



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2023 – 06:31 pm BST

PDB ID : 8AJT  
Title : Crystal structure of the H323A mutant of S-adenosyl-L-homocysteine hydro-  
lase from *Pseudomonas aeruginosa* cocrystallized with adenosine in the pres-  
ence of K<sup>+</sup> cations  
Authors : Drozdal, P.; Wozniak, K.; Malecki, P.; Gawel, M.; Komorowska, M.; Brzezini-  
ski, K.  
Deposited on : 2022-07-28  
Resolution : 1.50 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.34  
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) : 2.34

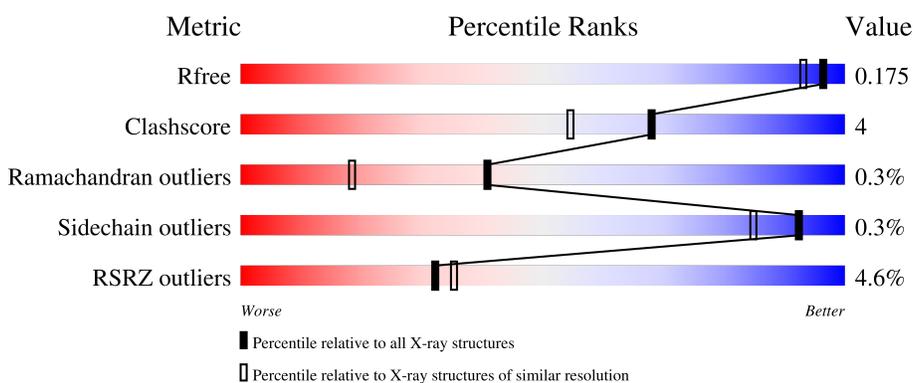
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	AAA	472	 2% 91% 6%
1	BBB	472	 8% 90% 7%
1	CCC	472	 % 93% 7%
1	DDD	472	 7% 92% 6%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 16457 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.

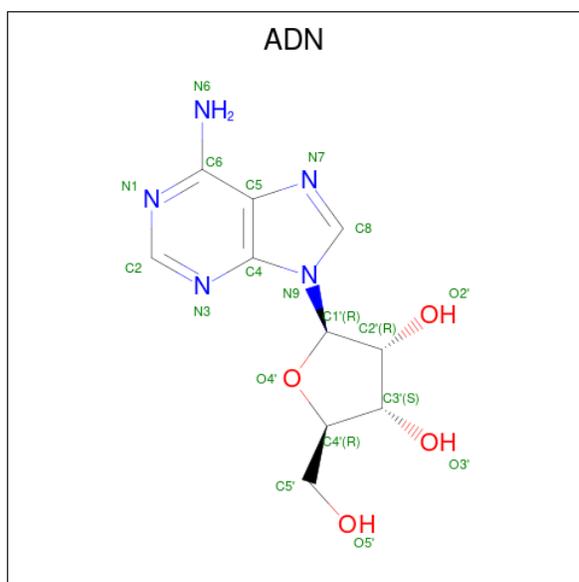
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	461	3631	2288	629	691	23	18	10	0
1	BBB	461	3650	2304	631	692	23	29	14	0
1	CCC	461	3608	2275	623	687	23	13	8	0
1	DDD	461	3604	2272	624	685	23	8	8	0

There are 16 discrepancies between the modelled and reference sequences:

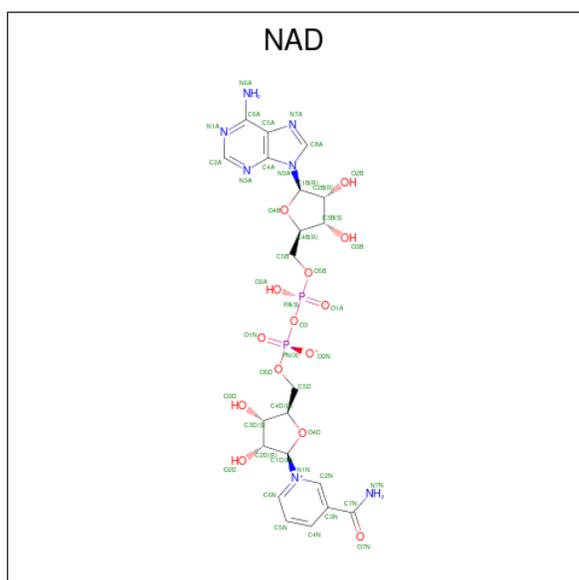
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	SER	-	expression tag	UNP Q9I685
AAA	-1	ASN	-	expression tag	UNP Q9I685
AAA	0	ALA	-	expression tag	UNP Q9I685
AAA	323	ALA	HIS	engineered mutation	UNP Q9I685
BBB	-2	SER	-	expression tag	UNP Q9I685
BBB	-1	ASN	-	expression tag	UNP Q9I685
BBB	0	ALA	-	expression tag	UNP Q9I685
BBB	323	ALA	HIS	engineered mutation	UNP Q9I685
CCC	-2	SER	-	expression tag	UNP Q9I685
CCC	-1	ASN	-	expression tag	UNP Q9I685
CCC	0	ALA	-	expression tag	UNP Q9I685
CCC	323	ALA	HIS	engineered mutation	UNP Q9I685
DDD	-2	SER	-	expression tag	UNP Q9I685
DDD	-1	ASN	-	expression tag	UNP Q9I685
DDD	0	ALA	-	expression tag	UNP Q9I685
DDD	323	ALA	HIS	engineered mutation	UNP Q9I685

- Molecule 2 is ADENOSINE (three-letter code: ADN) (formula:  $C_{10}H_{13}N_5O_4$ ) (labeled as "Ligand of Interest" by depositor).



