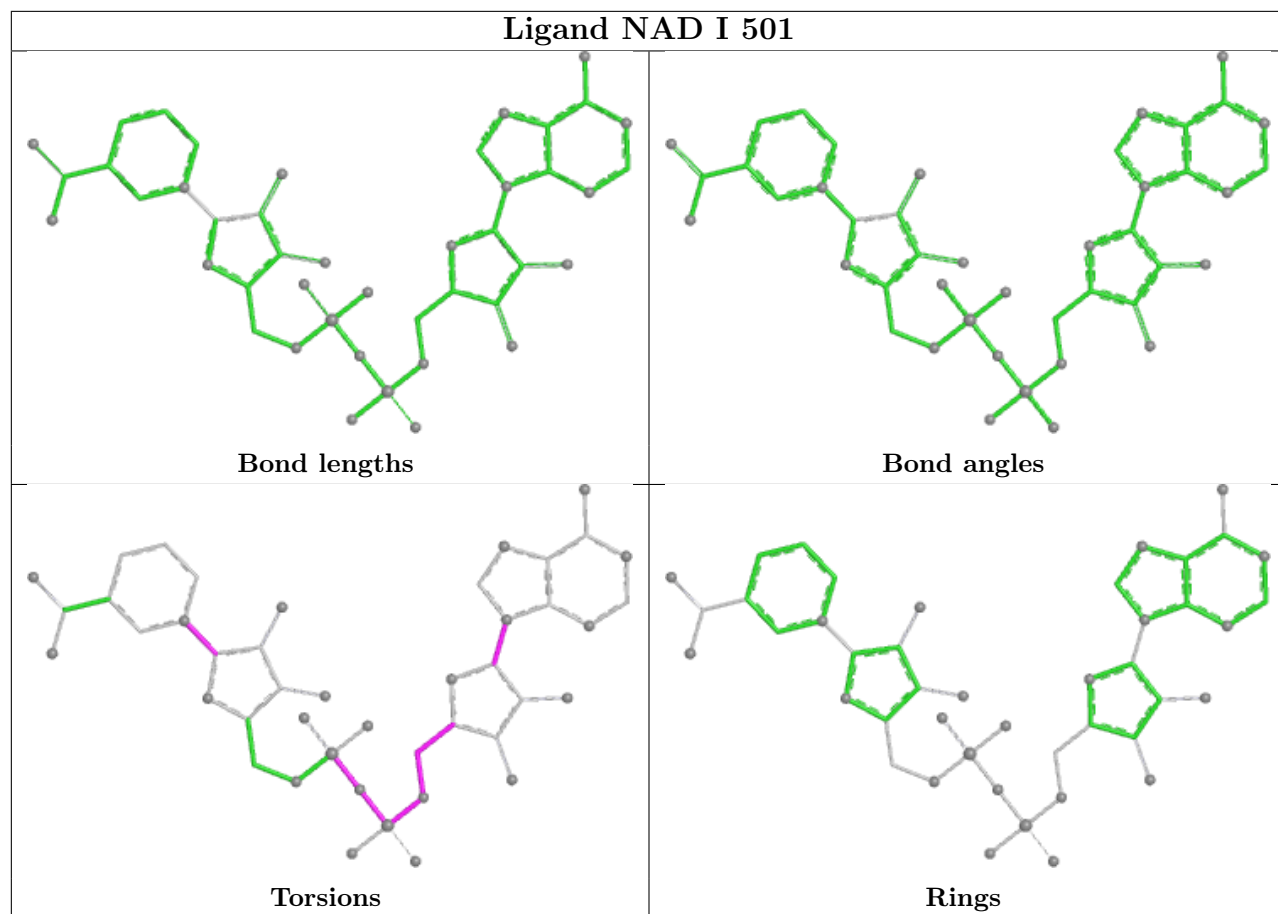












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	461/472 (97%)	-1.47	0 100 100	15, 28, 45, 63	3 (0%)
1	B	461/472 (97%)	-1.52	0 100 100	15, 25, 37, 58	2 (0%)
1	C	461/472 (97%)	-1.41	0 100 100	14, 29, 50, 74	5 (1%)
1	D	461/472 (97%)	-1.44	0 100 100	14, 29, 48, 69	2 (0%)
1	H	461/472 (97%)	-1.41	0 100 100	16, 31, 53, 68	3 (0%)
1	I	461/472 (97%)	-1.50	0 100 100	16, 26, 38, 49	3 (0%)
1	J	461/472 (97%)	-1.41	0 100 100	13, 28, 50, 67	5 (1%)
1	K	461/472 (97%)	-1.47	0 100 100	14, 28, 41, 51	2 (0%)
All	All	3688/3776 (97%)	-1.45	0 100 100	13, 28, 47, 74	25 (0%)

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

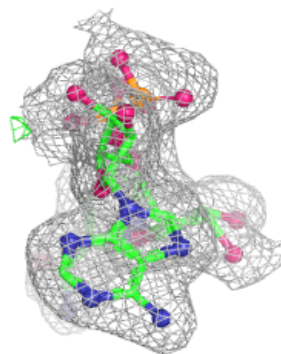
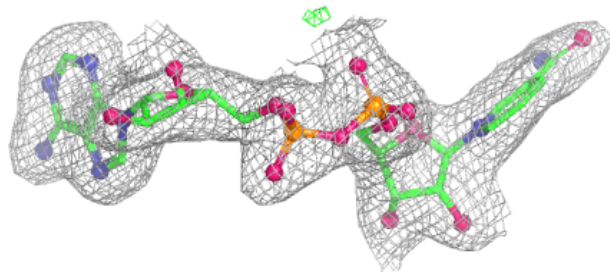
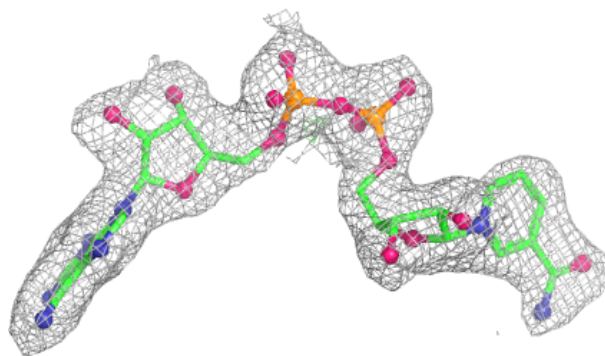
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	A	504	5/5	0.98	0.06	28,30,33,34	5
4	PO4	B	504	5/5	0.98	0.07	27,29,30,33	5
2	NAD	H	501	44/44	0.99	0.03	10,24,31,35	0
2	NAD	I	501	44/44	0.99	0.03	15,20,28,35	0
2	NAD	K	501	44/44	0.99	0.03	17,25,34,46	0
