



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:58 am BST

PDB ID : 5M5K  
Title : S-adenosyl-L-homocysteine hydrolase from *Bradyrhizobium elkanii* in complex with adenosine and cordycepin  
Authors : Manszewski, T.; Mueller-Dieckmann, J.; Jaskolski, M.  
Deposited on : 2016-10-21  
Resolution : 1.84 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 : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

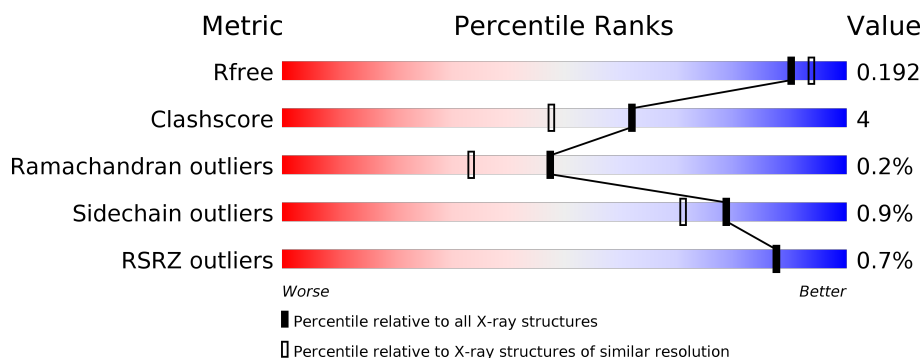
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	479	<div> <div>89%</div> <div>7% ..</div> </div>
1	B	479	<div> <div>92%</div> <div>5% ..</div> </div>
1	C	479	<div> <div>%</div> <div>89%</div> <div>9% .</div> </div>
1	D	479	<div> <div>%</div> <div>89%</div> <div>9% .</div> </div>

2 Entry composition ⓘ

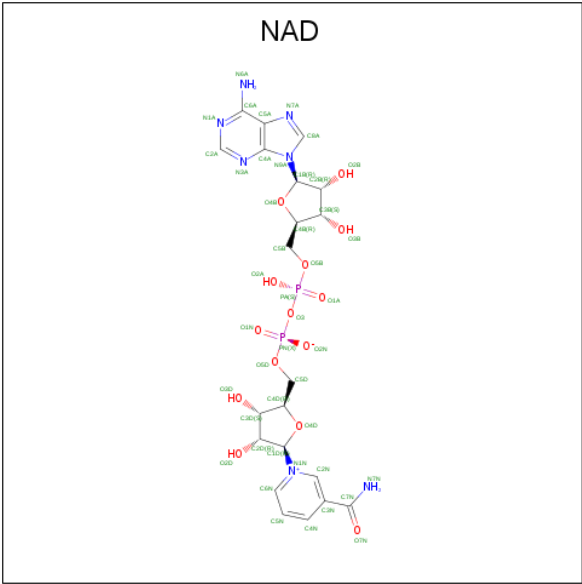
There are 9 unique types of molecules in this entry. The entry contains 16474 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	468	Total	C	N	O	S	0	8	0
			3670	2329	634	686	21			
1	B	468	Total	C	N	O	S	0	9	0
			3667	2325	629	692	21			
1	C	471	Total	C	N	O	S	0	10	0
			3696	2346	637	692	21			
1	D	468	Total	C	N	O	S	0	8	0
			3669	2322	634	691	22			

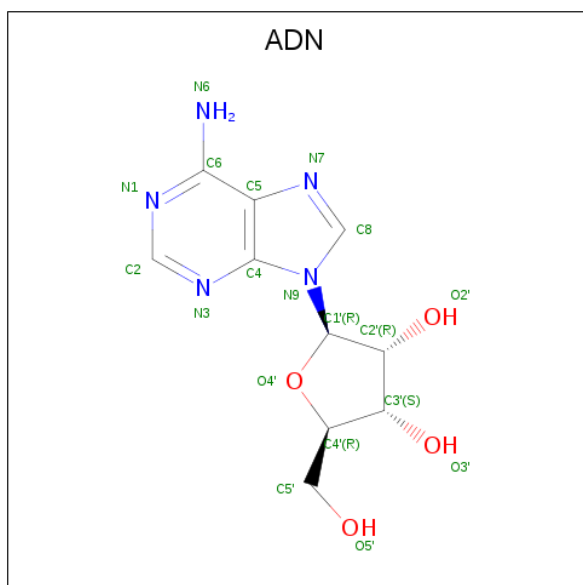
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

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

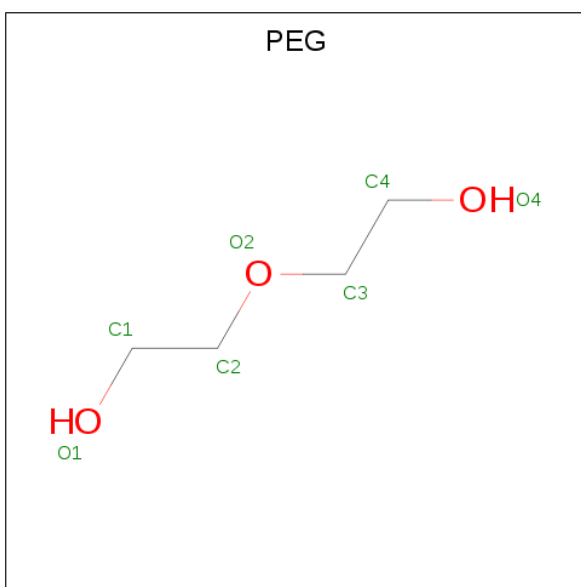


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	0
			19	10	5	4		
3	C	1	Total	C	N	O	0	0
			19	10	5	4		

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

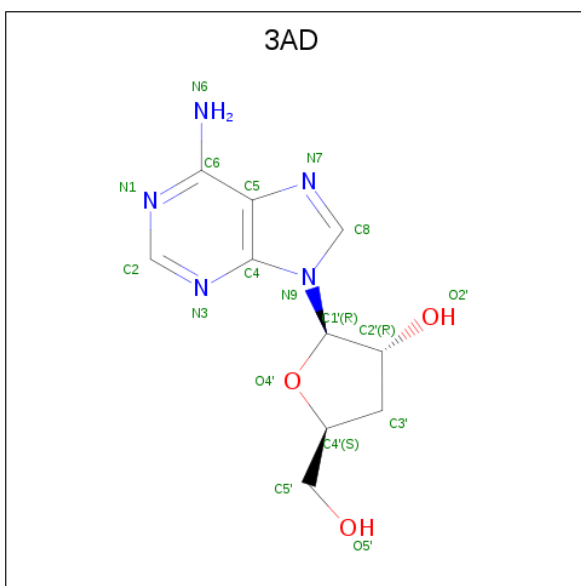
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



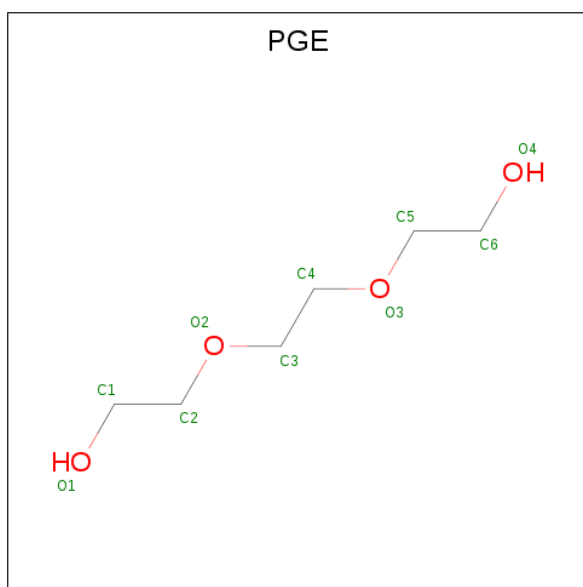
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is 3'-DEOXYADENOSINE (three-letter code: 3AD) (formula:  $\text{C}_{10}\text{H}_{13}\text{N}_5\text{O}_3$ ).



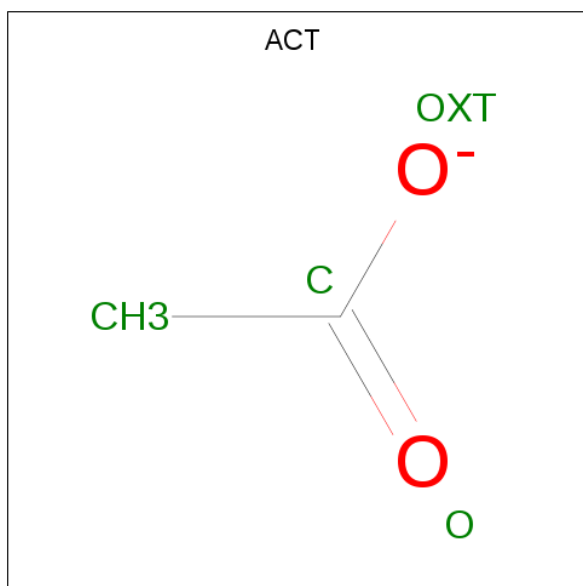
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $\text{C}_6\text{H}_{14}\text{O}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

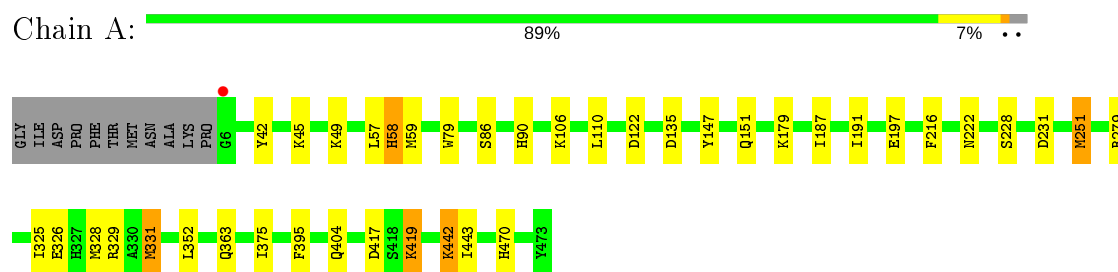
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	364	Total 364	O 364	0	0
9	B	395	Total 395	O 395	0	0
9	C	360	Total 360	O 360	0	0
9	D	371	Total 371	O 371	0	0