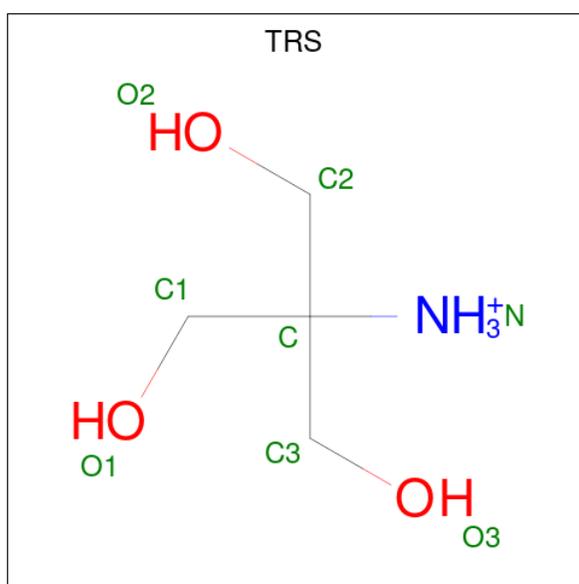
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	AAA	1	Total	C	N	O	0	0
			19	10	5	4		
2	BBB	1	Total	C	N	O	0	0
			19	10	5	4		
2	CCC	1	Total	C	N	O	0	0
			19	10	5	4		
2	DDD	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	AAA	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	BBB	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	CCC	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	DDD	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



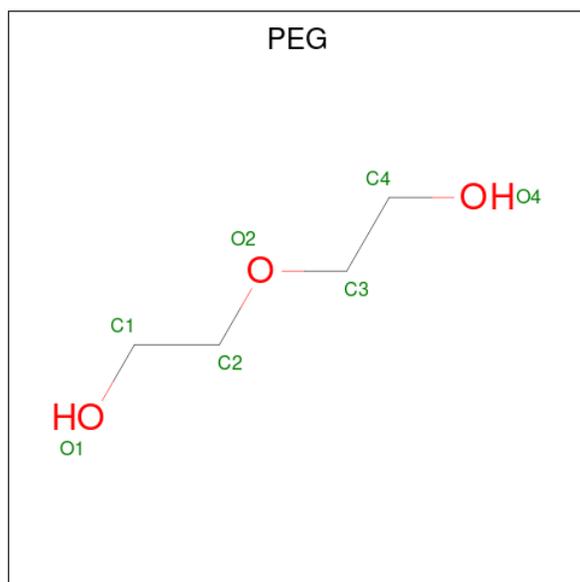
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	AAA	1	Total 10	C 5	N 1	O 4	0	1
4	AAA	1	Total 8	C 4	N 1	O 3	0	0
4	BBB	1	Total 10	C 5	N 1	O 4	0	1
4	BBB	1	Total 8	C 4	N 1	O 3	0	0
4	CCC	1	Total 10	C 5	N 1	O 4	0	1
4	CCC	1	Total 10	C 5	N 1	O 4	0	1
4	DDD	1	Total 10	C 5	N 1	O 4	0	1

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	DDD	1	8	4	1	3	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).

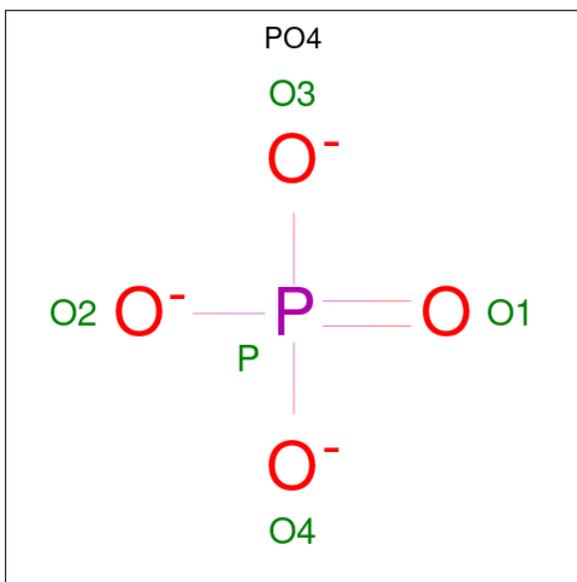


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	AAA	1	7	4	3	0	0
5	CCC	1	7	4	3	0	0
5	CCC	1	7	4	3	0	0
5	DDD	1	7	4	3	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
6	AAA	1	1	1	0	0
6	BBB	1	1	1	0	0
6	CCC	1	1	1	0	0
6	DDD	2	2	2	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total O P 5 4 1	0	0
7	CCC	1	Total O P 5 4 1	0	0
7	CCC	1	Total O P 5 4 1	1	0
7	DDD	1	Total O P 5 4 1	1	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	1	Total Cl 1 1	0	0
8	BBB	3	Total Cl 3 3	0	0
8	CCC	1	Total Cl 1 1	0	0
8	DDD	5	Total Cl 5 5	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	407	Total O 407 407	0	0