3	ADN	A	502	19/19	0.99	0.04	17,22,28,30	0
3	ADN	B	502[B]	19/19	0.99	0.04	17,21,24,28	0
3	ADN	C	502	19/19	0.99	0.04	20,27,34,36	0
3	ADN	D	502	19/19	0.99	0.02	13,17,26,37	0
3	ADN	H	502[B]	19/19	0.99	0.04	25,33,37,41	0
3	ADN	J	502	19/19	0.99	0.03	17,24,28,36	0
3	ADN	K	502[B]	19/19	0.99	0.04	17,24,28,28	0
2	NAD	C	501	44/44	0.99	0.03	9,22,29,32	0
4	PO4	B	503	5/5	0.99	0.05	17,23,30,36	5
2	NAD	D	501	44/44	0.99	0.03	19,24,34,38	0
4	PO4	C	503	5/5	0.99	0.04	37,38,53,60	0
4	PO4	D	503	5/5	0.99	0.05	16,26,30,36	0
4	PO4	H	505	5/5	0.99	0.04	30,32,42,55	5
4	PO4	H	506	5/5	0.99	0.05	30,35,38,55	5
4	PO4	K	503	5/5	0.99	0.05	20,27,28,29	5
4	PO4	K	504	5/5	0.99	0.05	36,38,42,49	5
4	PO4	K	505	5/5	0.99	0.04	26,39,42,54	5
4	PO4	H	503	5/5	1.00	0.03	24,33,38,48	0
4	PO4	H	504	5/5	1.00	0.04	18,32,38,40	0
2	NAD	J	501	44/44	1.00	0.02	12,21,31,34	0
3	ADN	I	502	19/19	1.00	0.02	10,16,23,31	0
4	PO4	J	503	5/5	1.00	0.03	26,39,42,44	0
2	NAD	A	501	44/44	1.00	0.02	13,20,28,34	0
2	NAD	B	501	44/44	1.00	0.02	8,18,24,30	0
4	PO4	A	503	5/5	1.00	0.05	28,35,37,42	0

