



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 12:11 am GMT

PDB ID : 6GBN  
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *Cytophaga hutchinsonii* in complex with adenosine  
Authors : Czyrko, J.; Jaskolski, M.; Brzezinski, K.  
Deposited on : 2018-04-15  
Resolution : 2.09 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.

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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

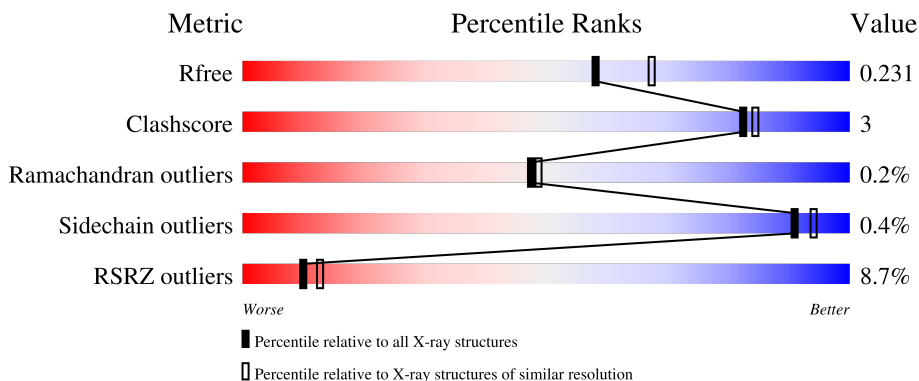
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	438	
1	B	438	
1	C	438	
1	D	438	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14484 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.

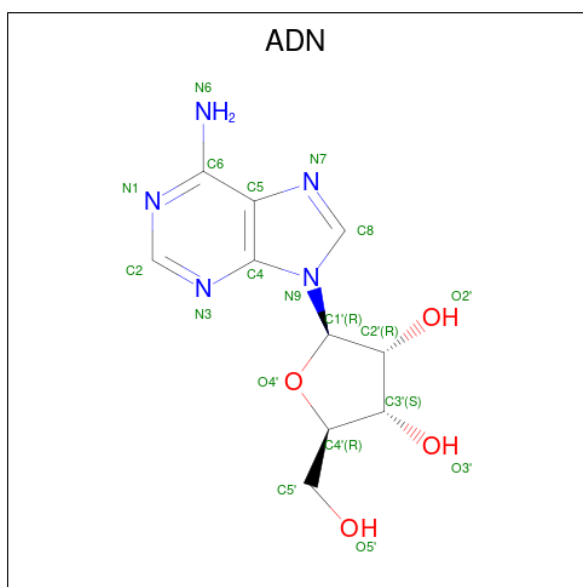
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	432	3400	2138	585	656	21	0	10	0
1	B	435	3383	2129	578	655	21	0	5	0
1	C	430	3319	2090	569	640	20	0	7	0
1	D	435	3355	2114	572	648	21	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

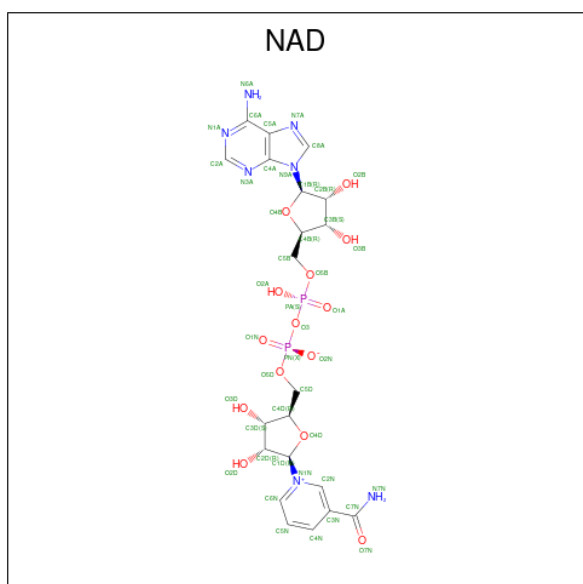
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q11XG9
A	-1	ASN	-	expression tag	UNP Q11XG9
A	0	ALA	-	expression tag	UNP Q11XG9
B	-2	SER	-	expression tag	UNP Q11XG9
B	-1	ASN	-	expression tag	UNP Q11XG9
B	0	ALA	-	expression tag	UNP Q11XG9
C	-2	SER	-	expression tag	UNP Q11XG9
C	-1	ASN	-	expression tag	UNP Q11XG9
C	0	ALA	-	expression tag	UNP Q11XG9
D	-2	SER	-	expression tag	UNP Q11XG9
D	-1	ASN	-	expression tag	UNP Q11XG9
D	0	ALA	-	expression tag	UNP Q11XG9

- Molecule 2 is ADENOSINE (three-letter code: ADN) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>4</sub>).



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).

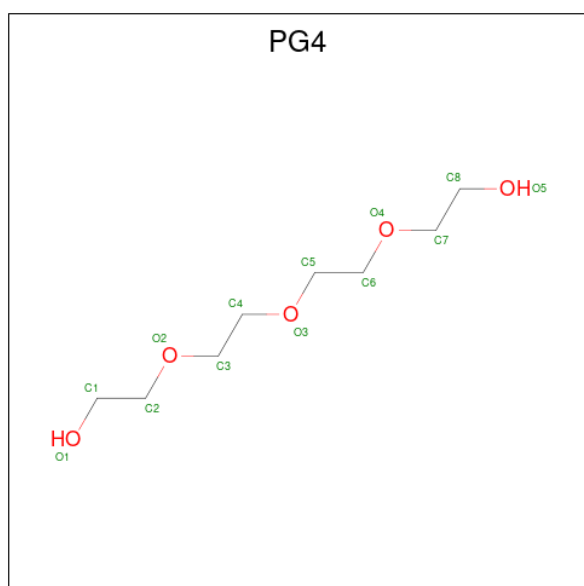


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	C O	0	0
			7	4 3		

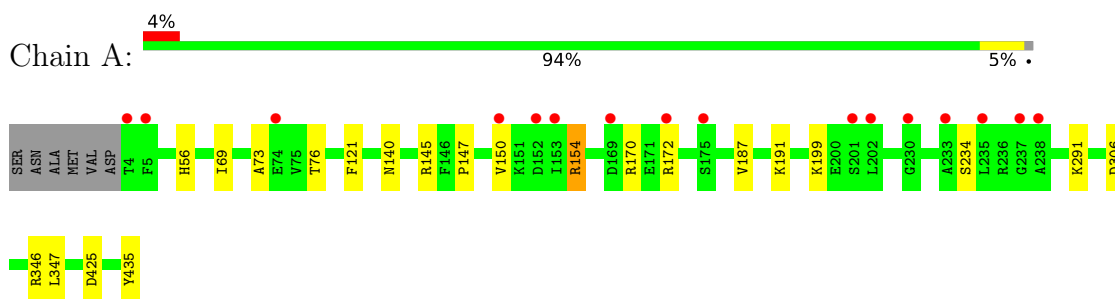
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	257	Total	O	0	11
			263	263		
7	B	286	Total	O	0	12
			292	292		
7	C	82	Total	O	0	3
			84	84		
7	D	109	Total	O	0	3
			112	112		

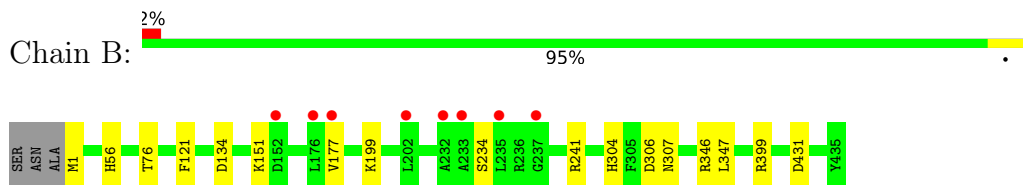
### 3 Residue-property plots [i](#)

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.