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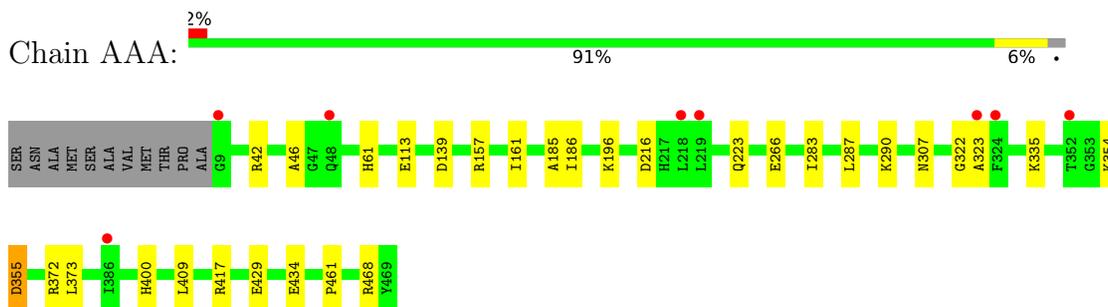
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
9	BBB	376	Total 376	O 376	0	0
9	CCC	430	Total 430	O 430	0	0
9	DDD	362	Total 362	O 362	0	0

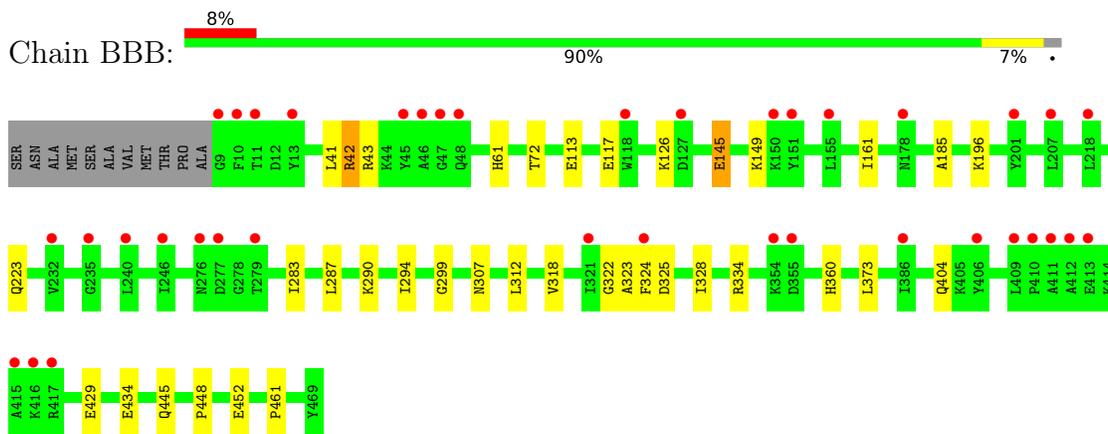
### 3 Residue-property plots [i](#)

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.

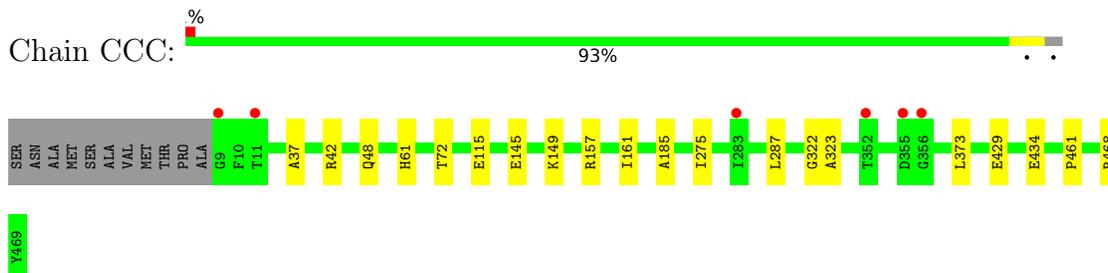
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase

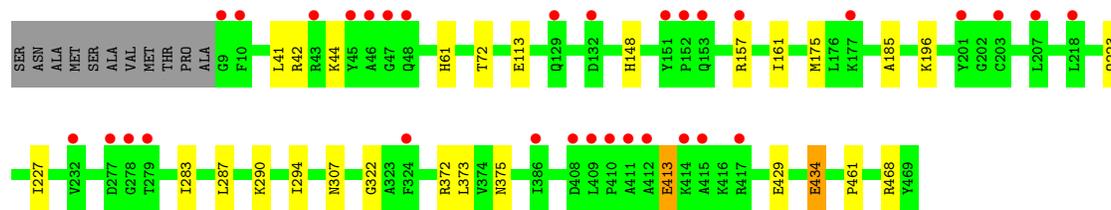


- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.71Å 134.56Å 108.09Å 90.00° 105.71° 90.00°	Depositor
Resolution (Å)	42.56 – 1.50 42.56 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.56-1.50) 99.8 (42.56-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.152 , 0.167 0.159 , 0.175	Depositor DCC
$R_{free}$ test set	1045 reflections (0.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtrriage
Anisotropy	0.379	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.000 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	16457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: PEG, K, ADN, NAD, PO4, CL, TRS