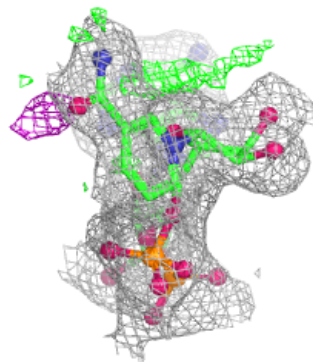
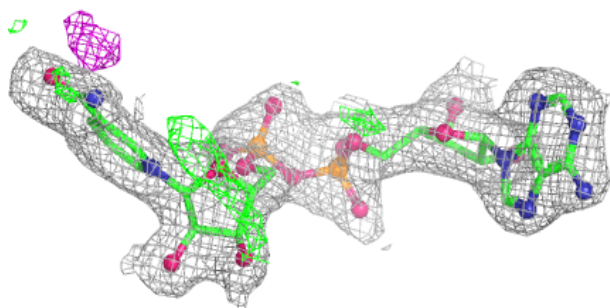
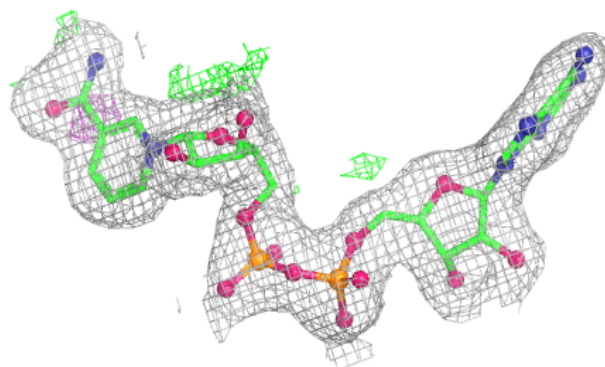
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD H 501:**

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

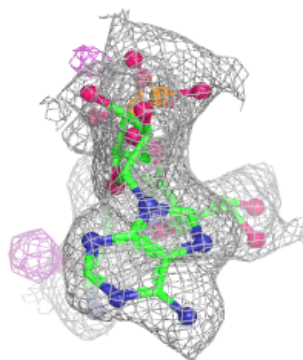
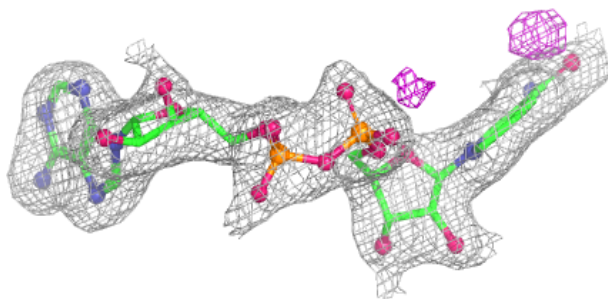
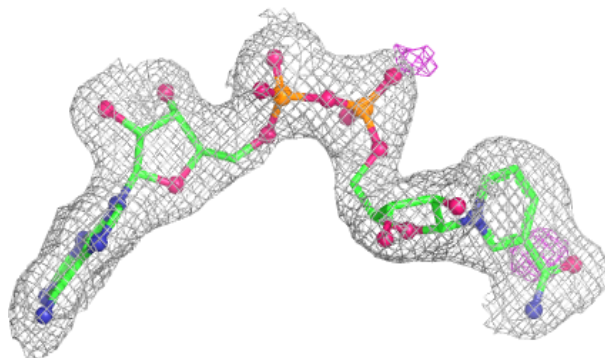
**Electron density around NAD I 501:**