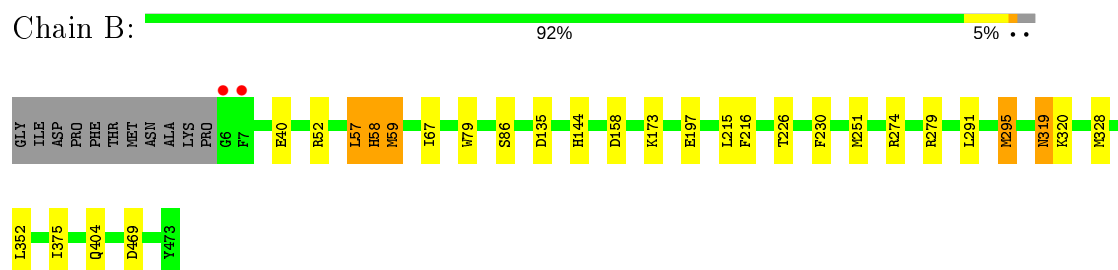
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

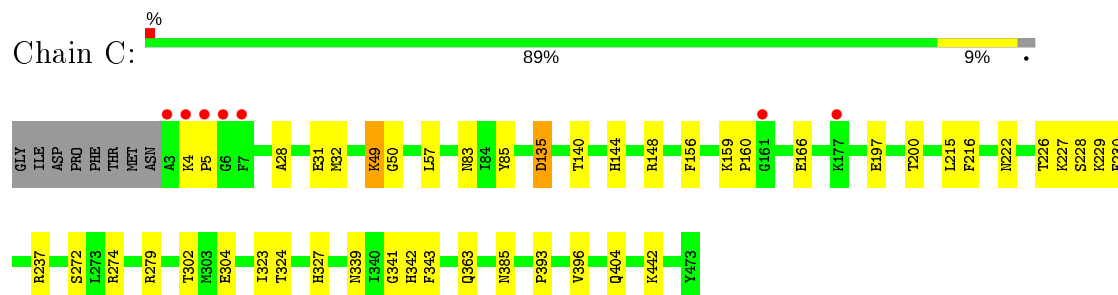
#### • Molecule 1: Adenosylhomocysteinase



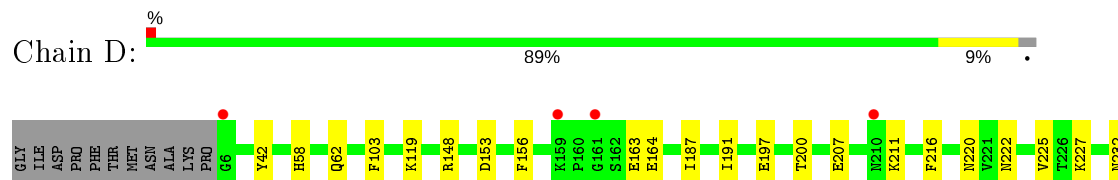
#### • Molecule 1: Adenosylhomocysteinase



#### • Molecule 1: Adenosylhomocysteinase



#### • Molecule 1: Adenosylhomocysteinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.16 Å   176.28 Å   102.35 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	47.82 – 1.84 47.82 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.82-1.84) 98.6 (47.82-1.83)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 1.83 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.146   ,   0.192 0.146   ,   0.192	Depositor DCC
$R_{free}$ test set	1243 reflections (0.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16474	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.99% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, NAD, NA, 3AD, ACT, ADN, 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	0.67	0/3762	0.77	3/5076 (0.1%)
1	B	0.68	0/3762	0.80	5/5080 (0.1%)
1	C	0.69	0/3795	0.77	1/5121 (0.0%)
1	D	0.69	0/3758	0.77	3/5072 (0.1%)
All	All	0.68	0/15077	0.78	12/20349 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	446	LYS	CD-CE-NZ	-10.69	87.12	111.70
1	B	59	MET	CG-SD-CE	9.75	115.80	100.20
1	A	331	MET	CG-SD-CE	9.25	115.00	100.20
1	A	251	MET	CG-SD-CE	8.68	114.08	100.20
1	D	390	MET	CG-SD-CE	7.67	112.47	100.20
1	D	446	LYS	CA-CB-CG	-6.23	99.69	113.40
1	B	52	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	295	MET	CG-SD-CE	5.71	109.34	100.20
1	A	231	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	274	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	135	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	469	ASP	CB-CG-OD1	5.32	123.08	118.30

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	3670	0	3713	33	0
1	B	3667	0	3695	29	0
1	C	3696	0	3745	38	0
1	D	3669	0	3688	36	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	1	0
3	A	19	0	13	2	0
3	B	19	0	13	2	0
3	C	19	0	13	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	7	0	10	0	0
5	B	7	0	10	0	0
6	D	18	0	13	2	0
7	D	10	0	14	0	0
8	D	4	0	3	0	0
9	A	364	0	0	4	0
9	B	395	0	0	3	0
9	C	360	0	0	7	0
9	D	371	0	0	5	0
All	All	16474	0	15034	132	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 4.