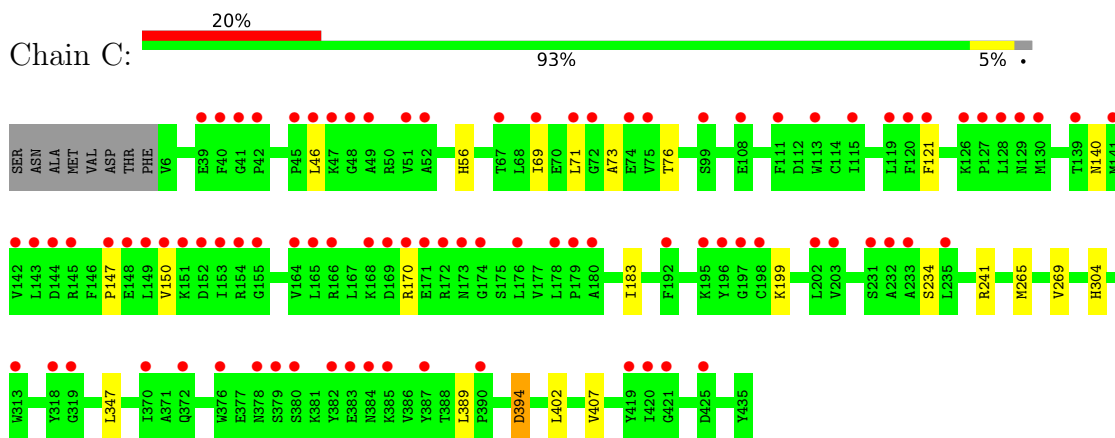
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase

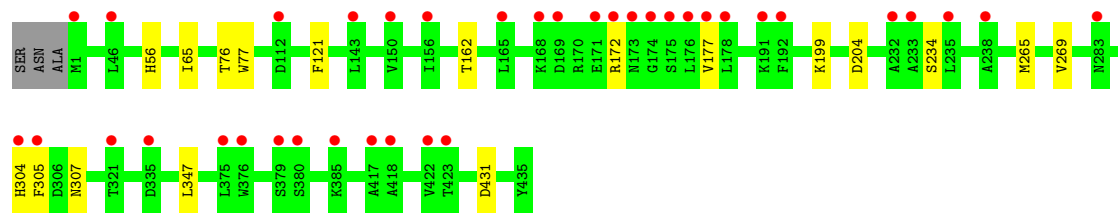


- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.28Å 102.44Å 188.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.09 48.14 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.14-2.09) 99.6 (48.14-2.09)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.08Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.210 , 0.231 0.216 , 0.231	Depositor DCC
$R_{free}$ test set	2101 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtrriage
Anisotropy	0.897	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1495e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PG4, ADN, NAD, PEG

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	0.62	0/3457	0.78	1/4668 (0.0%)
1	B	0.64	0/3437	0.80	8/4644 (0.2%)
1	C	0.53	0/3375	0.74	3/4560 (0.1%)
1	D	0.56	0/3409	0.74	2/4607 (0.0%)
All	All	0.59	0/13678	0.77	14/18479 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	C	394	ASP	CB-CA-C	7.21	124.83	110.40
1	D	307	ASN	CB-CA-C	-7.12	96.16	110.40
1	B	306	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	431	ASP	CB-CG-OD1	6.45	124.10	118.30
1	B	307	ASN	CB-CA-C	-6.43	97.53	110.40
1	C	241	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	306	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	D	431	ASP	CB-CG-OD1	5.62	123.35	118.30
1	C	394	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	145	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	B	134	ASP	CB-CG-OD1	5.09	122.89	118.30
1	B	346[A]	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	346[B]	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3400	0	3406	17	0
1	B	3383	0	3388	8	0
1	C	3319	0	3329	24	0
1	D	3355	0	3370	15	0
2	A	19	0	13	1	0
2	B	19	0	13	1	0
2	C	19	0	13	1	0
2	D	19	0	13	1	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
3	C	44	0	26	2	0
3	D	44	0	26	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	13	0	18	0	0
6	B	7	0	10	1	0
7	A	263	0	0	1	0
7	B	292	0	0	2	0
7	C	84	0	0	1	0
7	D	112	0	0	1	0
All	All	14484	0	13677	69	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 3.

All (69) 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:C:183:ILE:CD1	1:C:389:LEU:CD1	1.83	1.53
1:C:183:ILE:HD11	1:C:389:LEU:CD1	1.46	1.33
1:C:183:ILE:CD1	1:C:389:LEU:HD11	1.43	1.28
1:C:183:ILE:CD1	1:C:389:LEU:HD13	1.57	1.21
1:C:183:ILE:HD13	1:C:389:LEU:CD1	1.72	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154[A]:ARG:CG	1:A:154[A]:ARG:HH11	1.63	1.10
1:A:154[A]:ARG:HH11	1:A:154[A]:ARG:HG3	1.23	0.97
1:C:183:ILE:HD12	1:C:389:LEU:HD13	1.45	0.93
1:C:265:MET:SD	1:C:269:VAL:CG2	2.67	0.83
1:D:265:MET:SD	1:D:269:VAL:CG2	2.67	0.83
1:A:154[A]:ARG:HH11	1:A:154[A]:ARG:HG2	1.48	0.78
1:C:183:ILE:HD11	1:C:389:LEU:HD11	0.79	0.78
1:C:402:LEU:HD22	1:C:407:VAL:HG21	1.66	0.76
1:C:265:MET:SD	1:C:269:VAL:HG23	2.27	0.75
1:D:65:ILE:HD11	1:D:77:TRP:CD2	2.22	0.74
1:D:265:MET:SD	1:D:269:VAL:HG23	2.26	0.74
1:A:154[A]:ARG:HG3	1:A:154[A]:ARG:NH1	1.94	0.72
1:A:154[A]:ARG:CG	1:A:154[A]:ARG:NH1	2.36	0.69
1:D:65:ILE:CD1	1:D:77:TRP:CE3	2.76	0.69
1:D:65:ILE:HD12	1:D:77:TRP:CE3	2.31	0.65
1:C:304:HIS:O	1:C:347:LEU:HD11	1.96	0.65
1:C:402:LEU:HB3	1:C:407:VAL:HG23	1.79	0.64
1:A:306:ASP:HB3	1:A:346[B]:ARG:HG3	1.80	0.64
3:C:502:NAD:N1A	7:C:601:HOH:O	2.31	0.62
1:A:425[B]:ASP:HB3	7:A:823[B]:HOH:O	2.01	0.61
1:D:162:THR:HG21	1:D:305:PHE:CE2	2.36	0.61
1:C:402:LEU:HB3	1:C:407:VAL:CG2	2.31	0.60
1:C:69:ILE:HD13	1:C:73:ALA:O	2.01	0.60
1:A:69:ILE:HD13	1:A:73:ALA:O	2.02	0.58
2:A:501:ADN:H3'	3:A:502:NAD:C4N	2.33	0.58
1:B:304:HIS:O	1:B:347:LEU:HD11	2.05	0.57
1:C:183:ILE:HD13	1:C:389:LEU:HD13	1.52	0.57
1:A:191[B]:LYS:HD2	7:B:748[B]:HOH:O	2.06	0.55
1:C:147:PRO:O	1:C:150:VAL:HG22	2.08	0.54
1:D:65:ILE:CD1	1:D:77:TRP:CD2	2.91	0.54
1:D:65:ILE:HD11	1:D:77:TRP:CE2	2.44	0.53
1:C:402:LEU:HD22	1:C:407:VAL:CG2	2.38	0.52
1:A:147:PRO:O	1:A:150:VAL:HG22	2.10	0.51
2:B:501:ADN:H3'	3:B:502:NAD:C4N	2.42	0.49
1:B:151:LYS:HG3	7:B:607:HOH:O	2.13	0.49
1:B:399:ARG:HD3	6:B:504:PEG:H22	1.96	0.47
1:A:76:THR:HG23	1:A:121:PHE:CE2	2.50	0.47
1:B:76:THR:HG23	1:B:121:PHE:CE2	2.50	0.47
1:D:76:THR:HG23	1:D:121:PHE:CE2	2.50	0.47
1:A:154[A]:ARG:HG2	1:A:154[A]:ARG:NH1	2.19	0.46
1:D:65:ILE:CD1	1:D:77:TRP:CZ3	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:THR:HG23	1:C:121:PHE:CE2	2.50	0.46
1:C:347:LEU:H	1:C:347:LEU:HD12	1.81	0.46
1:D:177:VAL:HG22	1:D:177:VAL:O	2.16	0.45
1:A:140:ASN:OD1	1:A:170:ARG:NH1	2.50	0.44
1:B:177:VAL:O	1:B:177:VAL:HG22	2.16	0.44
2:D:501:ADN:H3'	3:D:502:NAD:C4N	2.48	0.44
1:A:187:VAL:HG21	1:A:435:TYR:CE1	2.53	0.44
1:C:46:LEU:HD13	1:C:71:LEU:HB3	2.01	0.43
1:A:191[B]:LYS:HD3	1:A:191[B]:LYS:HA	1.79	0.42
2:C:501:ADN:H3'	3:C:502:NAD:C4N	2.50	0.42
1:A:347:LEU:HA	1:A:347:LEU:HD23	1.86	0.42
1:C:140:ASN:OD1	1:C:170[A]:ARG:NH1	2.53	0.42
1:C:46:LEU:HD12	1:C:46:LEU:N	2.35	0.42
1:C:199:LYS:HA	1:C:234:SER:HB2	2.02	0.41
1:D:204:ASP:OD1	7:D:601:HOH:O	2.22	0.41
1:C:183:ILE:HD11	1:C:389:LEU:CD2	2.50	0.41
1:D:199:LYS:HA	1:D:234:SER:HB2	2.03	0.41
1:D:304:HIS:HA	1:D:347:LEU:HD21	2.03	0.41
1:A:199:LYS:HA	1:A:234:SER:HB2	2.03	0.40
1:B:199:LYS:HA	1:B:234:SER:HB2	2.03	0.40
1:D:265:MET:SD	1:D:269:VAL:HG22	2.58	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	439/438 (100%)	428 (98%)	10 (2%)	1 (0%)	47 49
1	B	437/438 (100%)	426 (98%)	10 (2%)	1 (0%)	47 49
1	C	430/438 (98%)	418 (97%)	11 (3%)	1 (0%)	47 49
1	D	434/438 (99%)	423 (98%)	10 (2%)	1 (0%)	47 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1740/1752 (99%)	1695 (97%)	41 (2%)	4 (0%)	47 49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	B	56	HIS
1	C	56	HIS
1	D	56	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	367/363 (101%)	363 (99%)	4 (1%)	73 79
1	B	365/363 (101%)	364 (100%)	1 (0%)	92 95
1	C	358/363 (99%)	357 (100%)	1 (0%)	92 95
1	D	362/363 (100%)	361 (100%)	1 (0%)	92 95
All	All	1452/1452 (100%)	1445 (100%)	7 (0%)	91 92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154[A]	ARG
1	A	154[B]	ARG
1	A	172	ARG
1	A	291	LYS
1	B	1	MET
1	C	394	ASP
1	D	172	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	D	307	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADN	D	501	-	18,21,21	0.93	1 (5%)	18,31,31	1.54	4 (22%)
3	NAD	C	502	-	42,48,48	0.89	2 (4%)	50,73,73	1.31	5 (10%)
2	ADN	A	501	-	18,21,21	0.84	0	18,31,31	1.53	2 (11%)
3	NAD	D	502	-	42,48,48	1.04	4 (9%)	50,73,73	1.35	8 (16%)
5	PG4	A	504	-	12,12,12	0.59	0	11,11,11	0.30	0
3	NAD	A	502	-	42,48,48	1.08	4 (9%)	50,73,73	1.39	7 (14%)
6	PEG	B	504	-	6,6,6	0.55	0	5,5,5	0.82	0
3	NAD	B	502	-	42,48,48	0.99	4 (9%)	50,73,73	1.27	6 (12%)
2	ADN	B	501	-	18,21,21	0.94	1 (5%)	18,31,31	1.69	4 (22%)
2	ADN	C	501	-	18,21,21	1.00	2 (11%)	18,31,31	1.53	3 (16%)