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

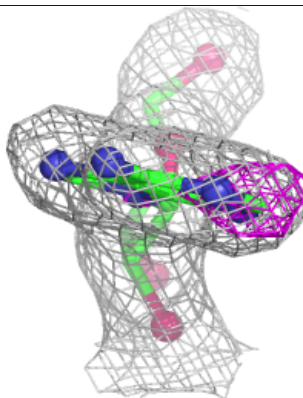
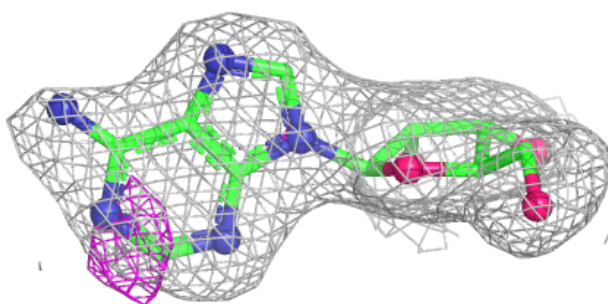
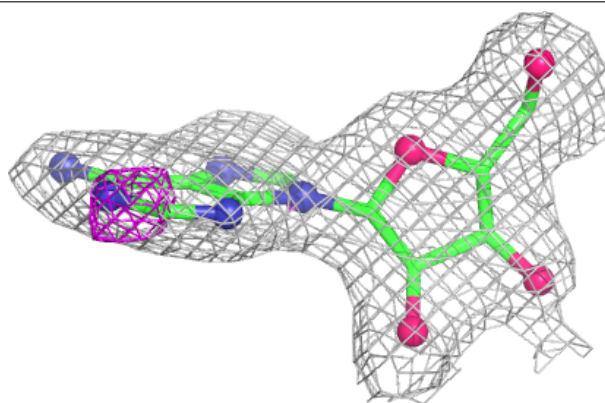


**Electron density around NAD K 501:**

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

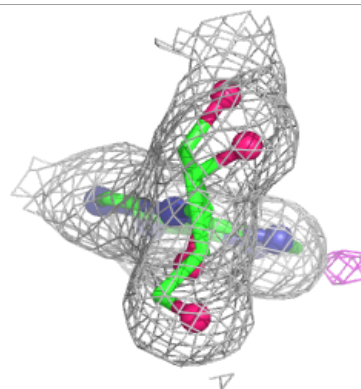
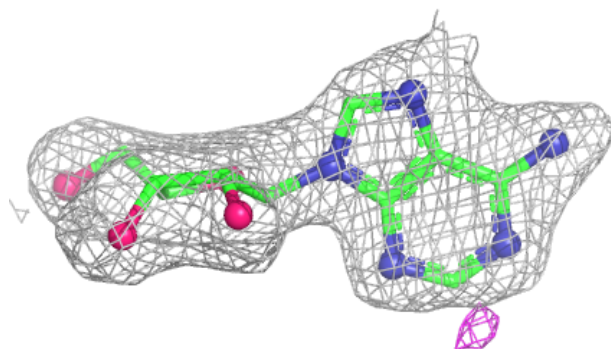
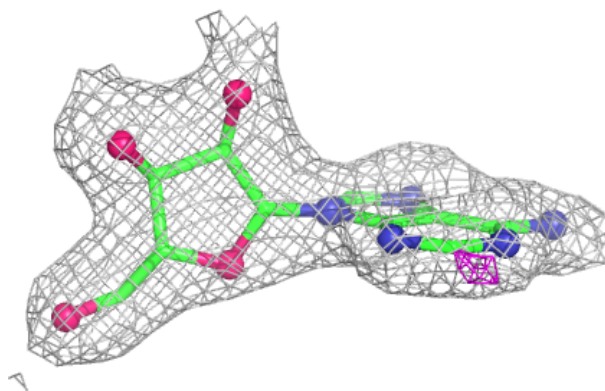
**Electron density around ADN A 502:**