All (132) 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:A:251:MET:HE2	1:C:393:PRO:HB2	1.49	0.95
1:B:59:MET:CE	1:B:79:TRP:CD1	2.59	0.84
1:A:328:MET:HG2	1:A:331:MET:HE1	1.59	0.84
1:A:331:MET:HE3	1:A:375:ILE:HG21	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:MET:CE	1:A:375:ILE:HG21	2.08	0.83
1:C:49:LYS:HD2	1:C:50:GLY:N	1.97	0.79
1:C:144:HIS:HE1	1:C:215:LEU:H	1.32	0.77
1:A:251:MET:HE2	1:C:393:PRO:CB	2.15	0.77
1:B:59:MET:HE2	1:B:79:TRP:CD1	2.20	0.77
1:D:207:GLU:O	1:D:211:LYS:HD3	1.86	0.76
1:C:385:ASN:HD21	2:C:501:NAD:H72N	1.34	0.76
1:B:279[A]:ARG:NH2	9:B:602:HOH:O	2.20	0.73
1:D:324:THR:H	1:D:327:HIS:HD2	1.34	0.73
1:B:328:MET:HE2	1:B:375:ILE:CD1	2.20	0.72
1:B:328:MET:HE2	1:B:375:ILE:HD11	1.72	0.72
1:D:324:THR:H	1:D:327:HIS:CD2	2.08	0.70
1:A:59:MET:CE	1:A:79:TRP:CD1	2.77	0.68
1:A:442[A]:LYS:HE3	9:C:656:HOH:O	1.94	0.67
1:D:197:GLU:HB2	1:D:227:LYS:HE3	1.79	0.65
1:B:319:ASN:HD22	1:B:320:LYS:H	1.46	0.64
1:C:159:LYS:HD3	9:C:723:HOH:O	1.97	0.64
1:D:279[A]:ARG:NH1	9:D:603:HOH:O	2.31	0.63
1:C:339:ASN:ND2	1:C:341:GLY:H	1.96	0.62
1:C:49:LYS:HD2	1:C:50:GLY:H	1.62	0.62
1:D:103:PHE:CE2	1:D:119:LYS:HE3	2.35	0.61
1:C:200[A]:THR:HG22	9:C:875:HOH:O	2.01	0.61
1:B:59:MET:HE3	1:B:79:TRP:CD1	2.36	0.60
1:A:331:MET:HE2	1:A:375:ILE:HG21	1.84	0.60
1:C:83:ASN:ND2	1:C:85:TYR:H	1.99	0.60
2:A:501:NAD:C4N	3:A:502:ADN:H3'	2.31	0.60
1:C:140:THR:O	1:C:144:HIS:HD2	1.83	0.60
1:A:279[A]:ARG:NH1	9:A:603:HOH:O	2.34	0.60
1:A:331:MET:HE3	1:A:375:ILE:CG2	2.31	0.58
1:C:279[B]:ARG:NH1	9:C:604:HOH:O	2.36	0.58
1:A:417:ASP:OD1	1:A:419:LYS:NZ	2.37	0.58
1:C:324:THR:H	1:C:327:HIS:CD2	2.22	0.57
1:B:251:MET:HE1	1:D:395:PHE:CD1	2.39	0.57
1:D:304:GLU:OE2	1:D:327:HIS:HE1	1.87	0.57
1:A:58:HIS:HD2	1:A:86:SER:OG	1.88	0.57
1:C:83:ASN:HD22	1:C:85:TYR:H	1.51	0.57
1:B:319:ASN:ND2	1:B:320:LYS:H	2.03	0.56
1:D:200:THR:HG23	9:D:848:HOH:O	2.04	0.56
1:A:328:MET:HG2	1:A:331:MET:CE	2.33	0.56
1:B:328:MET:CE	1:B:375:ILE:CD1	2.84	0.56
1:D:62:GLN:NE2	6:D:502:3AD:HN62	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:HIS:HE1	3:B:502:ADN:O5'	1.89	0.55
1:A:251:MET:HE2	1:C:393:PRO:CG	2.36	0.55
1:D:42:TYR:OH	1:D:434:LYS:NZ	2.40	0.55
1:B:135:ASP:OD2	1:B:197:GLU:HG2	2.05	0.55
1:B:58:HIS:HD2	1:B:86:SER:OG	1.89	0.55
1:B:251:MET:CE	1:D:395:PHE:CD1	2.90	0.55
2:C:501:NAD:C4N	3:C:502:ADN:H3'	2.37	0.54
1:A:197:GLU:HB2	1:A:404:GLN:HE21	1.73	0.54
1:C:49:LYS:C	1:C:49:LYS:HD2	2.26	0.54
1:A:49:LYS:NZ	9:A:602:HOH:O	2.33	0.54
1:B:197:GLU:HB2	1:B:404:GLN:HE21	1.72	0.53
1:B:279[A]:ARG:NH1	9:B:610:HOH:O	2.39	0.53
1:C:144:HIS:CE1	1:C:215:LEU:H	2.21	0.53
1:C:237:ARG:HA	1:C:272:SER:HB2	1.91	0.52
1:D:446:LYS:HE2	9:D:804:HOH:O	2.08	0.52
1:D:207:GLU:HG3	1:D:211:LYS:HE2	1.92	0.52
1:A:57:LEU:HG	1:A:135:ASP:HB2	1.91	0.51
2:B:501:NAD:C4N	3:B:502:ADN:H3'	2.40	0.51
1:D:207:GLU:O	1:D:211:LYS:CD	2.58	0.51
1:D:417:ASP:OD1	1:D:419:LYS:NZ	2.39	0.51
1:A:326:GLU:HG3	9:A:644:HOH:O	2.11	0.50
1:B:328:MET:HE1	1:B:352:LEU:HD11	1.93	0.50
1:B:40:GLU:OE1	9:B:601:HOH:O	2.19	0.50
1:C:197:GLU:HB2	1:C:404:GLN:HE21	1.77	0.50
1:C:302:THR:HG23	1:D:446:LYS:HG2	1.94	0.50
1:A:442[A]:LYS:HG2	1:A:443:ILE:HG23	1.94	0.49
1:D:187:ILE:O	1:D:191:ILE:HG12	2.12	0.49
1:C:222:ASN:HA	1:C:227:LYS:HD2	1.92	0.49
1:C:274[B]:ARG:HD2	9:C:751:HOH:O	2.12	0.49
1:A:58:HIS:HE1	3:A:502:ADN:O5'	1.94	0.49
1:D:350:ALA:O	1:D:353:ARG:HG2	2.13	0.48
1:C:222:ASN:O	1:C:228:SER:HB3	2.13	0.48
1:D:227:LYS:C	1:D:227:LYS:HD3	2.33	0.48
1:C:28:ALA:O	1:C:32:MET:HG3	2.13	0.48
1:A:147:TYR:O	1:A:151:GLN:HG2	2.14	0.48
1:C:226:THR:HA	1:C:230:PHE:CD1	2.49	0.48
1:C:363:GLN:NE2	9:C:607:HOH:O	2.39	0.48
1:D:163:GLU:HG3	1:D:164:GLU:N	2.29	0.48
1:A:251:MET:HE3	1:C:396:VAL:H	1.78	0.47
1:B:59:MET:HE1	1:B:67:ILE:HD11	1.96	0.47
1:D:422:LYS:O	1:D:423:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279[B]:ARG:NH2	9:C:617:HOH:O	2.48	0.47
1:D:220:ASN:OD1	1:D:222:ASN:HB3	2.15	0.47
1:B:59:MET:CE	1:B:67:ILE:HD11	2.44	0.47
1:C:57:LEU:HG	1:C:135:ASP:HB2	1.95	0.47
1:C:323:ILE:HA	1:C:327:HIS:HD2	1.79	0.47
1:A:122:ASP:OD1	1:A:179:LYS:NZ	2.43	0.46
1:D:232:ASN:OD1	2:D:501:NAD:H5N	2.16	0.46
1:C:342:HIS:CD2	1:C:343:PHE:CD2	3.03	0.46
1:D:274[A]:ARG:HD2	9:D:864:HOH:O	2.16	0.46
1:D:207:GLU:CG	1:D:211:LYS:HE2	2.46	0.46
1:B:144:HIS:CD2	1:B:215:LEU:HG	2.51	0.45
1:D:324:THR:N	1:D:327:HIS:HD2	2.10	0.45
1:C:31:GLU:OE2	1:C:442[B]:LYS:NZ	2.48	0.45
1:D:148:ARG:HD2	1:D:153:ASP:OD2	2.17	0.45
1:A:42:TYR:HA	1:A:45:LYS:HD3	1.97	0.45
1:D:339:ASN:ND2	1:D:341:GLY:H	2.15	0.45
1:B:291:LEU:O	1:B:295:MET:HG2	2.17	0.44
1:A:197:GLU:HB2	1:A:404:GLN:NE2	2.33	0.44
1:B:57:LEU:HG	1:B:135:ASP:HB2	2.00	0.44
1:A:187:ILE:O	1:A:191:ILE:HG12	2.17	0.44
1:C:304:GLU:OE2	1:C:327:HIS:HE1	2.00	0.44
1:A:470[B]:HIS:HD2	9:A:833:HOH:O	2.01	0.43
1:C:4:LYS:HB3	1:C:5:PRO:HD3	2.00	0.43
1:A:395:PHE:CD1	1:A:442[A]:LYS:HD3	2.53	0.43
1:D:62:GLN:HE21	6:D:502:3AD:HN62	1.65	0.43
1:D:211:LYS:N	1:D:211:LYS:HD3	2.34	0.43
1:B:328:MET:CE	1:B:352:LEU:HD11	2.49	0.42
1:C:342:HIS:HD2	1:C:343:PHE:CD2	2.37	0.42
1:D:148:ARG:HG2	1:D:156:PHE:CE1	2.54	0.42
1:A:106:LYS:HE3	1:A:363:GLN:NE2	2.34	0.42
1:D:292:GLN:O	1:D:296:GLU:HG2	2.20	0.42
1:B:319:ASN:HD22	1:B:320:LYS:N	2.15	0.42
1:C:324:THR:H	1:C:327:HIS:HD2	1.63	0.42
1:B:158:ASP:OD1	1:B:173:LYS:NZ	2.37	0.41
1:C:148:ARG:HG2	1:C:156:PHE:CE1	2.55	0.41
1:D:442:LYS:HE2	9:D:900:HOH:O	2.20	0.41
1:C:160:PRO:CB	1:C:166:GLU:HG2	2.50	0.41
1:B:328:MET:HE3	1:B:375:ILE:HD12	2.03	0.41
1:A:325[A]:ILE:HD13	1:A:352:LEU:HD23	2.03	0.40
1:D:225:VAL:HG21	1:D:473:TYR:CE1	2.56	0.40
1:B:226:THR:HA	1:B:230:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HA	1:A:110:LEU:HD23	1.94	0.40
1:A:222:ASN:O	1:A:228:SER:HB3	2.21	0.40
1:B:328:MET:CE	1:B:375:ILE:HD12	2.51	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	474/479 (99%)	463 (98%)	10 (2%)	1 (0%)	47	33
1	B	475/479 (99%)	461 (97%)	13 (3%)	1 (0%)	47	33
1	C	479/479 (100%)	462 (96%)	17 (4%)	0	100	100
1	D	474/479 (99%)	464 (98%)	9 (2%)	1 (0%)	47	33
All	All	1902/1916 (99%)	1850 (97%)	49 (3%)	3 (0%)	47	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	58	HIS
1	A	58	HIS
1	B	58	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	386/387 (100%)	381 (99%)	5 (1%)	69	58
1	B	387/387 (100%)	384 (99%)	3 (1%)	81	75
1	C	390/387 (101%)	387 (99%)	3 (1%)	81	75
1	D	386/387 (100%)	383 (99%)	3 (1%)	81	75
All	All	1549/1548 (100%)	1535 (99%)	14 (1%)	78	71

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	216	PHE
1	A	419	LYS
1	A	442[A]	LYS
1	A	442[B]	LYS
1	B	57	LEU
1	B	216	PHE
1	B	319	ASN
1	C	49	LYS
1	C	216	PHE
1	C	229	LYS
1	D	216	PHE
1	D	252	LEU
1	D	419	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	58	HIS
1	A	363	GLN
1	B	58	HIS
1	B	319	ASN
1	C	83	ASN
1	C	144	HIS
1	C	327	HIS
1	C	339	ASN
1	C	403	ASN
1	C	462	GLN
1	D	46	GLN
1	D	62	GLN