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	AAA	0.74	1/3696 (0.0%)	0.77	2/4995 (0.0%)
1	BBB	0.83	4/3722 (0.1%)	0.74	1/5031 (0.0%)
1	CCC	0.76	0/3674	0.77	1/4965 (0.0%)
1	DDD	0.74	2/3672 (0.1%)	0.73	0/4963
All	All	0.77	7/14764 (0.0%)	0.75	4/19954 (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	DDD	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	145	GLU	CD-OE1	-18.21	1.05	1.25
1	BBB	117	GLU	CG-CD	-11.63	1.34	1.51
1	DDD	413	GLU	CG-CD	9.65	1.66	1.51
1	BBB	434	GLU	CD-OE2	8.64	1.35	1.25
1	DDD	434	GLU	CD-OE2	5.77	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	157	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	CCC	157	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	BBB	117	GLU	CB-CG-CD	6.45	131.60	114.20
1	AAA	157	ARG	NE-CZ-NH1	5.37	122.98	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DDD	413	GLU	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	AAA	3631	0	3639	24	0
1	BBB	3650	0	3664	34	0
1	CCC	3608	0	3618	23	0
1	DDD	3604	0	3617	26	0
2	AAA	19	0	13	2	0
2	BBB	19	0	13	1	0
2	CCC	19	0	13	1	0
2	DDD	19	0	13	1	0
3	AAA	44	0	26	1	0
3	BBB	44	0	26	1	0
3	CCC	44	0	26	1	0
3	DDD	44	0	26	3	0
4	AAA	18	0	18	4	0
4	BBB	18	0	24	4	0
4	CCC	20	0	18	2	0
4	DDD	18	0	18	6	0
5	AAA	7	0	10	0	0
5	CCC	14	0	20	1	0
5	DDD	7	0	10	1	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
6	DDD	2	0	0	0	0
7	AAA	5	0	0	0	0
7	CCC	10	0	0	0	0
7	DDD	5	0	0	0	0
8	AAA	1	0	0	0	0
8	BBB	3	0	0	0	0
8	CCC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	DDD	5	0	0	0	0
9	AAA	407	0	0	7	0
9	BBB	376	0	0	8	0
9	CCC	430	0	0	6	0
9	DDD	362	0	0	5	0
All	All	16457	0	14812	112	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.

The worst 5 of 112 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)
4:DDD:503[A]:TRS:H31	9:DDD:601:HOH:O	1.33	1.26
4:CCC:703[A]:TRS:H31	9:CCC:801:HOH:O	1.38	1.21
4:DDD:503[A]:TRS:C3	9:DDD:601:HOH:O	1.91	1.08
1:CCC:322[B]:GLY:O	1:CCC:373:LEU:CD2	2.06	1.03
1:AAA:322:GLY:O	1:AAA:373:LEU:CD2	2.06	1.03

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	AAA	469/472 (99%)	458 (98%)	9 (2%)	2 (0%)	34 13
1	BBB	473/472 (100%)	457 (97%)	15 (3%)	1 (0%)	47 23
1	CCC	467/472 (99%)	458 (98%)	8 (2%)	1 (0%)	47 23
1	DDD	467/472 (99%)	459 (98%)	7 (2%)	1 (0%)	47 23
All	All	1876/1888 (99%)	1832 (98%)	39 (2%)	5 (0%)	41 18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	355	ASP
1	BBB	61	HIS
1	DDD	61	HIS
1	AAA	61	HIS
1	CCC	61	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	AAA	386/384 (100%)	385 (100%)	1 (0%)	92 85
1	BBB	388/384 (101%)	386 (100%)	2 (0%)	88 78
1	CCC	383/384 (100%)	382 (100%)	1 (0%)	92 85
1	DDD	383/384 (100%)	383 (100%)	0	100 100
All	All	1540/1536 (100%)	1536 (100%)	4 (0%)	92 85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	223	GLN
1	BBB	42	ARG
1	BBB	334	ARG
1	CCC	48	GLN