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

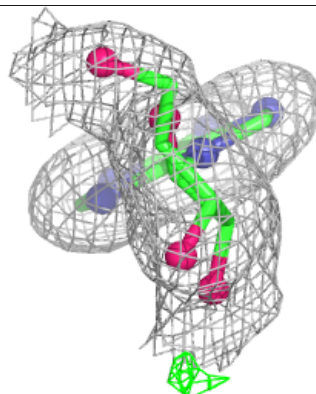
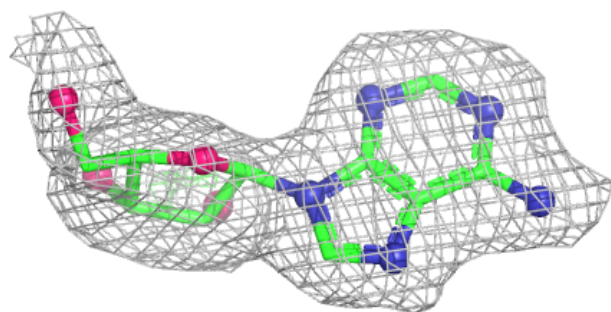
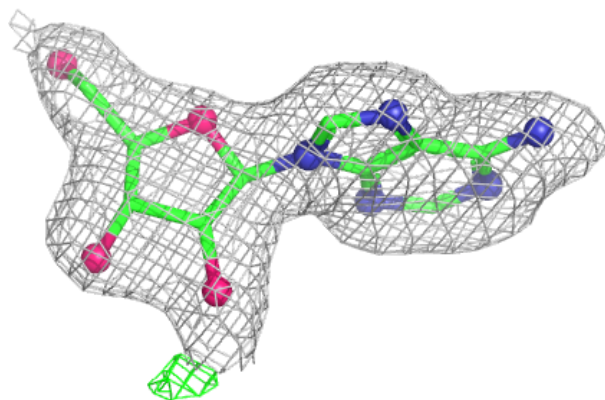


**Electron density around ADN C 502:**

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

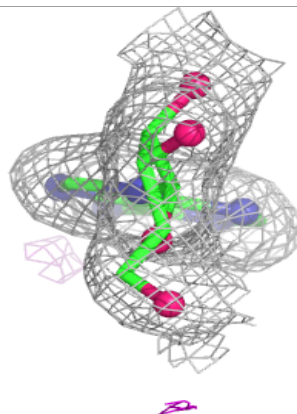
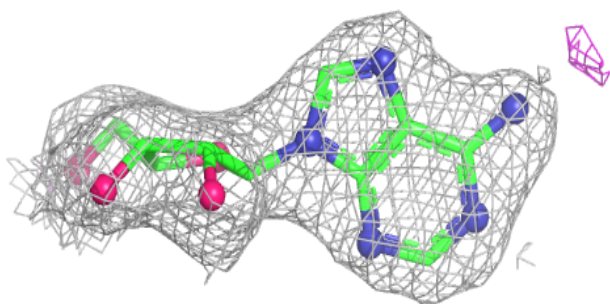
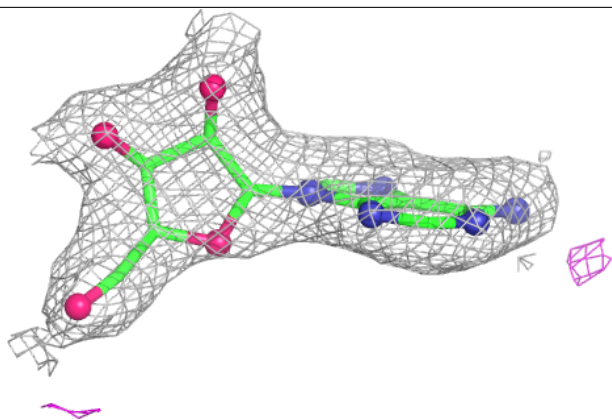
**Electron density around ADN D 502:**