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Mol	Chain	Res	Type
1	D	327	HIS
1	D	339	ASN
1	D	345	ASN
1	D	408	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAD	B	501	-	42,48,48	1.83	9 (21%)	50,73,73	1.64	10 (20%)
7	PGE	D	503	-	9,9,9	0.70	0	8,8,8	1.51	1 (12%)
3	ADN	C	502	-	18,21,21	1.19	2 (11%)	18,31,31	1.52	3 (16%)
3	ADN	A	502	-	18,21,21	0.98	1 (5%)	18,31,31	1.77	3 (16%)
2	NAD	C	501	-	42,48,48	1.81	10 (23%)	50,73,73	1.66	7 (14%)
8	ACT	D	504	-	1,3,3	1.68	0	0,3,3	0.00	-
2	NAD	A	501	-	42,48,48	1.82	11 (26%)	50,73,73	1.61	9 (18%)
6	3AD	D	502	-	17,20,20	1.83	3 (17%)	16,29,29	1.70	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	B	504	-	6,6,6	0.59	0	5,5,5	0.76	0
5	PEG	A	504	-	6,6,6	0.60	0	5,5,5	0.90	0
2	NAD	D	501	-	42,48,48	1.85	12 (28%)	50,73,73	1.51	7 (14%)
3	ADN	B	502	-	18,21,21	1.01	2 (11%)	18,31,31	1.47	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	NAD	B	501	-	-	5/26/62/62	0/5/5/5
7	PGE	D	503	-	-	3/7/7/7	-
3	ADN	C	502	-	-	0/2/22/22	0/3/3/3
3	ADN	A	502	-	-	0/2/22/22	0/3/3/3
2	NAD	C	501	-	-	5/26/62/62	0/5/5/5
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
6	3AD	D	502	-	-	1/2/18/18	0/3/3/3
5	PEG	B	504	-	-	3/4/4/4	-
5	PEG	A	504	-	-	2/4/4/4	-
2	NAD	D	501	-	-	5/26/62/62	0/5/5/5
3	ADN	B	502	-	-	0/2/22/22	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	502	3AD	C2'-C1'	-5.70	1.48	1.54
2	D	501	NAD	C7N-N7N	5.08	1.42	1.33
2	A	501	NAD	C2B-C1B	-4.66	1.46	1.53
2	B	501	NAD	C2B-C1B	-4.22	1.47	1.53
2	B	501	NAD	C7N-N7N	3.97	1.40	1.33
2	B	501	NAD	C5N-C4N	3.90	1.47	1.38
2	C	501	NAD	C5N-C4N	3.83	1.47	1.38
2	C	501	NAD	C2B-C3B	-3.73	1.43	1.53
2	C	501	NAD	C4N-C3N	3.65	1.45	1.39
2	C	501	NAD	C2B-C1B	-3.60	1.48	1.53
2	A	501	NAD	C7N-N7N	3.54	1.39	1.33
2	A	501	NAD	C8A-N7A	3.46	1.40	1.34
2	B	501	NAD	C2B-C3B	-3.40	1.44	1.53
2	B	501	NAD	C4N-C3N	3.37	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	C6A-N6A	3.37	1.46	1.34
2	C	501	NAD	C6A-N6A	3.28	1.46	1.34
2	D	501	NAD	C2D-C1D	-3.25	1.48	1.53
2	A	501	NAD	C2B-C3B	-3.24	1.44	1.53
2	D	501	NAD	C4N-C3N	3.18	1.44	1.39
2	B	501	NAD	O4B-C4B	-3.17	1.37	1.45
2	B	501	NAD	C2D-C1D	-3.07	1.49	1.53
2	D	501	NAD	C8A-N7A	3.05	1.40	1.34
3	C	502	ADN	C8-N7	3.04	1.40	1.34
2	A	501	NAD	C6A-N6A	3.03	1.45	1.34
2	D	501	NAD	C2N-N1N	3.02	1.38	1.35
2	C	501	NAD	C2D-C1D	-3.01	1.49	1.53
2	D	501	NAD	C2B-C1B	-2.98	1.49	1.53
2	D	501	NAD	C2B-C3B	-2.97	1.45	1.53
2	A	501	NAD	O4D-C1D	2.95	1.45	1.41
2	C	501	NAD	C7N-N7N	2.89	1.38	1.33
2	D	501	NAD	C6A-N6A	2.82	1.44	1.34
2	A	501	NAD	C5N-C4N	2.81	1.44	1.38
2	A	501	NAD	C2N-N1N	2.79	1.38	1.35
2	A	501	NAD	C2D-C1D	-2.78	1.49	1.53
2	D	501	NAD	C2N-C3N	2.76	1.43	1.39
2	D	501	NAD	C5N-C4N	2.74	1.44	1.38
6	D	502	3AD	O2'-C2'	-2.70	1.37	1.43
3	B	502	ADN	C6-N6	2.70	1.43	1.34
3	A	502	ADN	C6-N6	2.68	1.43	1.34
2	C	501	NAD	C2N-N1N	2.61	1.38	1.35
2	C	501	NAD	O4B-C4B	-2.58	1.39	1.45
2	A	501	NAD	C4N-C3N	2.49	1.43	1.39
2	D	501	NAD	C4A-N3A	2.25	1.38	1.35
6	D	502	3AD	C6-N6	2.20	1.42	1.34
3	C	502	ADN	C6-N6	2.20	1.42	1.34
2	A	501	NAD	C2A-N3A	2.18	1.35	1.32
2	D	501	NAD	C6N-N1N	2.18	1.40	1.35
3	B	502	ADN	C8-N7	2.17	1.38	1.34
2	C	501	NAD	C2A-N3A	2.07	1.35	1.32
2	B	501	NAD	C6N-N1N	2.02	1.40	1.35

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	N3A-C2A-N1A	-6.77	118.10	128.68
2	D	501	NAD	N3A-C2A-N1A	-6.07	119.19	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	N3A-C2A-N1A	-5.74	119.71	128.68
3	A	502	ADN	N3-C2-N1	-4.88	121.05	128.68
2	A	501	NAD	O4B-C1B-C2B	-4.83	99.87	106.93
2	A	501	NAD	N3A-C2A-N1A	-4.47	121.69	128.68
3	B	502	ADN	N3-C2-N1	-4.35	121.89	128.68
2	C	501	NAD	O7N-C7N-C3N	4.29	124.77	119.63
2	A	501	NAD	O4D-C1D-C2D	-4.09	100.94	106.93
2	C	501	NAD	O4D-C1D-C2D	-4.08	100.96	106.93
3	C	502	ADN	N3-C2-N1	-4.05	122.34	128.68
6	D	502	3AD	C4'-O4'-C1'	-4.02	104.23	109.75
2	B	501	NAD	O4D-C1D-C2D	-3.86	101.28	106.93
2	C	501	NAD	O4B-C1B-C2B	-3.73	101.47	106.93
2	B	501	NAD	C4A-C5A-N7A	-3.67	105.58	109.40
2	A	501	NAD	C6N-N1N-C2N	-3.59	118.70	121.97
2	D	501	NAD	O4D-C1D-C2D	-3.48	101.84	106.93
3	A	502	ADN	C5-C6-N6	3.26	125.30	120.35
3	C	502	ADN	C1'-N9-C4	-3.15	121.10	126.64
2	A	501	NAD	C5N-C4N-C3N	-3.01	116.78	120.34
2	D	501	NAD	PN-O3-PA	-3.00	122.54	132.83
3	A	502	ADN	C4-C5-N7	-2.95	106.33	109.40
2	D	501	NAD	O4B-C1B-C2B	-2.90	102.68	106.93
2	B	501	NAD	C1B-N9A-C4A	-2.83	121.67	126.64
2	A	501	NAD	C2N-C3N-C4N	2.72	121.34	118.26
2	C	501	NAD	PN-O3-PA	-2.67	123.65	132.83
6	D	502	3AD	N3-C2-N1	-2.52	124.75	128.68
3	B	502	ADN	C1'-N9-C4	-2.51	122.22	126.64
6	D	502	3AD	O4'-C4'-C5'	-2.46	105.84	109.50
2	B	501	NAD	C2A-N1A-C6A	2.42	122.89	118.75
2	C	501	NAD	O7N-C7N-N7N	-2.42	119.14	122.58
2	A	501	NAD	C3B-C2B-C1B	2.41	104.61	100.98
2	A	501	NAD	C1B-N9A-C4A	-2.40	122.42	126.64
2	D	501	NAD	C5N-C4N-C3N	-2.37	117.54	120.34
2	B	501	NAD	C5N-C4N-C3N	-2.37	117.54	120.34
2	A	501	NAD	C4A-C5A-N7A	-2.34	106.96	109.40
2	D	501	NAD	C2A-N1A-C6A	2.33	122.75	118.75
2	B	501	NAD	PN-O3-PA	-2.33	124.84	132.83
2	B	501	NAD	C3N-C7N-N7N	2.22	120.42	117.75
2	C	501	NAD	C6N-C5N-C4N	-2.21	116.23	119.44
3	B	502	ADN	C5-C6-N6	2.20	123.70	120.35
2	D	501	NAD	C5B-C4B-C3B	-2.12	107.23	115.18
2	B	501	NAD	O7N-C7N-N7N	-2.09	119.60	122.58
3	C	502	ADN	C3'-C2'-C1'	2.05	104.06	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	C6N-N1N-C2N	-2.04	120.11	121.97
7	D	503	PGE	O2-C2-C1	2.04	119.01	110.07

There are no chirality outliers.

All (29) torsion outliers are listed below:

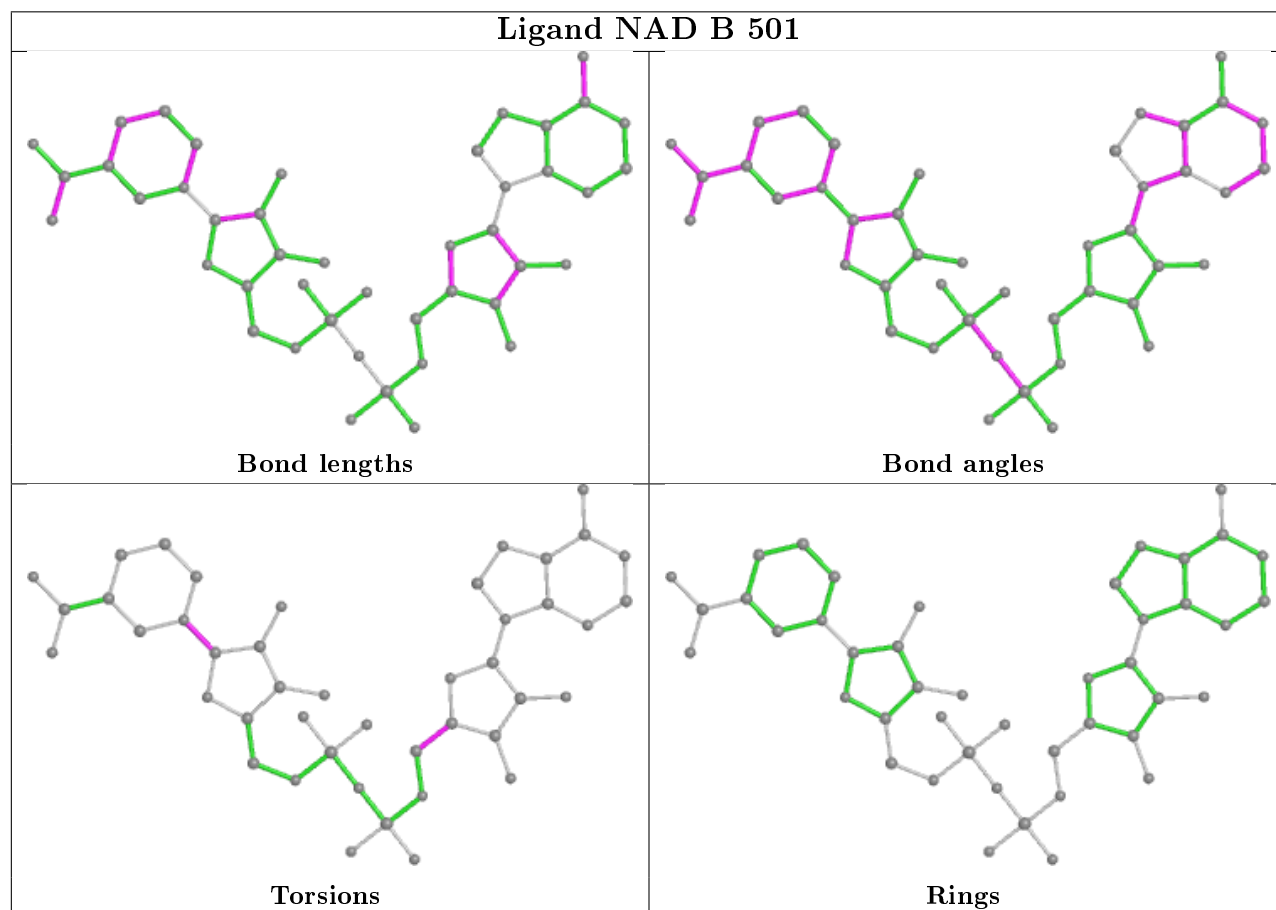
Mol	Chain	Res	Type	Atoms
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	C	501	NAD	C2D-C1D-N1N-C6N
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
7	D	503	PGE	O2-C3-C4-O3
5	A	504	PEG	O1-C1-C2-O2
7	D	503	PGE	O3-C5-C6-O4
5	B	504	PEG	O1-C1-C2-O2
5	B	504	PEG	O2-C3-C4-O4
7	D	503	PGE	C3-C4-O3-C5
5	B	504	PEG	C4-C3-O2-C2
5	A	504	PEG	O2-C3-C4-O4
2	D	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B
6	D	502	3AD	O4'-C4'-C5'-O5'

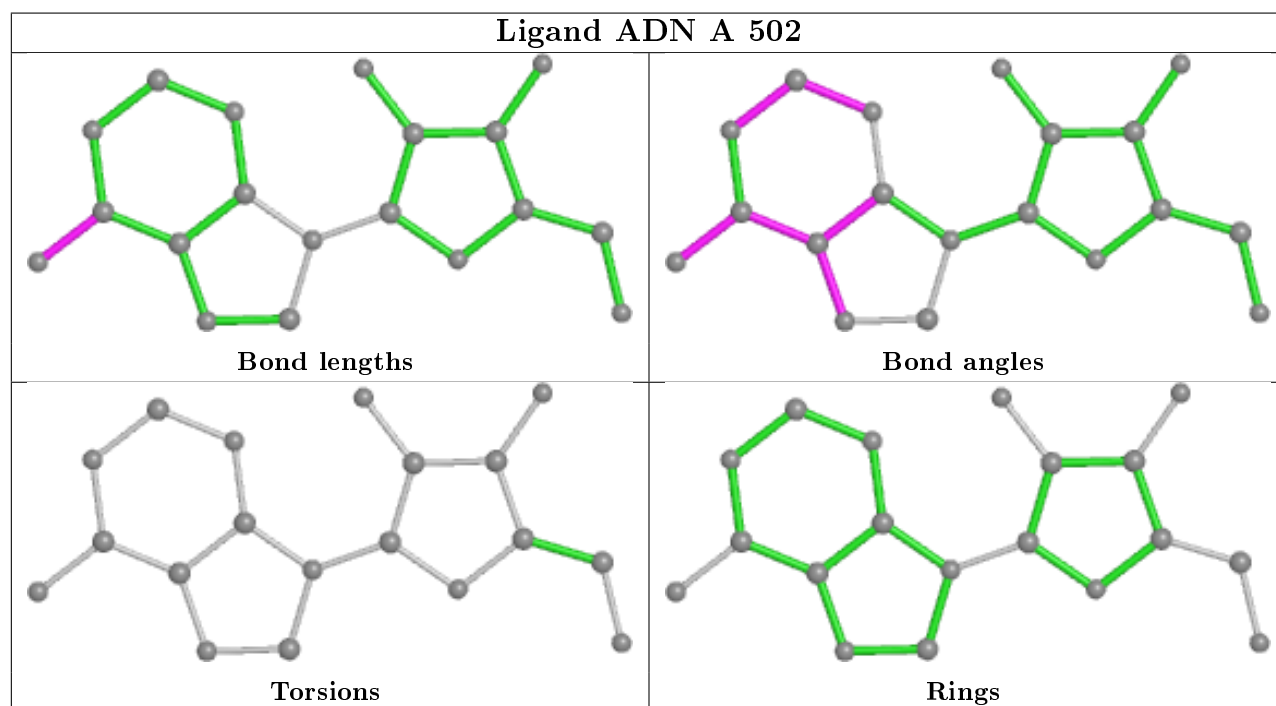
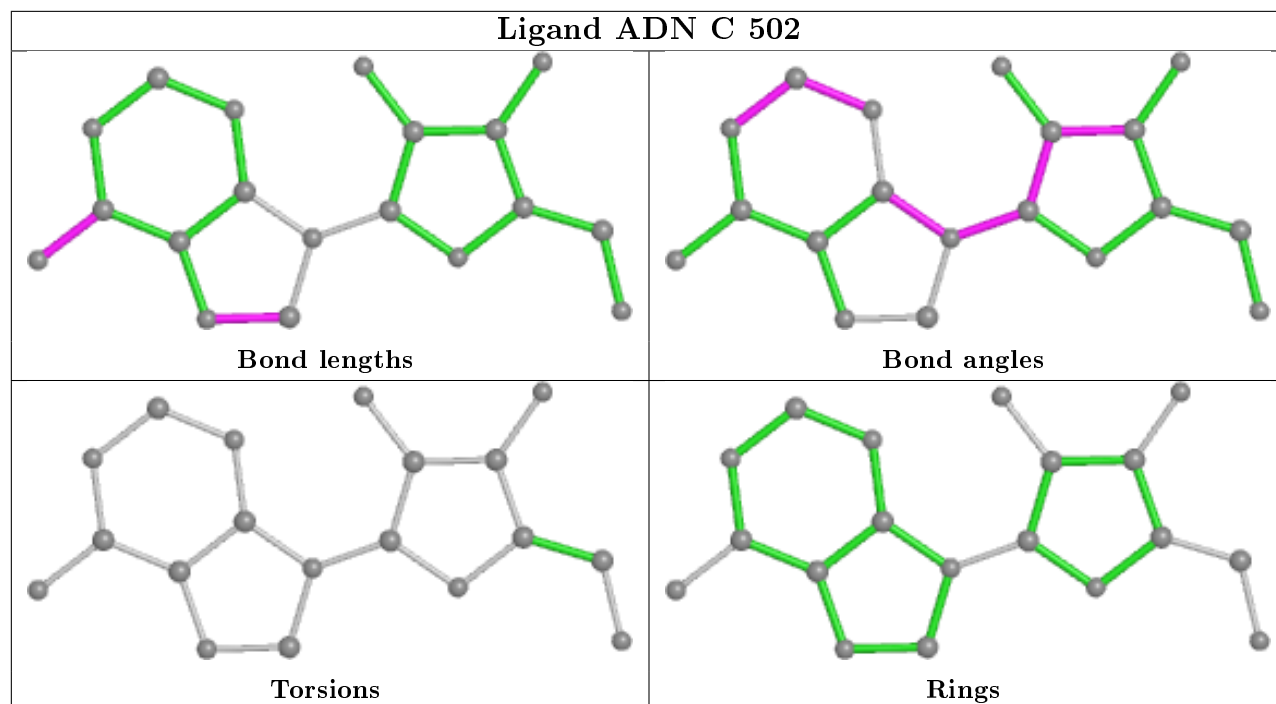
There are no ring outliers.