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	ADN	D	501	-	-	2/2/22/22	0/3/3/3
3	NAD	C	502	-	-	5/26/62/62	0/5/5/5
2	ADN	A	501	-	-	2/2/22/22	0/3/3/3
3	NAD	D	502	-	-	6/26/62/62	0/5/5/5
5	PG4	A	504	-	-	4/10/10/10	-
3	NAD	A	502	-	-	5/26/62/62	0/5/5/5
6	PEG	B	504	-	-	2/4/4/4	-
3	NAD	B	502	-	-	5/26/62/62	0/5/5/5
2	ADN	B	501	-	-	2/2/22/22	0/3/3/3
2	ADN	C	501	-	-	2/2/22/22	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NAD	C2A-N3A	2.94	1.36	1.32
3	B	502	NAD	C2A-N3A	2.85	1.36	1.32
3	D	502	NAD	O4B-C1B	2.79	1.45	1.41
3	A	502	NAD	O4D-C1D	2.77	1.44	1.41
3	A	502	NAD	C2A-N3A	2.56	1.36	1.32
3	D	502	NAD	C5A-C4A	2.43	1.47	1.40
3	B	502	NAD	O4D-C1D	2.41	1.44	1.41
2	C	501	ADN	C5-C4	2.38	1.47	1.40
3	A	502	NAD	C5A-C4A	2.37	1.47	1.40
3	B	502	NAD	C5A-C4A	2.34	1.47	1.40
3	C	502	NAD	C5A-C4A	2.29	1.47	1.40
3	A	502	NAD	C2N-N1N	2.26	1.37	1.35
2	D	501	ADN	C5-C4	2.25	1.46	1.40
2	C	501	ADN	C2-N3	2.23	1.35	1.32
2	B	501	ADN	C5-C4	2.20	1.46	1.40
3	D	502	NAD	O4D-C1D	2.18	1.44	1.41
3	B	502	NAD	O4B-C1B	2.17	1.44	1.41
3	C	502	NAD	O4D-C1D	2.04	1.43	1.41

All (39) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ADN	N3-C2-N1	-4.14	122.21	128.68
3	C	502	NAD	N3A-C2A-N1A	-4.08	122.30	128.68
3	A	502	NAD	PN-O3-PA	-3.77	119.88	132.83
3	A	502	NAD	N3A-C2A-N1A	-3.75	122.82	128.68
2	B	501	ADN	N3-C2-N1	-3.67	122.94	128.68
3	D	502	NAD	PN-O3-PA	-3.60	120.49	132.83
3	B	502	NAD	N3A-C2A-N1A	-3.46	123.27	128.68
3	C	502	NAD	PN-O3-PA	-3.45	121.00	132.83
2	D	501	ADN	N3-C2-N1	-3.42	123.33	128.68
3	B	502	NAD	PN-O3-PA	-3.30	121.49	132.83
2	C	501	ADN	N3-C2-N1	-3.25	123.61	128.68
3	D	502	NAD	N3A-C2A-N1A	-3.23	123.63	128.68
3	D	502	NAD	C4A-C5A-N7A	-3.19	106.07	109.40
3	D	502	NAD	O4B-C1B-C2B	-3.16	102.31	106.93
3	A	502	NAD	O4D-C1D-C2D	-3.14	102.34	106.93
2	B	501	ADN	O4'-C1'-C2'	-2.87	102.72	106.93
2	A	501	ADN	C1'-N9-C4	-2.77	121.78	126.64
2	C	501	ADN	C4-C5-N7	-2.69	106.60	109.40
3	A	502	NAD	C4A-C5A-N7A	-2.61	106.67	109.40
2	B	501	ADN	C4-C5-N7	-2.56	106.73	109.40
2	D	501	ADN	C4-C5-N7	-2.47	106.82	109.40
3	B	502	NAD	C4A-C5A-N7A	-2.46	106.84	109.40
2	D	501	ADN	C1'-N9-C4	-2.44	122.35	126.64
3	B	502	NAD	C1B-N9A-C4A	-2.41	122.41	126.64
3	C	502	NAD	C4A-C5A-N7A	-2.36	106.94	109.40
3	C	502	NAD	C1B-N9A-C4A	-2.29	122.61	126.64
2	C	501	ADN	C1'-N9-C4	-2.26	122.67	126.64
3	D	502	NAD	C3B-C2B-C1B	2.18	104.27	100.98
3	D	502	NAD	O7N-C7N-N7N	-2.17	119.49	122.58
2	D	501	ADN	C2-N1-C6	2.16	122.45	118.75
2	B	501	ADN	C3'-C2'-C1'	2.16	104.23	100.98
3	D	502	NAD	C3N-C2N-N1N	2.11	122.49	120.43
3	D	502	NAD	C3N-C7N-N7N	2.11	120.28	117.75
3	A	502	NAD	C6N-N1N-C2N	-2.11	120.05	121.97
3	B	502	NAD	C2N-N1N-C1D	-2.10	114.47	119.14
3	C	502	NAD	C2N-N1N-C1D	-2.09	114.48	119.14
3	A	502	NAD	C1B-N9A-C4A	-2.06	123.02	126.64
3	B	502	NAD	C3N-C7N-N7N	2.06	120.22	117.75
3	A	502	NAD	O7N-C7N-N7N	-2.03	119.70	122.58