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

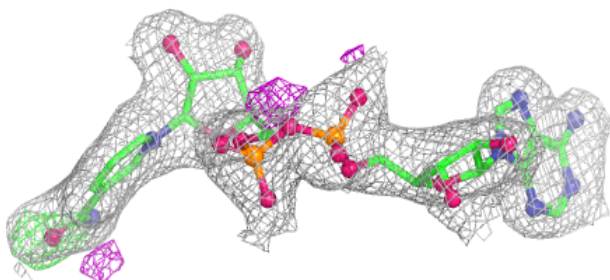
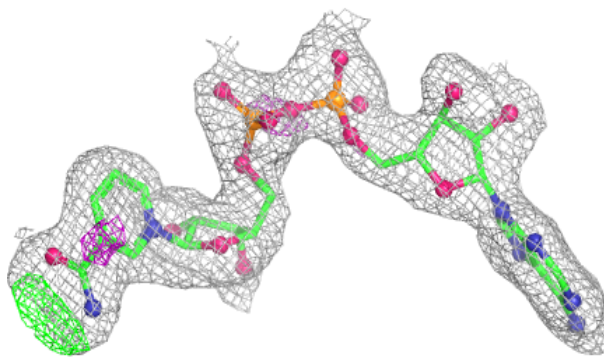


**Electron density around ADN J 502:**

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

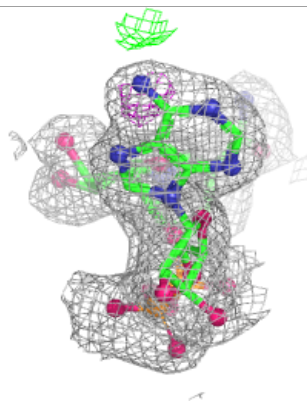
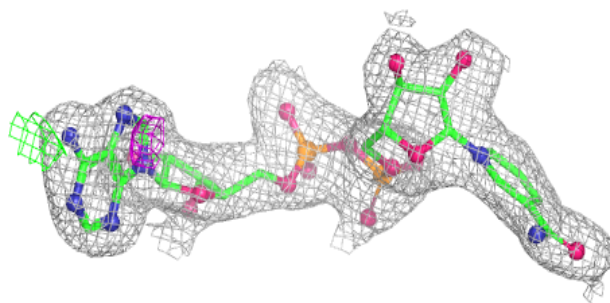
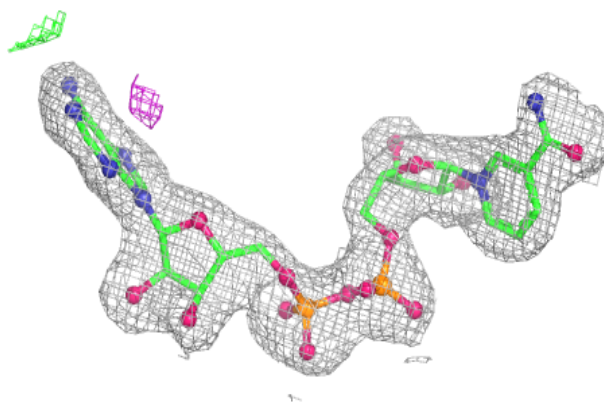
**Electron density around NAD C 501:**