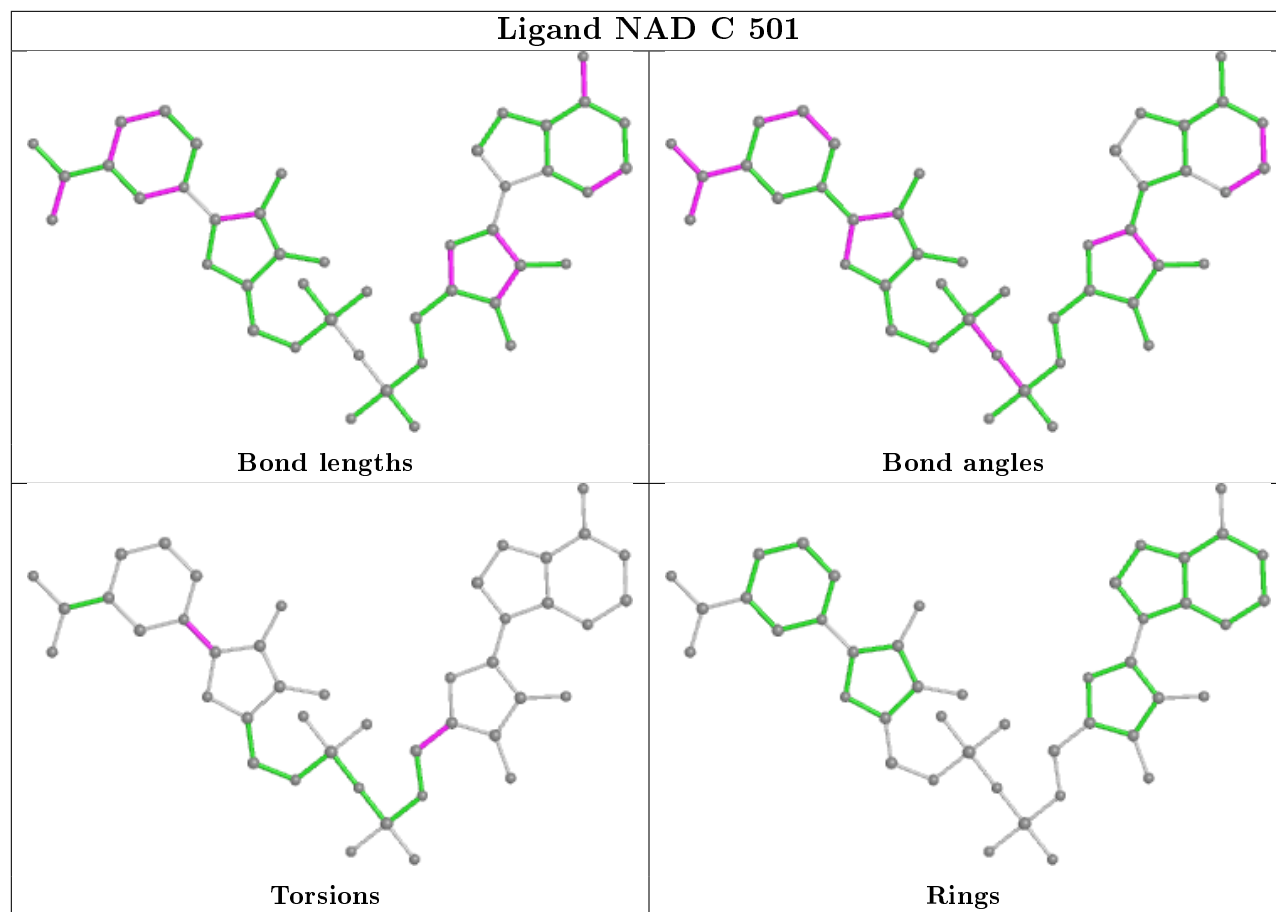
8 monomers are involved in 9 short contacts:

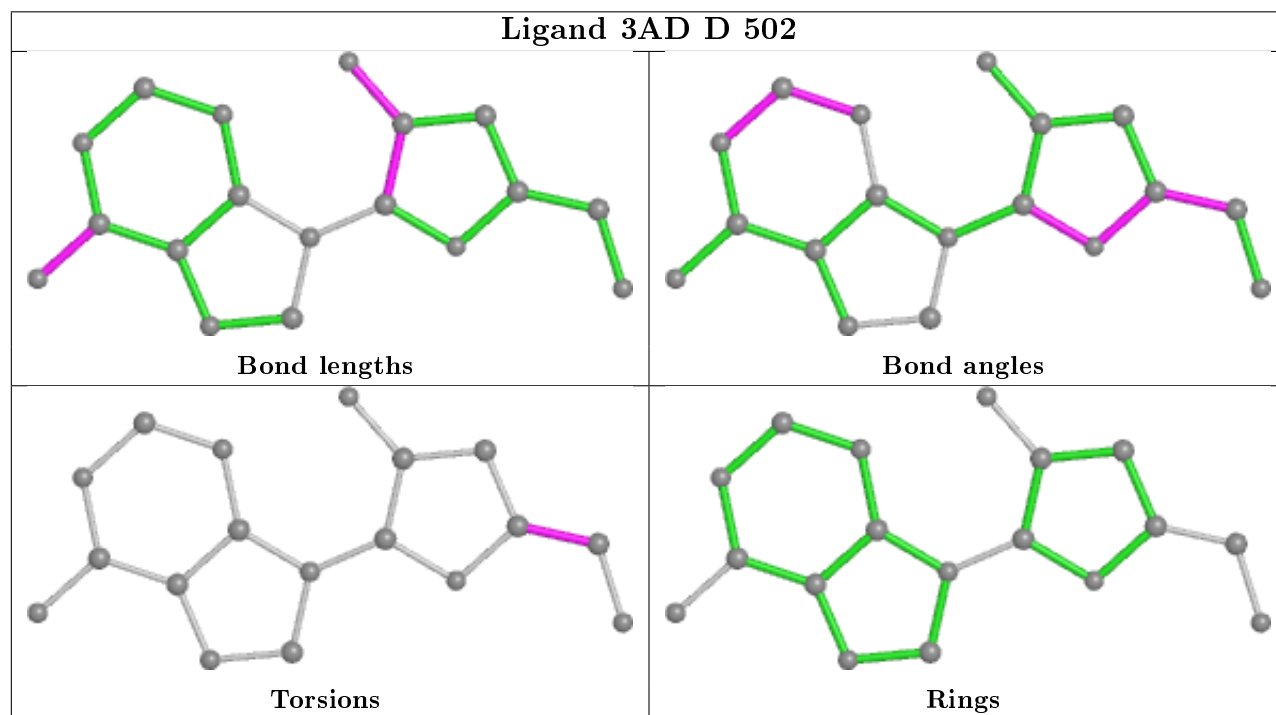
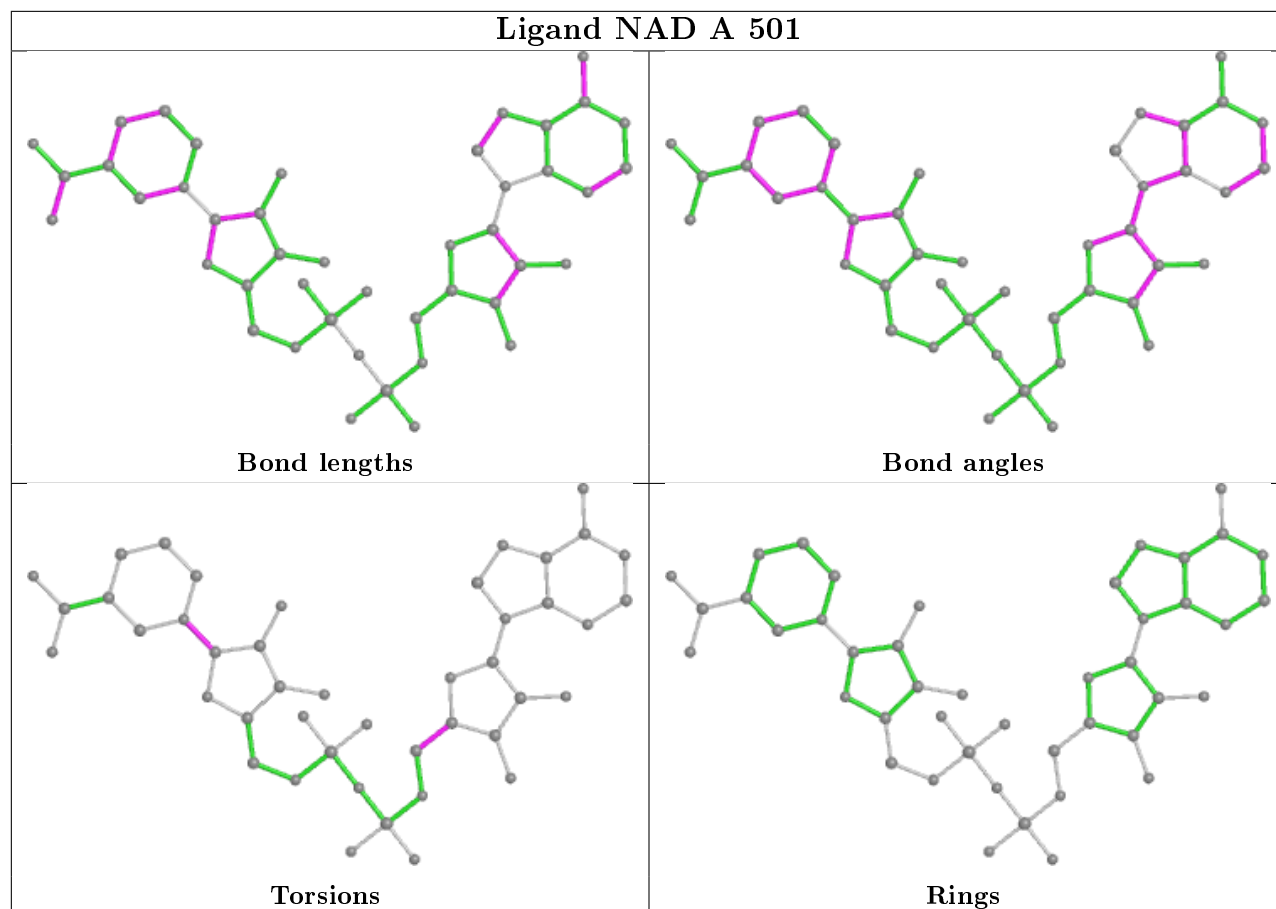
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NAD	1	0
3	C	502	ADN	1	0
3	A	502	ADN	2	0
2	C	501	NAD	2	0
2	A	501	NAD	1	0
6	D	502	3AD	2	0
2	D	501	NAD	1	0
3	B	502	ADN	2	0