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

### 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 44 ligands modelled in this entry, 15 are monoatomic - leaving 29 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	CCC	702	-	18,21,21	0.48	0	18,31,31	0.99	1 (5%)
3	NAD	CCC	701	-	42,48,48	0.83	1 (2%)	50,73,73	0.94	2 (4%)
7	PO4	DDD	508	-	4,4,4	1.34	1 (25%)	6,6,6	0.65	0
5	PEG	CCC	706	-	6,6,6	0.11	0	5,5,5	0.06	0
4	TRS	DDD	505	-	7,7,7	0.21	0	9,9,9	0.32	0
4	TRS	BBB	503[A]	-	7,7,7	0.40	0	9,9,9	0.62	0
3	NAD	DDD	502	-	42,48,48	0.91	2 (4%)	50,73,73	1.09	5 (10%)
4	TRS	AAA	703[A]	-	7,7,7	0.36	0	9,9,9	0.62	0
4	TRS	BBB	503[B]	-	7,7,7	0.42	0	9,9,9	0.67	0
4	TRS	AAA	703[B]	-	7,7,7	0.36	0	9,9,9	0.66	0
7	PO4	CCC	709	-	4,4,4	1.25	1 (25%)	6,6,6	1.04	0
5	PEG	AAA	705	-	6,6,6	0.12	0	5,5,5	0.07	0
4	TRS	CCC	704[A]	-	7,7,7	0.20	0	9,9,9	0.14	0
2	ADN	AAA	701	-	18,21,21	0.55	0	18,31,31	1.32	1 (5%)
4	TRS	DDD	503[A]	-	7,7,7	0.47	0	9,9,9	0.71	0
2	ADN	DDD	501	-	18,21,21	0.54	0	18,31,31	0.93	0
3	NAD	BBB	502	-	42,48,48	0.95	3 (7%)	50,73,73	1.13	5 (10%)
2	ADN	BBB	501	-	18,21,21	0.59	0	18,31,31	0.98	1 (5%)
5	PEG	CCC	707	-	6,6,6	0.21	0	5,5,5	0.12	0
4	TRS	CCC	703[A]	-	7,7,7	0.47	0	9,9,9	0.81	0
4	TRS	CCC	704[B]	-	7,7,7	0.21	0	9,9,9	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TRS	DDD	503[B]	-	7,7,7	0.45	0	9,9,9	0.51	0
4	TRS	BBB	504	-	7,7,7	0.24	0	9,9,9	0.28	0
4	TRS	CCC	703[B]	-	7,7,7	0.46	0	9,9,9	0.77	0
3	NAD	AAA	702	-	42,48,48	0.86	1 (2%)	50,73,73	0.91	3 (6%)
4	TRS	AAA	704	-	7,7,7	0.23	0	9,9,9	0.28	0
5	PEG	DDD	504	-	6,6,6	0.17	0	5,5,5	0.04	0
7	PO4	AAA	707	-	4,4,4	0.81	0	6,6,6	0.41	0
7	PO4	CCC	705	-	4,4,4	0.55	0	6,6,6	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	ADN	CCC	702	-	-	0/2/22/22	0/3/3/3
3	NAD	CCC	701	-	-	5/26/62/62	0/5/5/5
5	PEG	CCC	706	-	-	1/4/4/4	-
4	TRS	DDD	505	-	-	6/9/9/9	-
4	TRS	BBB	503[A]	-	-	6/9/9/9	-
3	NAD	DDD	502	-	-	5/26/62/62	0/5/5/5
4	TRS	AAA	703[A]	-	-	6/9/9/9	-
4	TRS	BBB	503[B]	-	-	6/9/9/9	-
4	TRS	AAA	703[B]	-	-	6/9/9/9	-
5	PEG	AAA	705	-	-	0/4/4/4	-
4	TRS	CCC	704[A]	-	-	3/9/9/9	-
2	ADN	AAA	701	-	-	0/2/22/22	0/3/3/3
4	TRS	DDD	503[A]	-	-	6/9/9/9	-
2	ADN	DDD	501	-	-	0/2/22/22	0/3/3/3
3	NAD	BBB	502	-	-	5/26/62/62	0/5/5/5
2	ADN	BBB	501	-	-	0/2/22/22	0/3/3/3
5	PEG	CCC	707	-	-	3/4/4/4	-
4	TRS	CCC	703[A]	-	-	3/9/9/9	-
4	TRS	CCC	704[B]	-	-	3/9/9/9	-
4	TRS	DDD	503[B]	-	-	6/9/9/9	-
4	TRS	BBB	504	-	-	1/9/9/9	-
4	TRS	CCC	703[B]	-	-	4/9/9/9	-
3	NAD	AAA	702	-	-	5/26/62/62	0/5/5/5
4	TRS	AAA	704	-	-	6/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	DDD	504	-	-	3/4/4/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DDD	502	NAD	C2N-N1N	3.68	1.39	1.35
3	CCC	701	NAD	O4D-C1D	3.17	1.45	1.41
3	BBB	502	NAD	C2N-N1N	3.05	1.38	1.35
3	AAA	702	NAD	O4D-C1D	2.95	1.45	1.41
3	BBB	502	NAD	O4D-C1D	2.80	1.45	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	502	NAD	C6N-N1N-C2N	-4.05	118.28	121.97
2	AAA	701	ADN	C5-C6-N6	3.62	125.86	120.35
3	AAA	702	NAD	C6N-N1N-C2N	-3.09	119.15	121.97
3	DDD	502	NAD	C6N-N1N-C2N	-3.05	119.19	121.97
3	CCC	701	NAD	C5A-C6A-N6A	2.91	124.77	120.35

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	702	NAD	O4D-C1D-N1N-C2N
3	AAA	702	NAD	O4D-C1D-N1N-C6N
3	AAA	702	NAD	C2D-C1D-N1N-C2N
3	AAA	702	NAD	C2D-C1D-N1N-C6N
3	BBB	502	NAD	O4D-C1D-N1N-C2N

There are no ring outliers.

15 monomers are involved in 25 short contacts:

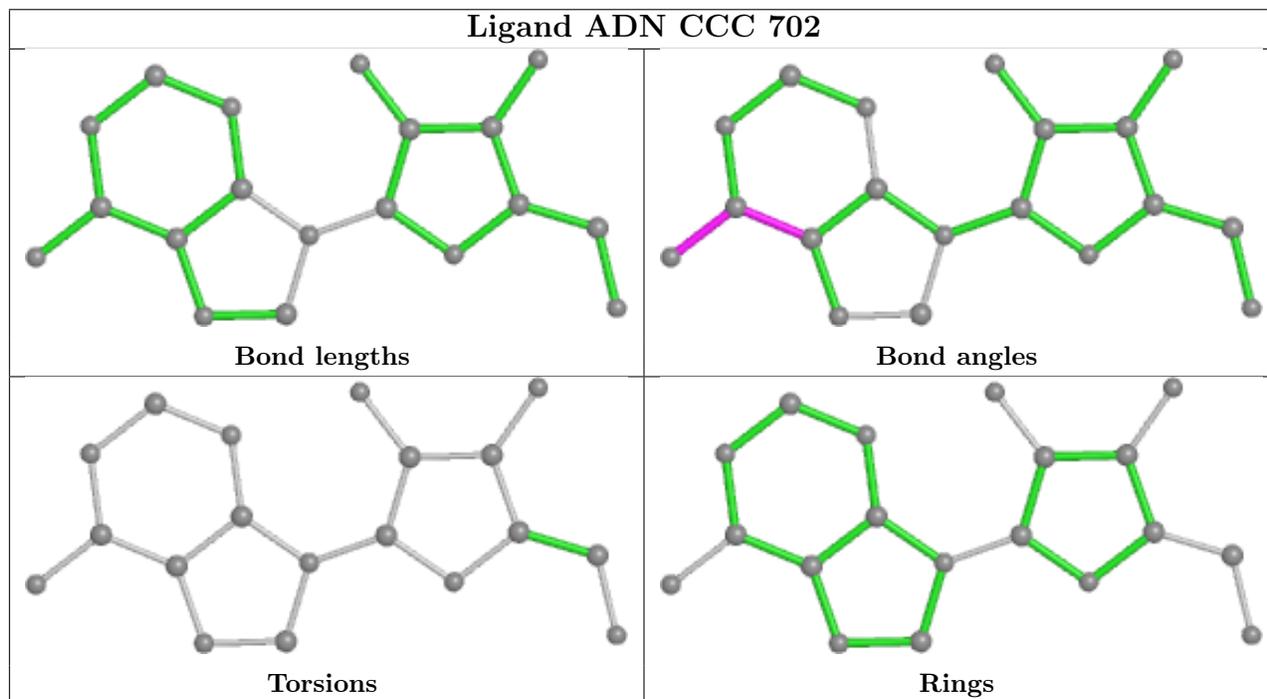
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	702	ADN	1	0
3	CCC	701	NAD	1	0
4	DDD	505	TRS	4	0
3	DDD	502	NAD	3	0
2	AAA	701	ADN	2	0
4	DDD	503[A]	TRS	2	0
2	DDD	501	ADN	1	0