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

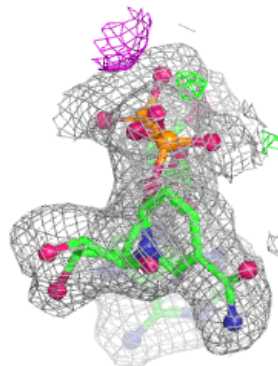
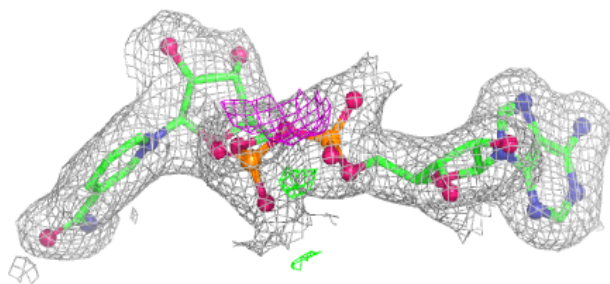
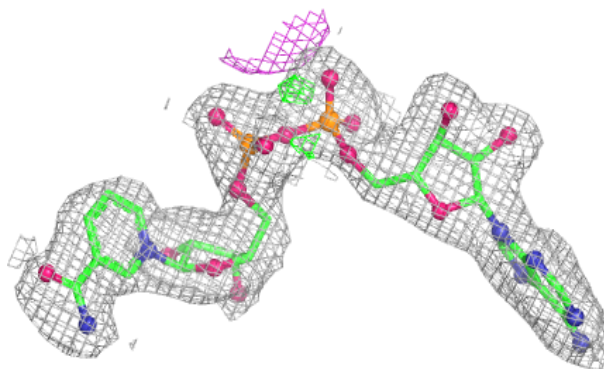


**Electron density around NAD D 501:**

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

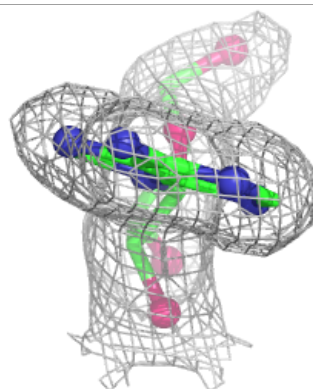
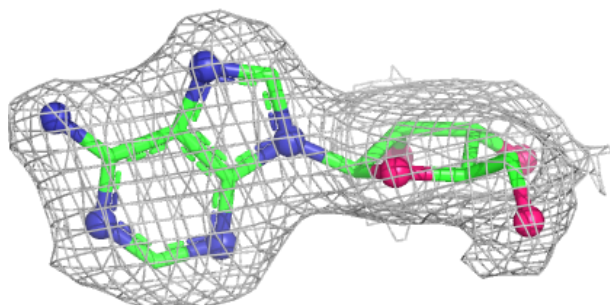
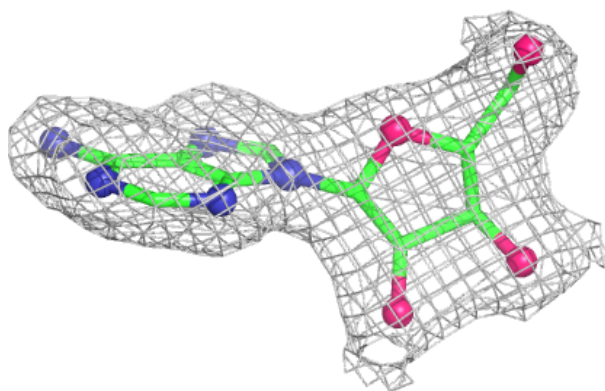
**Electron density around NAD J 501:**

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

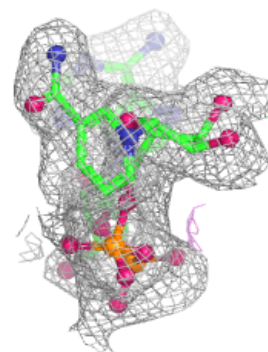
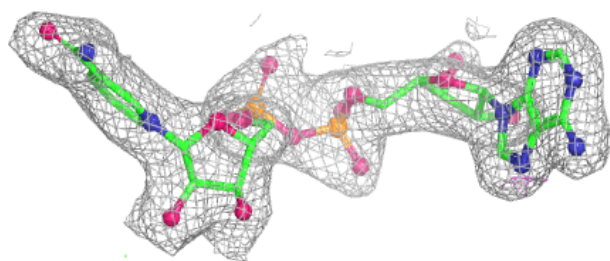
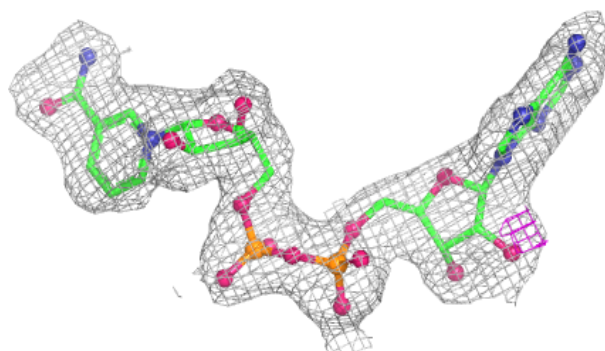