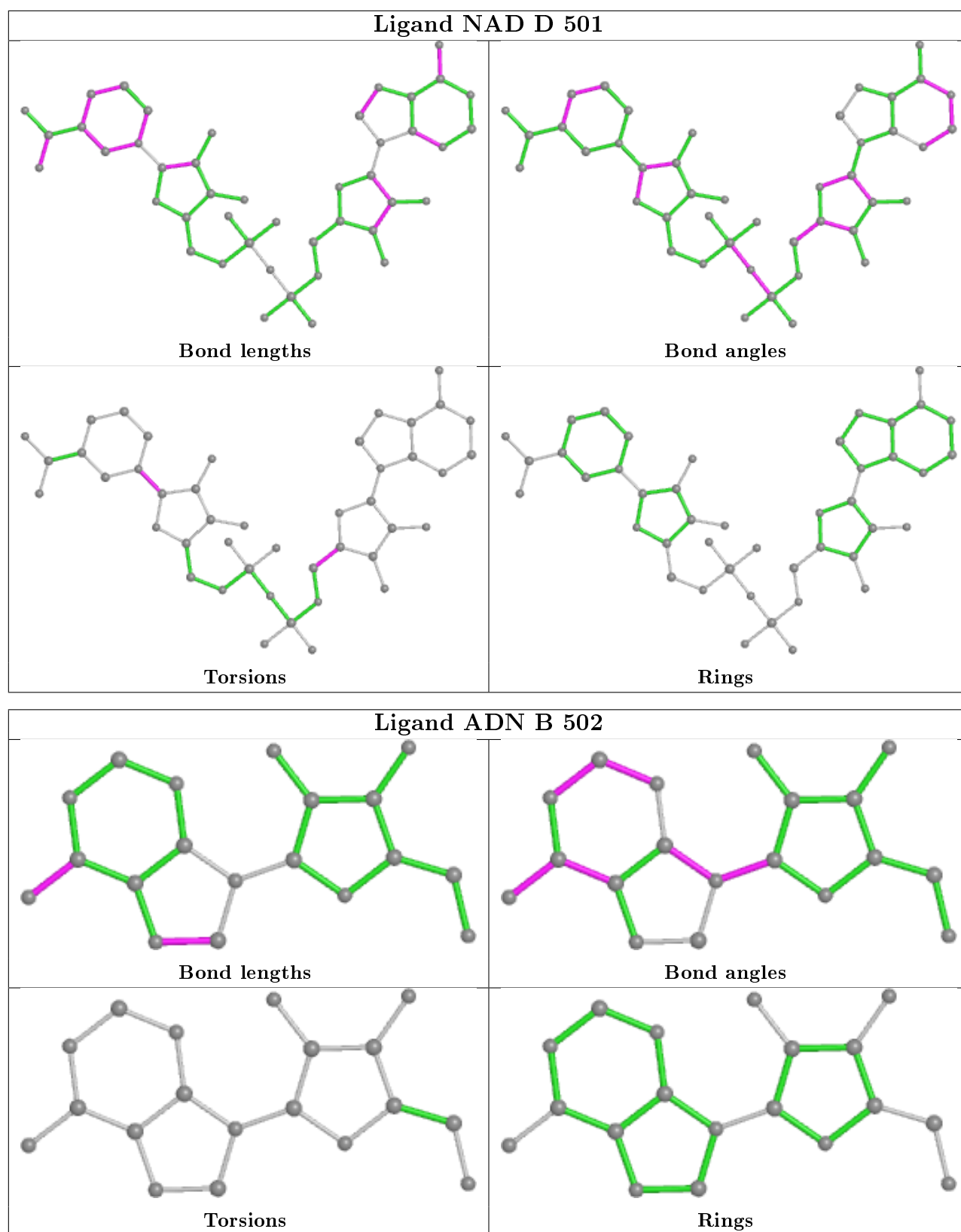
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	468/479 (97%)	-0.54	1 (0%) 95 94	14, 26, 47, 73	0
1	B	468/479 (97%)	-0.52	2 (0%) 92 92	13, 23, 42, 75	0
1	C	471/479 (98%)	-0.47	7 (1%) 73 73	14, 25, 47, 93	0
1	D	468/479 (97%)	-0.52	4 (0%) 84 84	15, 25, 46, 82	0
All	All	1875/1916 (97%)	-0.51	14 (0%) 87 87	13, 25, 46, 93	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	ALA	7.6
1	B	6	GLY	4.7
1	C	4	LYS	3.1
1	C	7	PHE	3.1
1	A	6	GLY	2.8
1	C	5	PRO	2.8
1	D	159	LYS	2.7
1	B	7	PHE	2.6
1	D	161	GLY	2.4
1	D	210	ASN	2.3
1	C	161	GLY	2.2
1	D	6	GLY	2.2
1	C	6	GLY	2.2
1	C	177	LYS	2.2

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

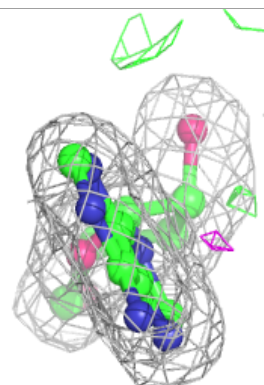
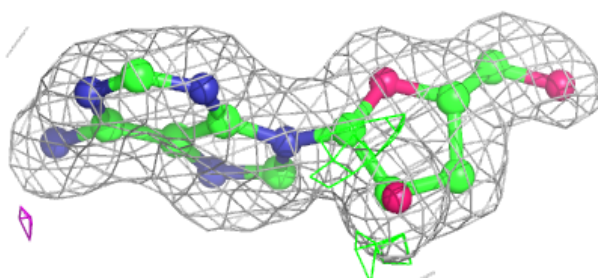
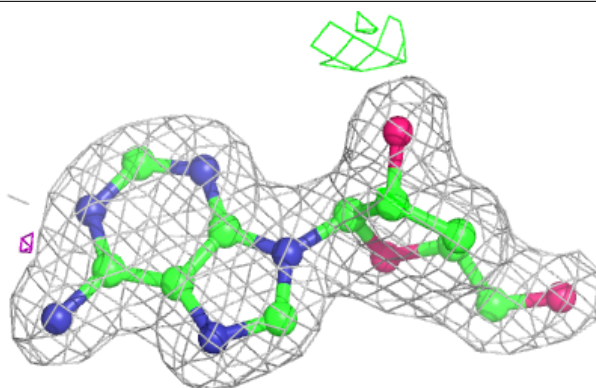
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEG	A	504	7/7	0.84	0.35	61,65,73,75	0
7	PGE	D	503	10/10	0.86	0.14	45,58,63,63	0
8	ACT	D	504	4/4	0.88	0.29	51,58,59,63	0
5	PEG	B	504	7/7	0.90	0.14	50,54,69,75	0
6	3AD	D	502	18/18	0.97	0.12	16,21,27,32	0
3	ADN	A	502	19/19	0.97	0.09	14,18,30,31	0
3	ADN	C	502	19/19	0.97	0.11	15,20,31,33	0
2	NAD	C	501	44/44	0.98	0.08	14,18,22,29	0
2	NAD	B	501	44/44	0.98	0.09	15,19,22,25	0
2	NAD	A	501	44/44	0.98	0.07	15,19,23,25	0
3	ADN	B	502	19/19	0.98	0.11	13,18,25,30	0
4	NA	B	503	1/1	0.99	0.10	23,23,23,23	0
4	NA	A	503	1/1	0.99	0.05	25,25,25,25	0
2	NAD	D	501	44/44	0.99	0.06	13,18,23,25	0
4	NA	C	503	1/1	0.99	0.05	25,25,25,25	0

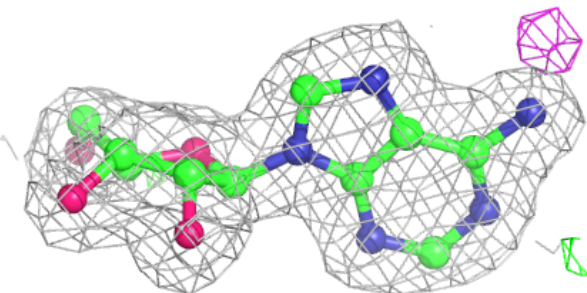
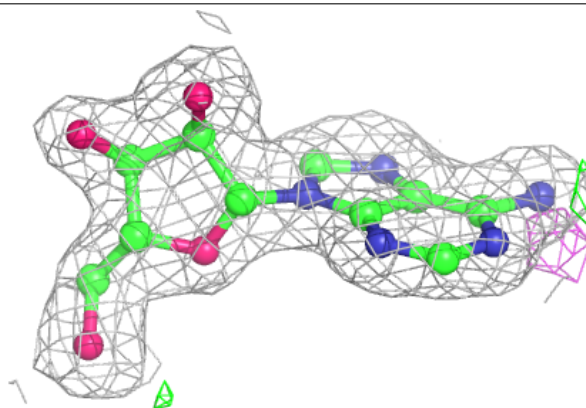
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 3AD 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)

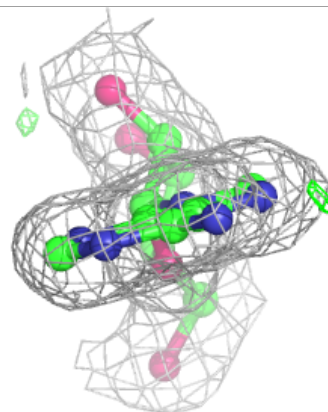
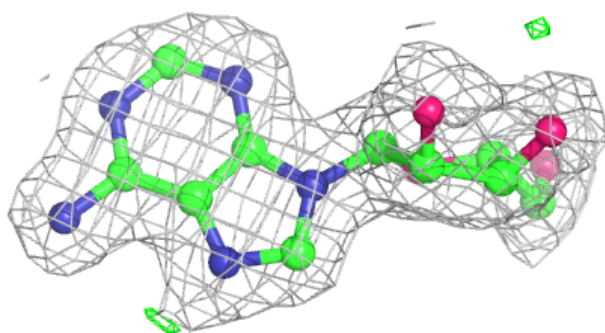
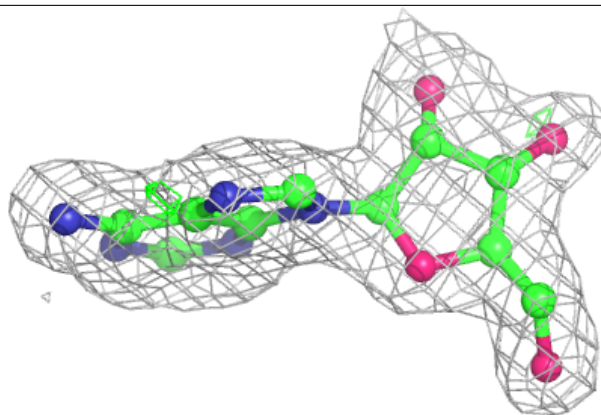
**Electron density around ADN A 502:**