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NAD	O4D-C1D-N1N-C2N
3	A	502	NAD	O4D-C1D-N1N-C6N
3	A	502	NAD	C2D-C1D-N1N-C2N
3	A	502	NAD	C2D-C1D-N1N-C6N
3	B	502	NAD	O4D-C1D-N1N-C2N
3	B	502	NAD	O4D-C1D-N1N-C6N
3	B	502	NAD	C2D-C1D-N1N-C2N
3	B	502	NAD	C2D-C1D-N1N-C6N
3	C	502	NAD	O4D-C1D-N1N-C2N
3	C	502	NAD	O4D-C1D-N1N-C6N
3	C	502	NAD	C2D-C1D-N1N-C2N
3	C	502	NAD	C2D-C1D-N1N-C6N
3	D	502	NAD	O4D-C1D-N1N-C2N
3	D	502	NAD	O4D-C1D-N1N-C6N
3	D	502	NAD	C2D-C1D-N1N-C2N
3	D	502	NAD	C2D-C1D-N1N-C6N
2	D	501	ADN	C3'-C4'-C5'-O5'
5	A	504	PG4	O2-C3-C4-O3
2	C	501	ADN	C3'-C4'-C5'-O5'
2	A	501	ADN	C3'-C4'-C5'-O5'
6	B	504	PEG	O2-C3-C4-O4
2	C	501	ADN	O4'-C4'-C5'-O5'
2	D	501	ADN	O4'-C4'-C5'-O5'
2	B	501	ADN	C3'-C4'-C5'-O5'
5	A	504	PG4	O1-C1-C2-O2
3	D	502	NAD	O4B-C4B-C5B-O5B
5	A	504	PG4	O3-C5-C6-O4
2	A	501	ADN	O4'-C4'-C5'-O5'
6	B	504	PEG	C4-C3-O2-C2
5	A	504	PG4	C3-C4-O3-C5
3	A	502	NAD	O4B-C4B-C5B-O5B
2	B	501	ADN	O4'-C4'-C5'-O5'
3	B	502	NAD	O4B-C4B-C5B-O5B
3	C	502	NAD	O4B-C4B-C5B-O5B
3	D	502	NAD	C3B-C4B-C5B-O5B

There are no ring outliers.

9 monomers are involved in 6 short contacts:

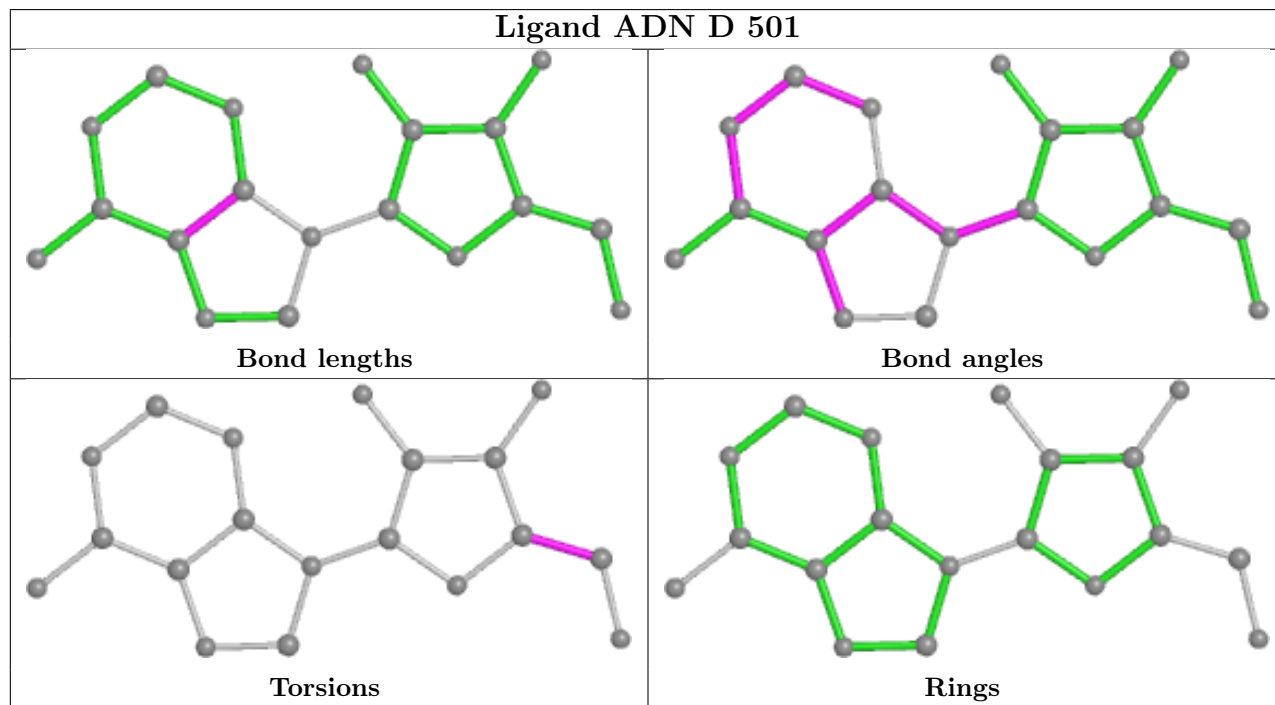
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	ADN	1	0
3	C	502	NAD	2	0
2	A	501	ADN	1	0