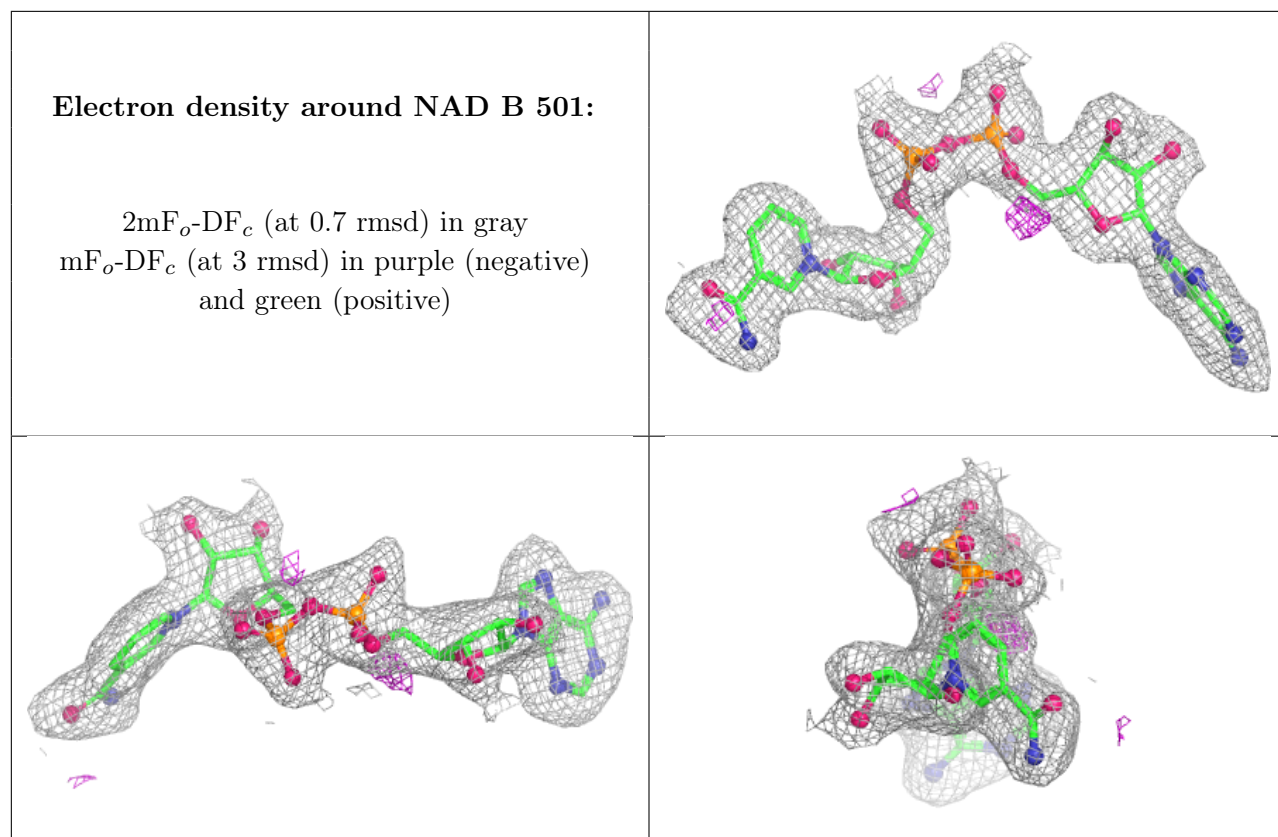
**Electron density around ADN I 502:**

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

**Electron density around NAD 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.