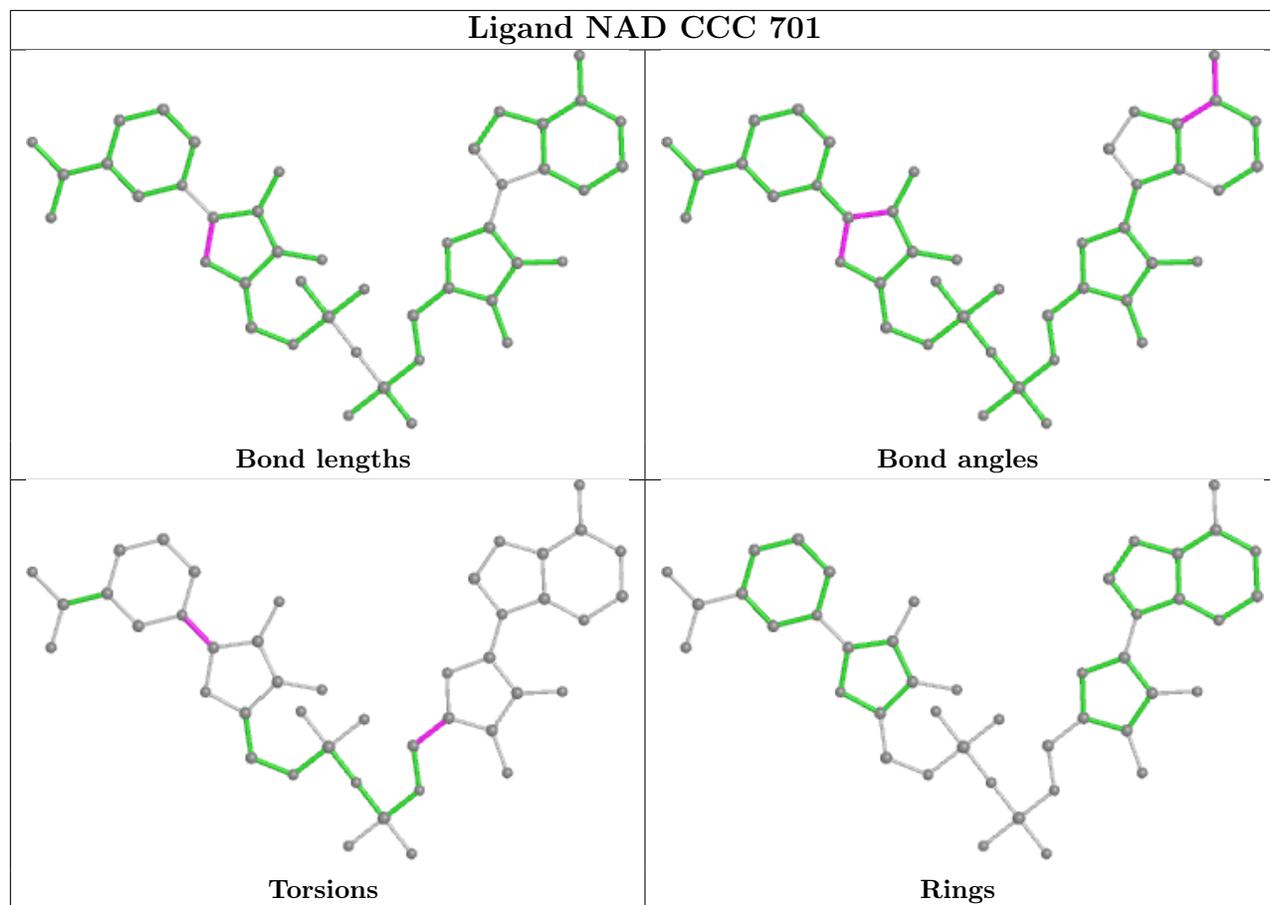
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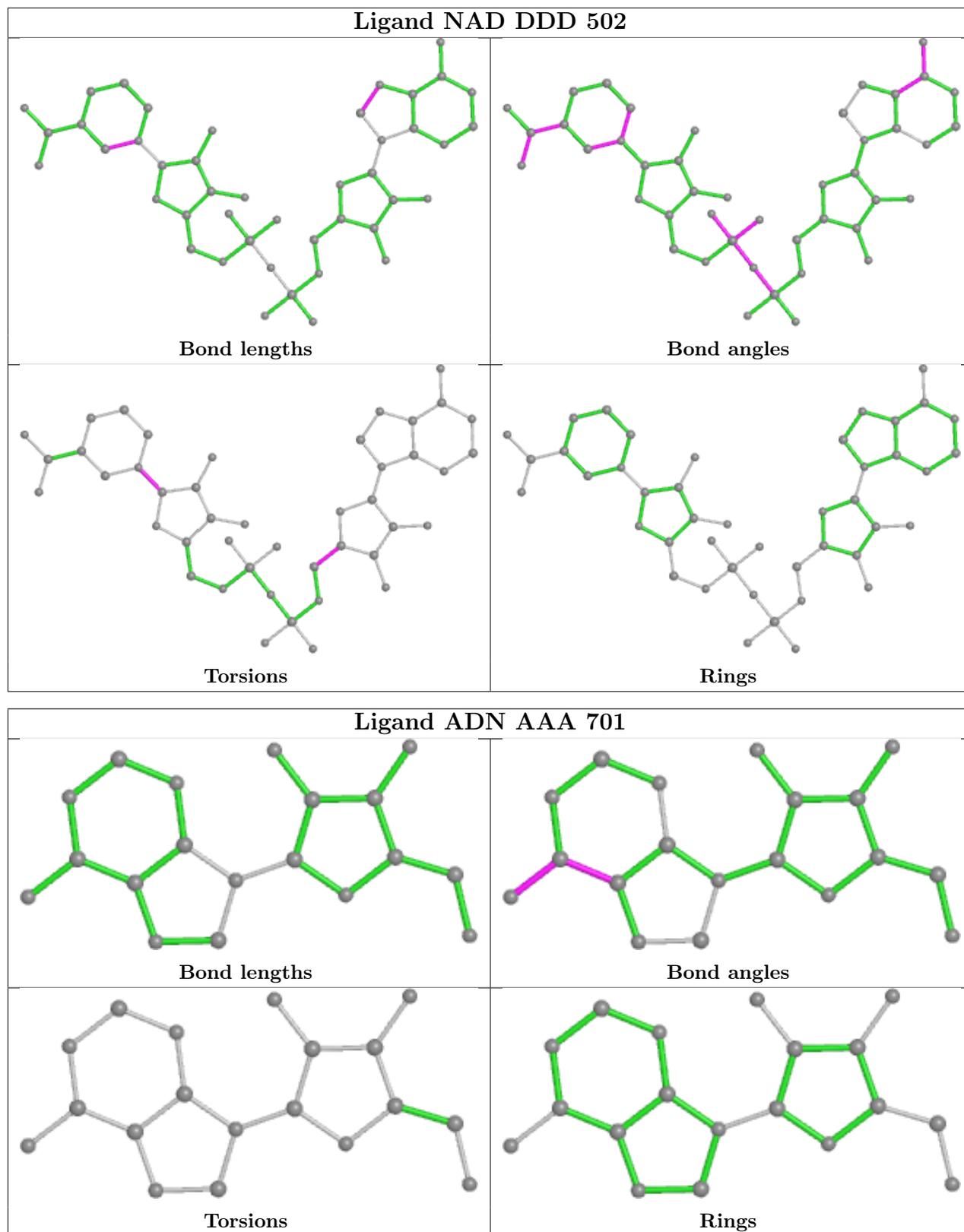
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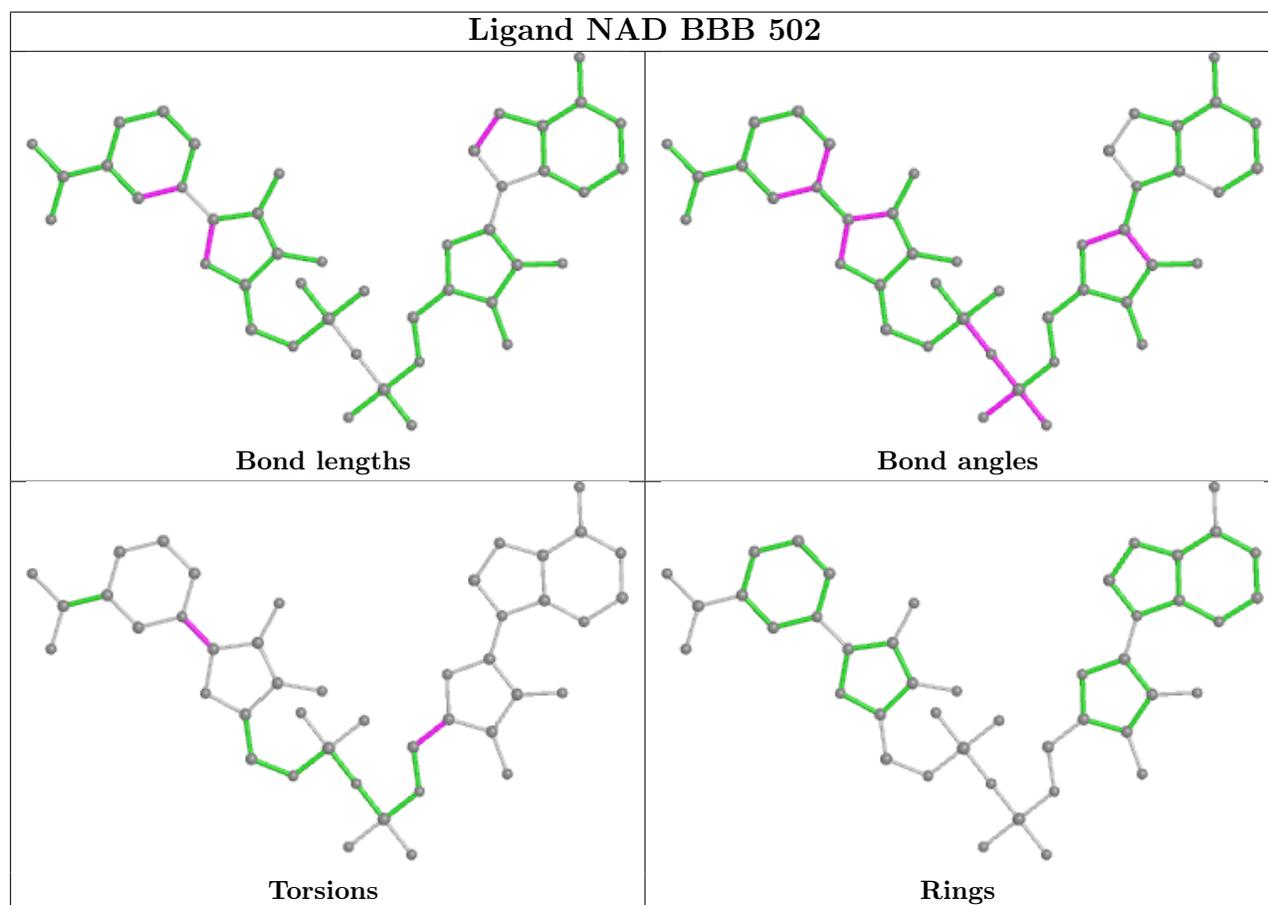