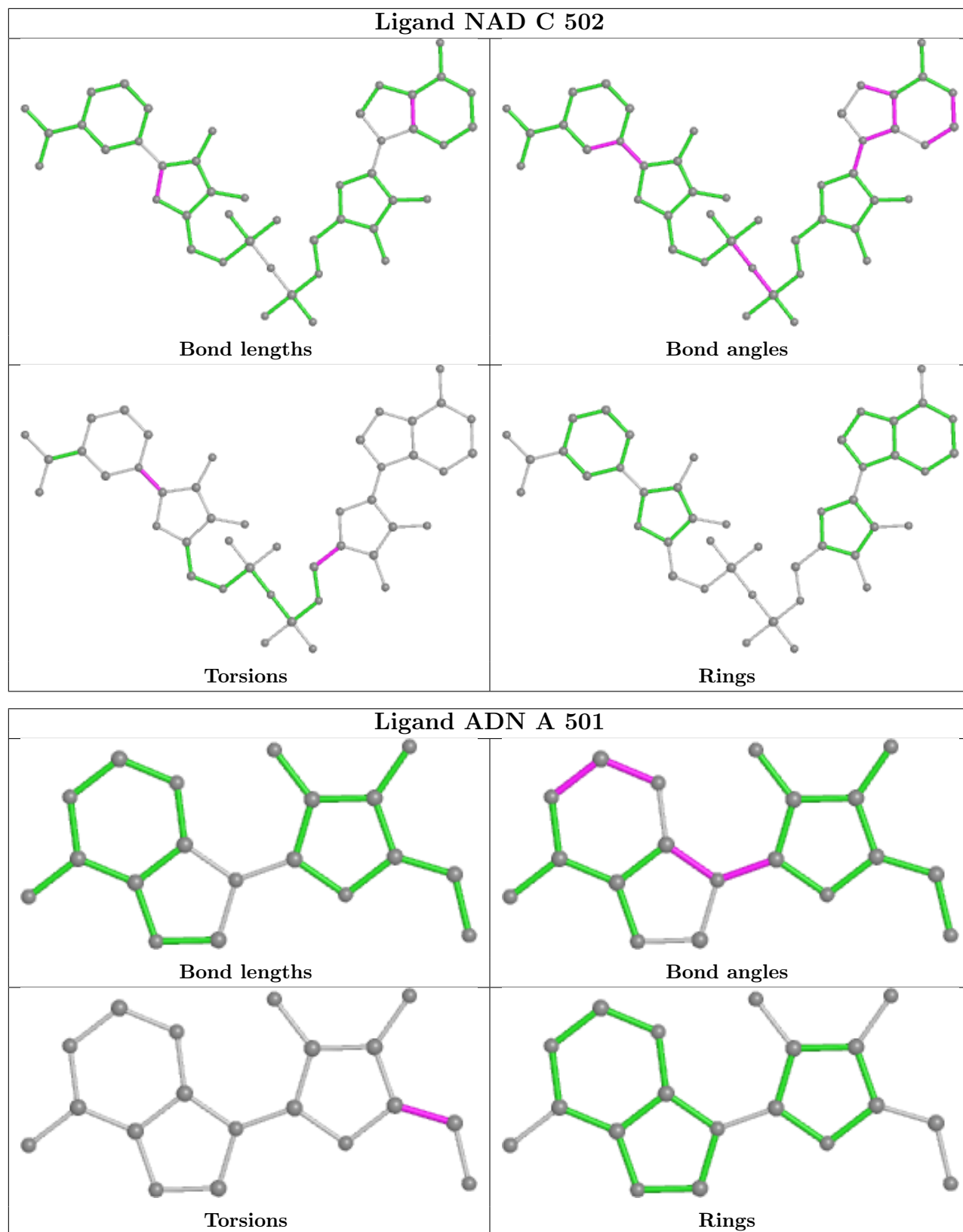
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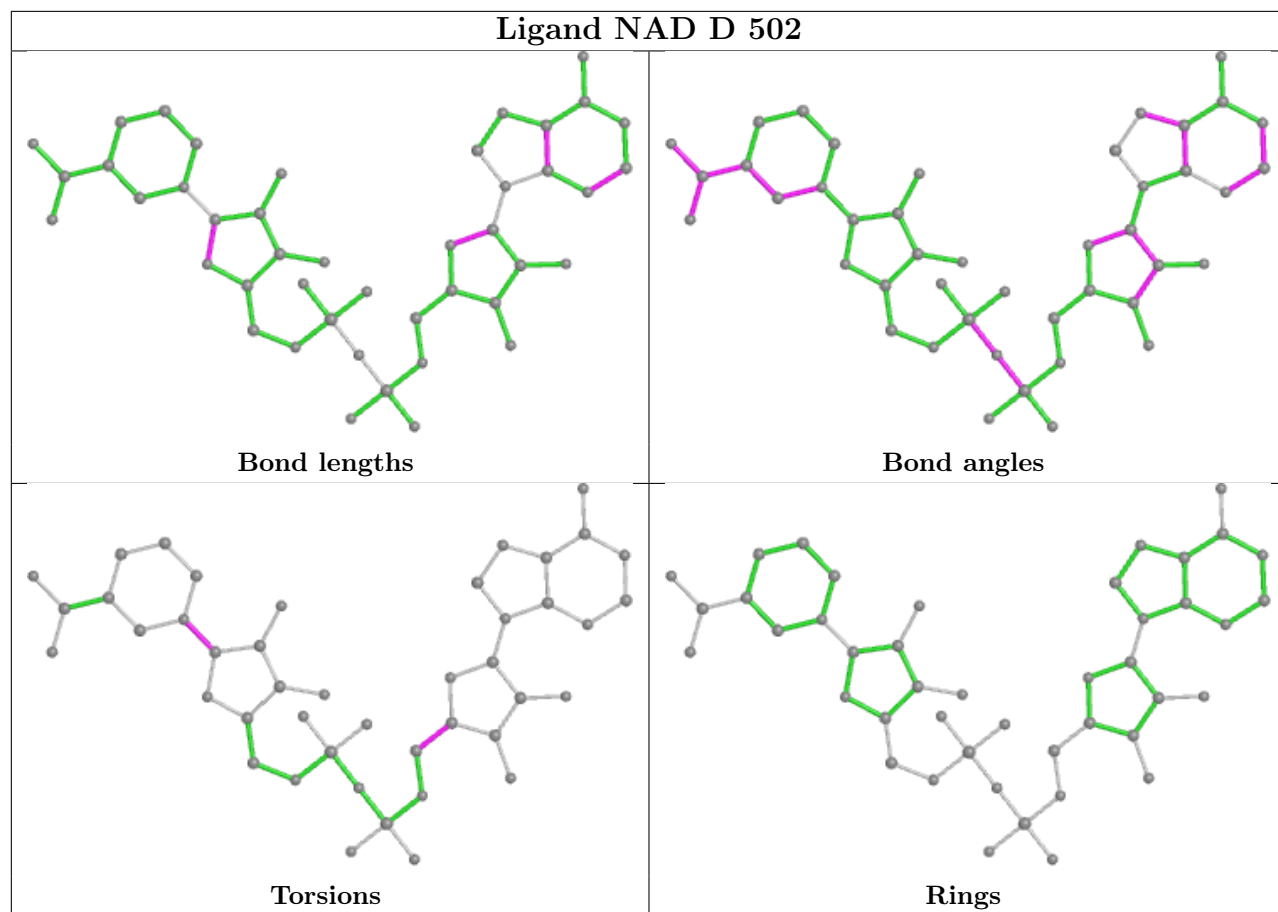
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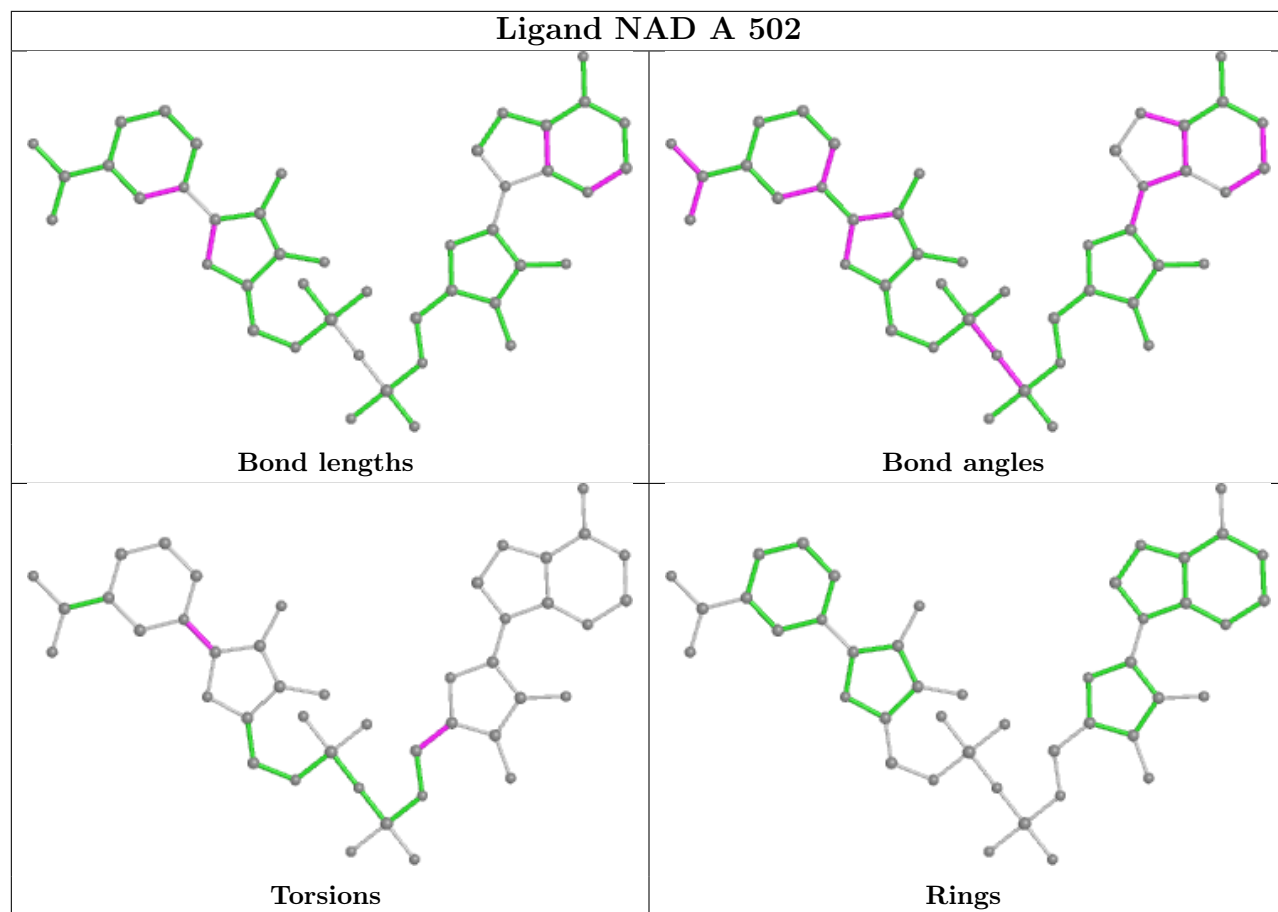
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	NAD	1	0
3	A	502	NAD	1	0
6	B	504	PEG	1	0
3	B	502	NAD	1	0
2	B	501	ADN	1	0
2	C	501	ADN	1	0