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

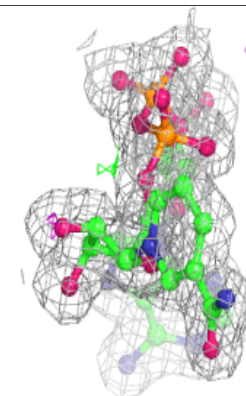
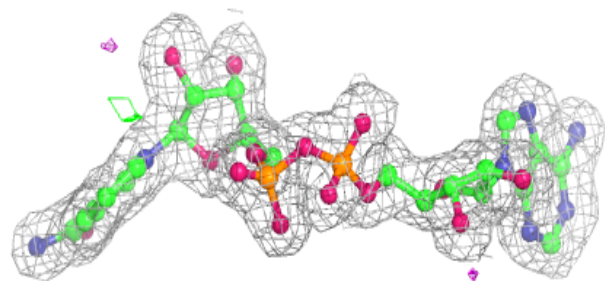
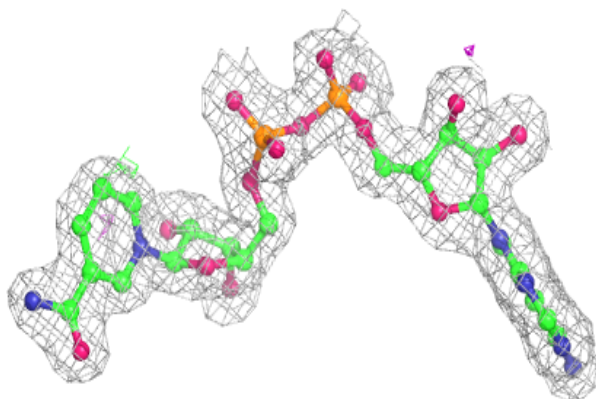


**Electron density around ADN C 502:**

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

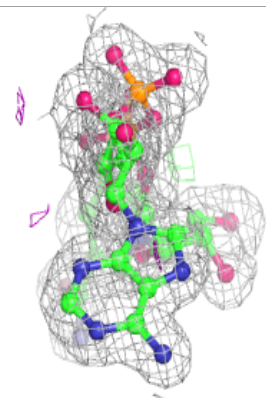
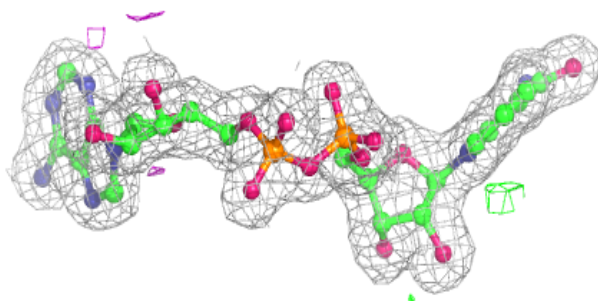
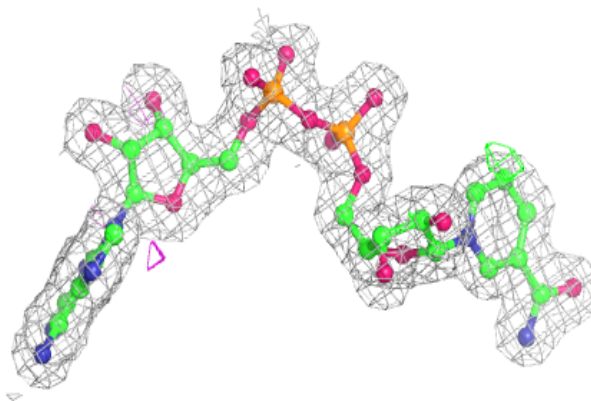
**Electron density around NAD C 501:**

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

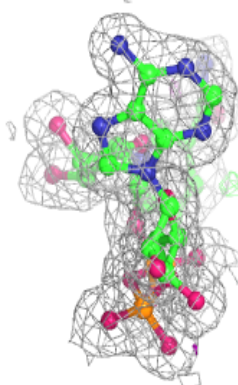
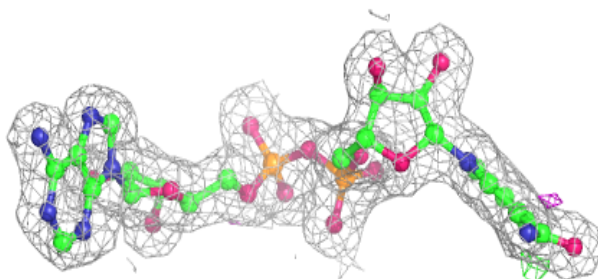
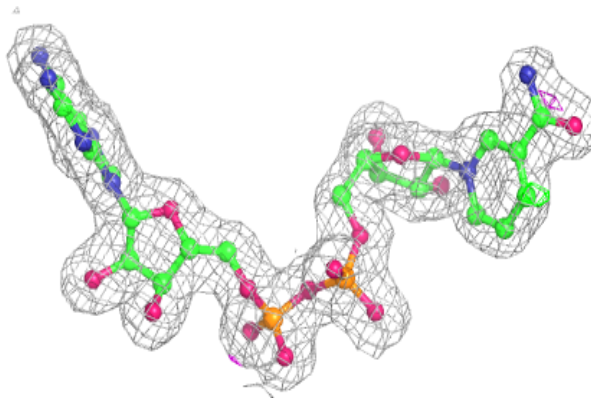


**Electron density around NAD B 501:**

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

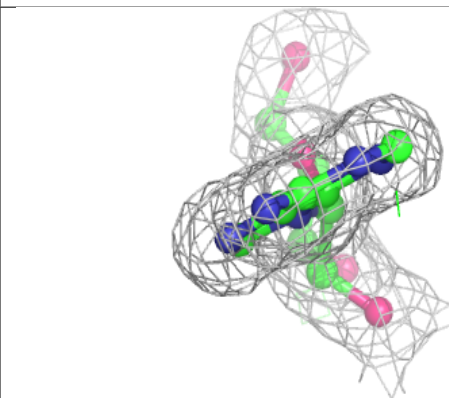
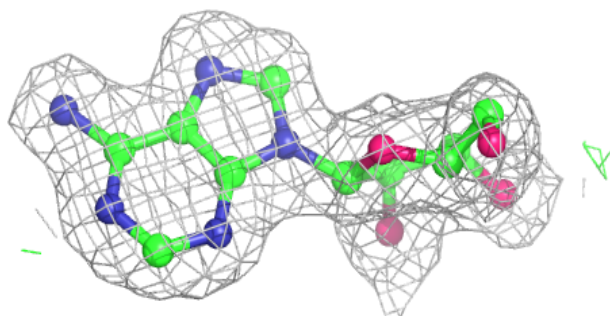
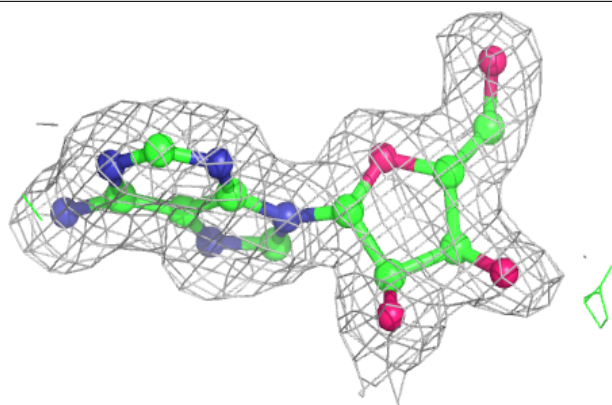
**Electron density around NAD A 501:**

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

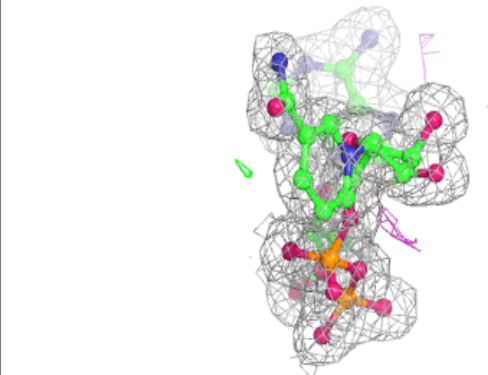
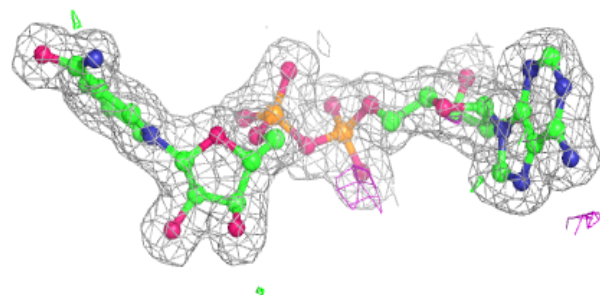
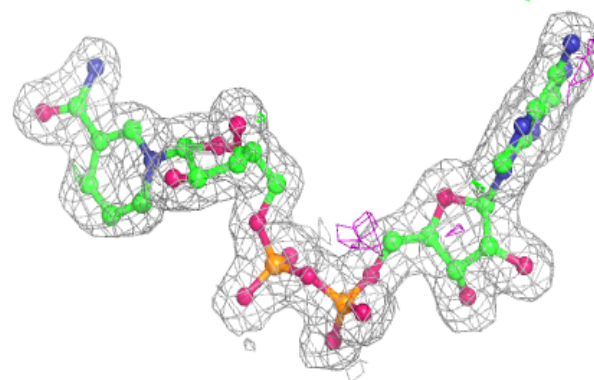


**Electron density around ADN B 502:**

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

**Electron density around NAD 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.