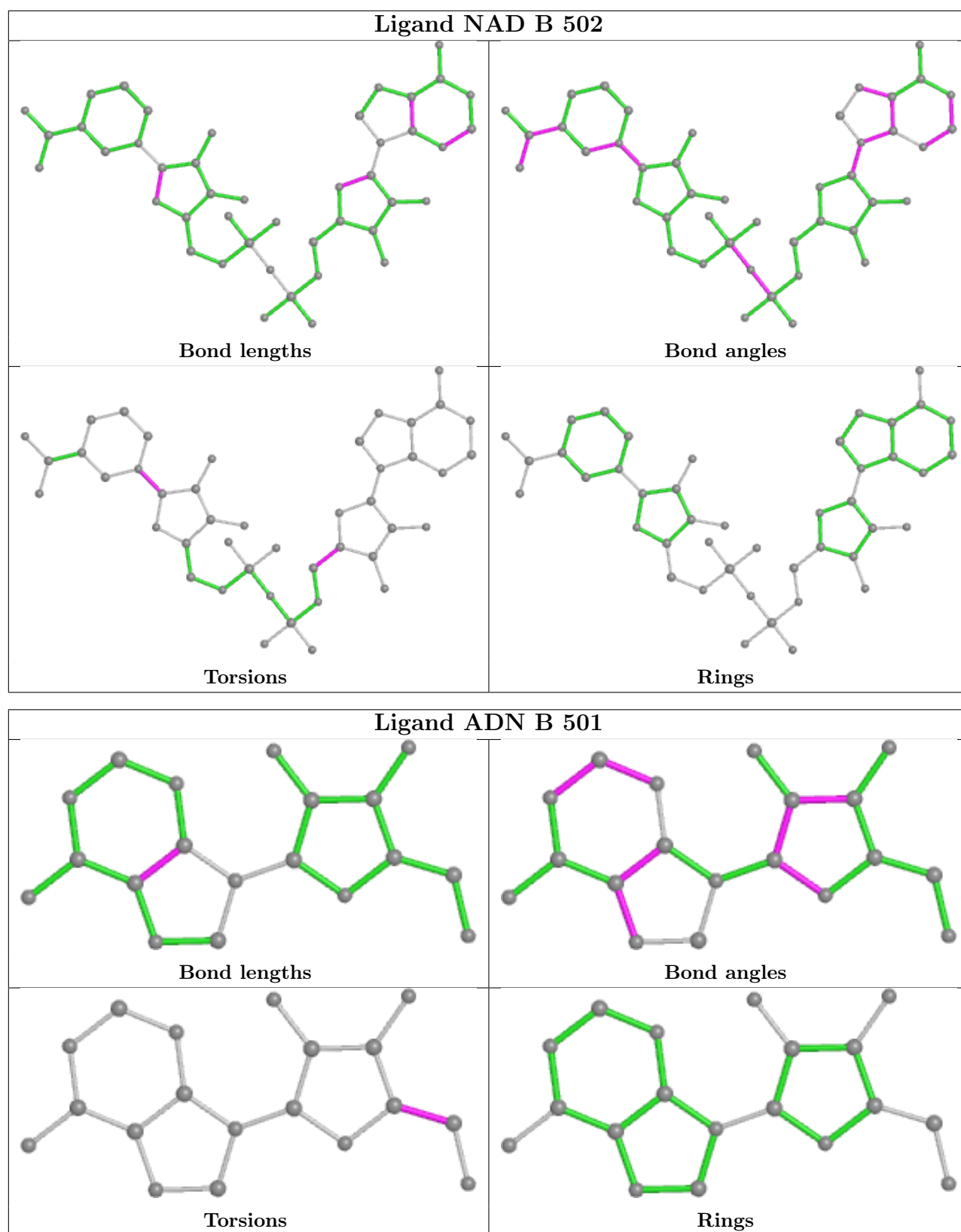
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

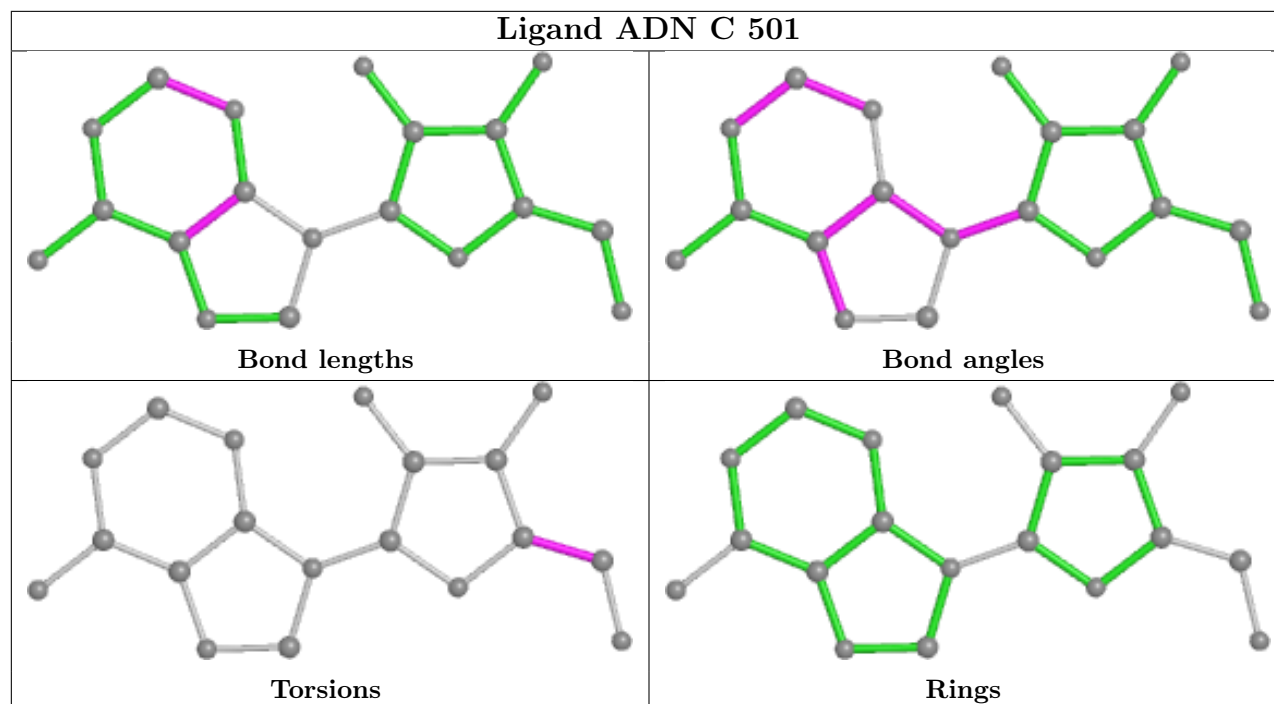












## 5.7 Other polymers [i](#)

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	432/438 (98%)	0.07	16 (3%) 41 48	16, 31, 58, 70	23 (5%)
1	B	435/438 (99%)	-0.09	8 (1%) 68 72	17, 29, 50, 61	14 (3%)
1	C	430/438 (98%)	0.98	89 (20%) 1 1	26, 54, 97, 120	57 (13%)
1	D	435/438 (99%)	0.53	37 (8%) 10 13	27, 47, 79, 107	33 (7%)
All	All	1732/1752 (98%)	0.37	150 (8%) 10 13	16, 39, 80, 120	127 (7%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	174	GLY	6.8
1	C	143	LEU	5.8
1	C	128	LEU	5.6
1	C	49	ALA	5.5
1	C	153	ILE	5.4
1	C	46	LEU	5.3
1	C	166[A]	ARG	5.0
1	C	380	SER	5.0
1	D	380	SER	4.9
1	C	420	ILE	4.7
1	C	127	PRO	4.6
1	C	170[A]	ARG	4.6
1	C	419	TYR	4.4
1	C	180	ALA	4.3
1	C	41	GLY	4.3
1	C	171	GLU	4.1
1	D	173	ASN	4.1
1	D	178	LEU	4.1
1	C	202	LEU	4.0
1	D	46	LEU	4.0
1	C	74	GLU	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	168	LYS	3.9
1	C	384	ASN	3.9
1	C	421	GLY	3.8
1	D	165	LEU	3.8
1	C	174	GLY	3.8
1	D	176	LEU	3.8
1	C	139	THR	3.7
1	C	39	GLU	3.7
1	D	191	LYS	3.7
1	C	378	ASN	3.7
1	C	51	VAL	3.7
1	D	379	SER	3.7
1	C	155	GLY	3.6
1	C	173	ASN	3.6
1	C	203	VAL	3.6
1	C	52	ALA	3.6
1	C	179	PRO	3.5
1	C	149	LEU	3.5
1	C	176	LEU	3.5
1	C	72	GLY	3.5
1	C	318	TYR	3.5
1	D	112	ASP	3.4
1	D	305	PHE	3.4
1	A	169	ASP	3.3
1	D	375	LEU	3.2
1	A	233	ALA	3.2
1	D	1	MET	3.2
1	C	151	LYS	3.2
1	C	154	ARG	3.1
1	A	153	ILE	3.1
1	C	319	GLY	3.1
1	C	126	LYS	3.1
1	C	150	VAL	3.1
1	D	417	ALA	3.0
1	C	313	TRP	3.0
1	D	422	VAL	3.0
1	C	71	LEU	3.0
1	C	195	LYS	3.0
1	D	172	ARG	3.0
1	C	119	LEU	3.0
1	D	233	ALA	3.0
1	C	147	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	5	PHE	2.9
1	D	232	ALA	2.9
1	C	130	MET	2.9
1	A	230	GLY	2.9
1	C	196	TYR	2.8
1	C	385	LYS	2.8
1	D	175	SER	2.8
1	C	121	PHE	2.8
1	D	321	THR	2.8
1	C	48	GLY	2.8
1	C	113	TRP	2.8
1	D	304	HIS	2.8
1	C	168	LYS	2.8
1	B	176	LEU	2.7
1	C	178	LEU	2.7
1	C	42	PRO	2.7
1	C	111	PHE	2.7
1	A	4	THR	2.6
1	D	169	ASP	2.6
1	C	142	VAL	2.6
1	C	382[A]	TYR	2.6
1	A	238	ALA	2.6
1	C	40	PHE	2.6
1	C	152	ASP	2.6
1	D	171	GLU	2.6
1	D	238	ALA	2.6
1	C	376	TRP	2.6
1	C	69	ILE	2.5
1	C	192	PHE	2.5
1	D	376	TRP	2.5
1	A	237	GLY	2.5
1	C	198	CYS	2.5
1	C	75	VAL	2.5
1	A	175	SER	2.5
1	C	169	ASP	2.5
1	A	74	GLU	2.5
1	C	165	LEU	2.4
1	D	235	LEU	2.4
1	D	283	ASN	2.4
1	A	235	LEU	2.4
1	C	235	LEU	2.4
1	C	115	ILE	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	418	ALA	2.4
1	C	233	ALA	2.4
1	C	390	PRO	2.4
1	C	370	ILE	2.4
1	D	423	THR	2.4
1	A	202	LEU	2.3
1	D	150	VAL	2.3
1	C	172	ARG	2.3
1	C	197	GLY	2.3
1	C	67	THR	2.3
1	C	47	LYS	2.3
1	A	172	ARG	2.3
1	C	99	SER	2.3
1	C	379	SER	2.3
1	C	141	MET	2.3
1	C	372	GLN	2.3
1	D	192	PHE	2.3
1	C	108	GLU	2.3
1	C	383	GLU	2.3
1	B	232	ALA	2.2
1	C	144	ASP	2.2
1	D	143	LEU	2.2
1	C	148	GLU	2.2
1	C	387	TYR	2.2
1	B	202	LEU	2.2
1	C	129	ASN	2.2
1	D	385	LYS	2.2
1	B	152	ASP	2.2
1	A	150	VAL	2.1
1	C	45	PRO	2.1
1	D	335	ASP	2.1
1	C	120	PHE	2.1
1	C	231	SER	2.1
1	B	233	ALA	2.1
1	D	156	ILE	2.1
1	B	177	VAL	2.1
1	B	237	GLY	2.1
1	A	201	SER	2.0
1	B	235	LEU	2.0
1	A	152	ASP	2.0
1	C	145	ARG	2.0
1	C	232	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	164	VAL	2.0
1	C	425	ASP	2.0
1	D	177	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

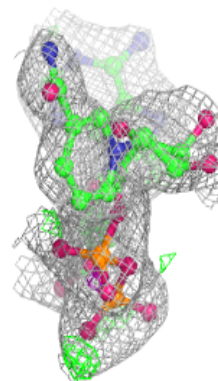
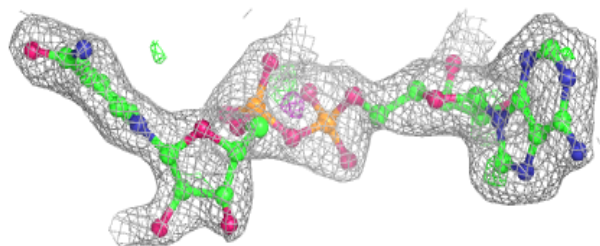
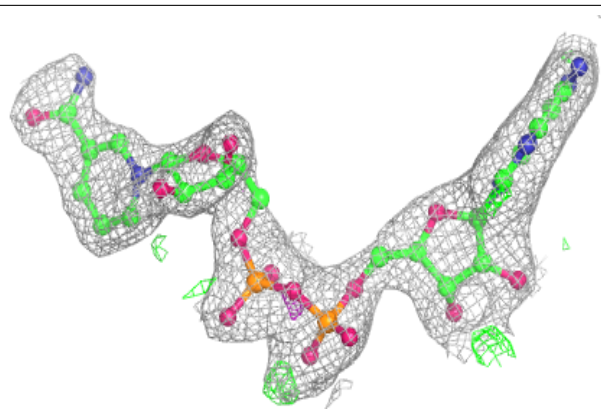
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	PG4	A	504	13/13	0.70	0.17	68,69,71,71	0
6	PEG	B	504	7/7	0.79	0.28	55,55,56,57	0
3	NAD	D	502	44/44	0.90	0.14	35,49,59,60	0
3	NAD	C	502	44/44	0.91	0.12	34,46,55,59	0
2	ADN	B	501	19/19	0.91	0.13	24,26,37,39	0
2	ADN	C	501	19/19	0.92	0.11	34,38,49,52	0
2	ADN	D	501	19/19	0.92	0.12	34,40,56,56	0
3	NAD	A	502	44/44	0.93	0.11	21,31,35,38	0
3	NAD	B	502	44/44	0.93	0.11	18,33,38,42	0
2	ADN	A	501	19/19	0.94	0.12	22,25,36,41	0
4	NA	C	503	1/1	0.98	0.22	41,41,41,41	0
4	NA	D	503	1/1	0.98	0.09	42,42,42,42	0
4	NA	A	503	1/1	0.98	0.10	26,26,26,26	0
4	NA	B	503	1/1	0.98	0.14	27,27,27,27	0

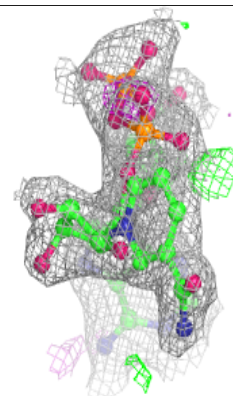
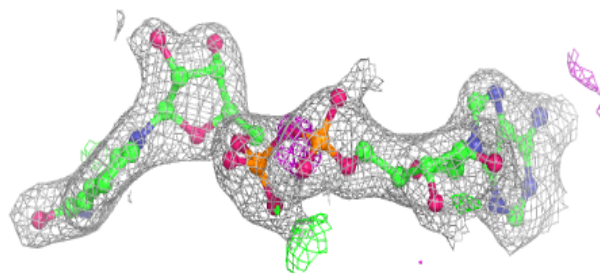
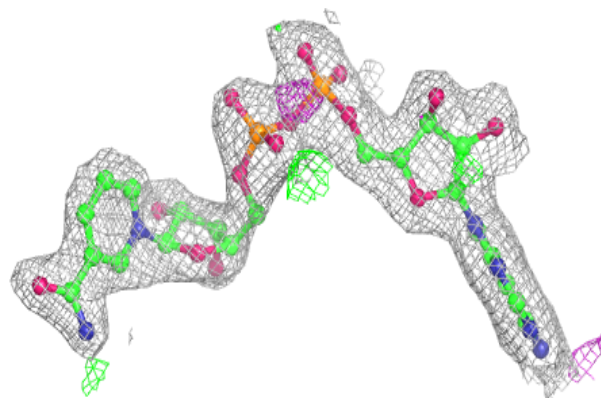
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD 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)

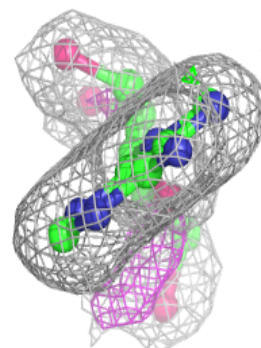
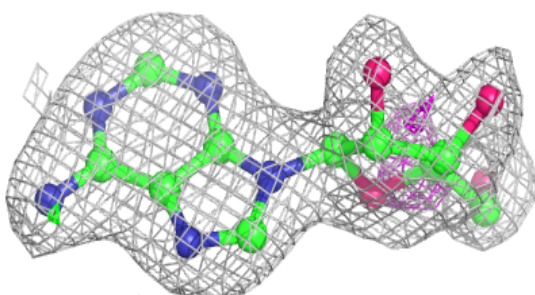
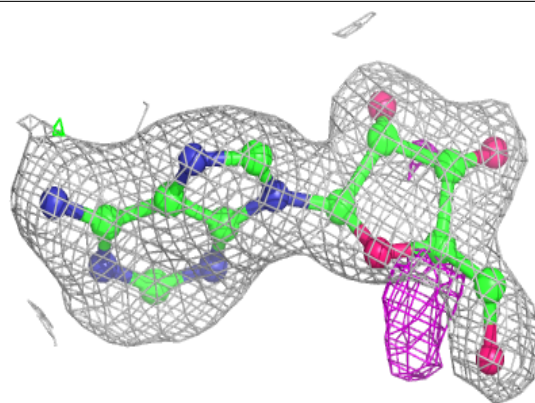
**Electron density around NAD C 502:**

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

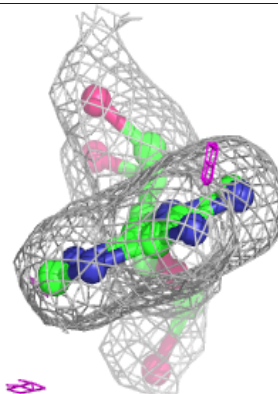
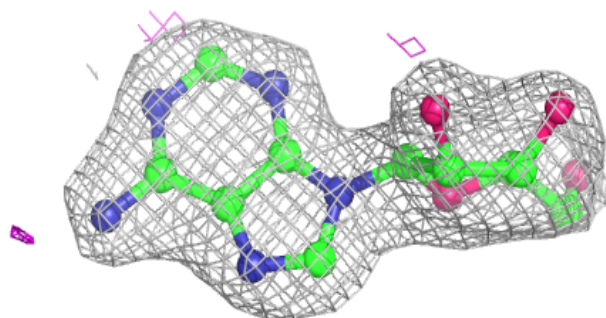
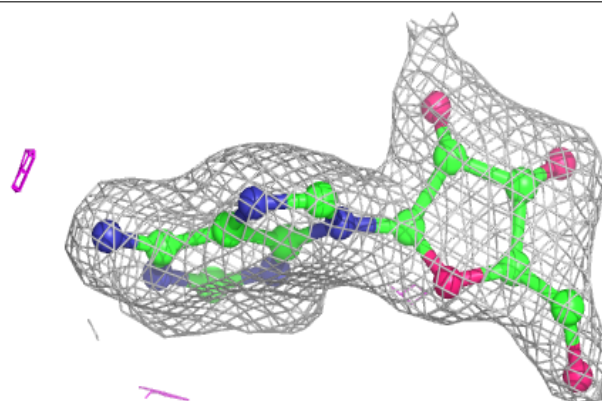


**Electron density around ADN B 501:**

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

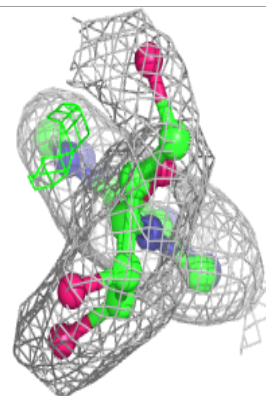
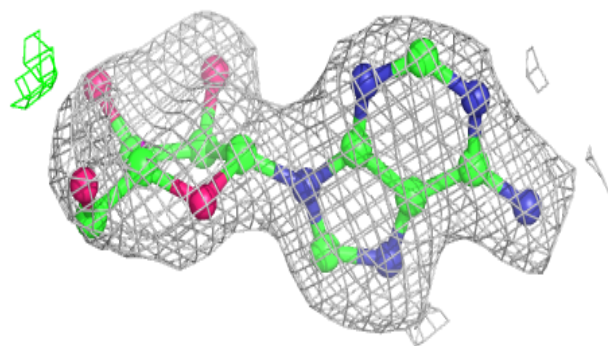
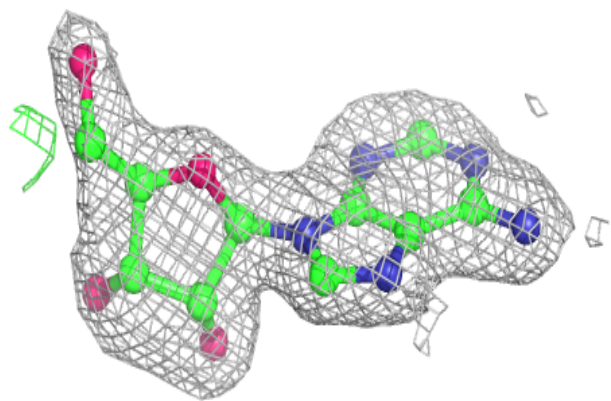
**Electron density around ADN C 501:**

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

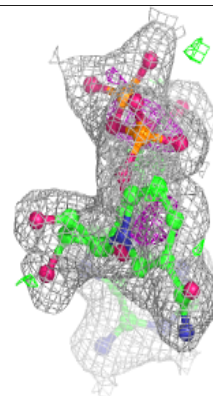
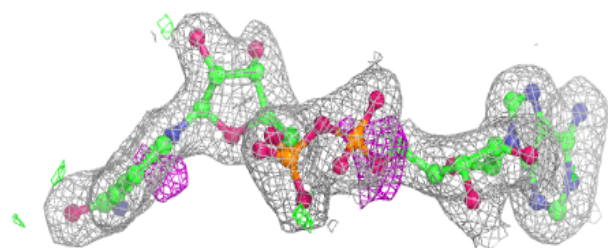
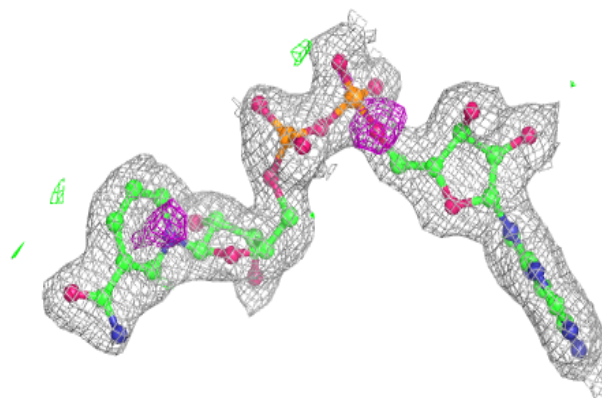


**Electron density around ADN D 501:**

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

**Electron density around NAD A 502:**

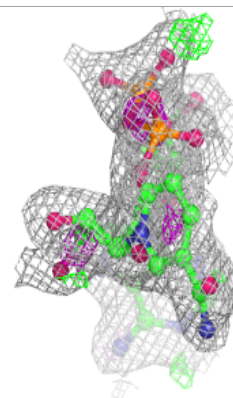
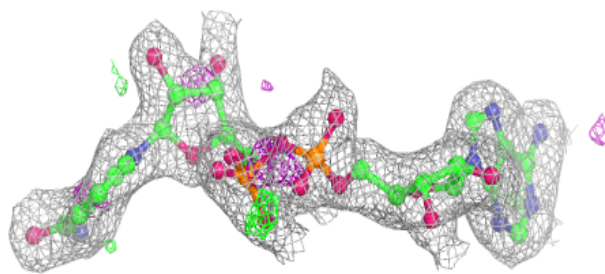
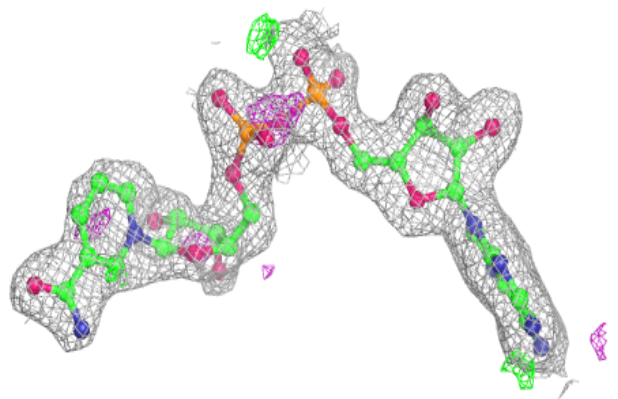
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



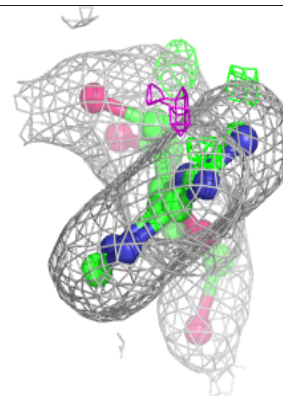
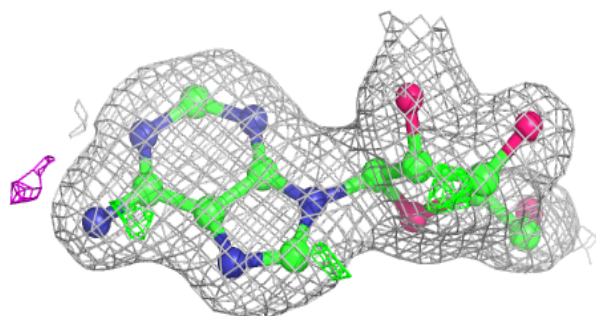
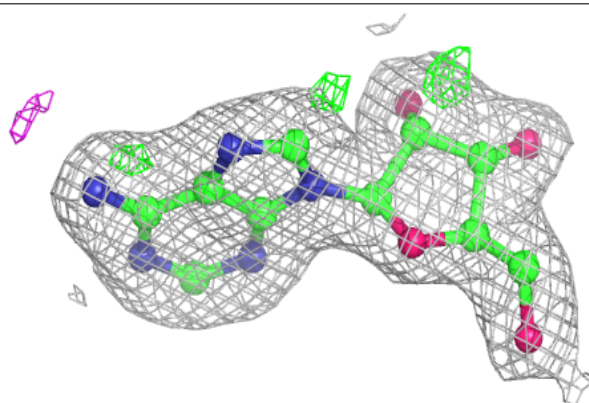


**Electron density around NAD B 502:**

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

**Electron density around ADN 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.