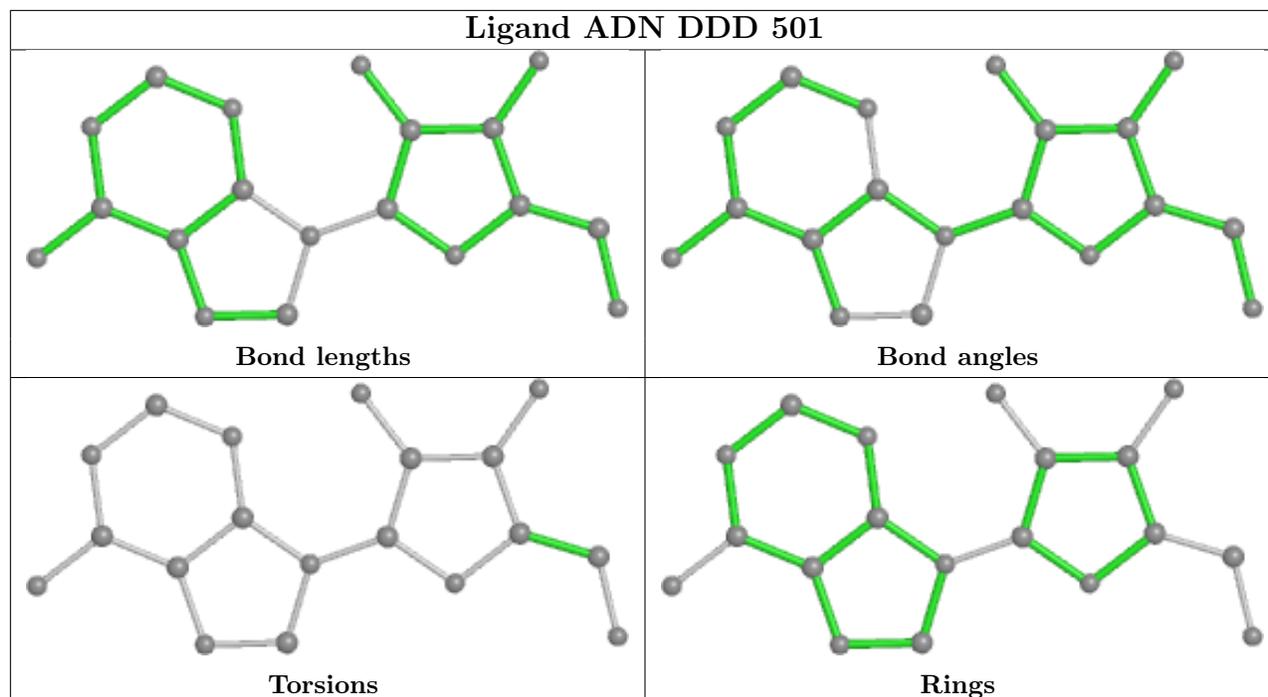
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	502	NAD	1	0
2	BBB	501	ADN	1	0
5	CCC	707	PEG	1	0
4	CCC	703[A]	TRS	2	0
4	BBB	504	TRS	4	0
3	AAA	702	NAD	1	0
4	AAA	704	TRS	4	0
5	DDD	504	PEG	1	0

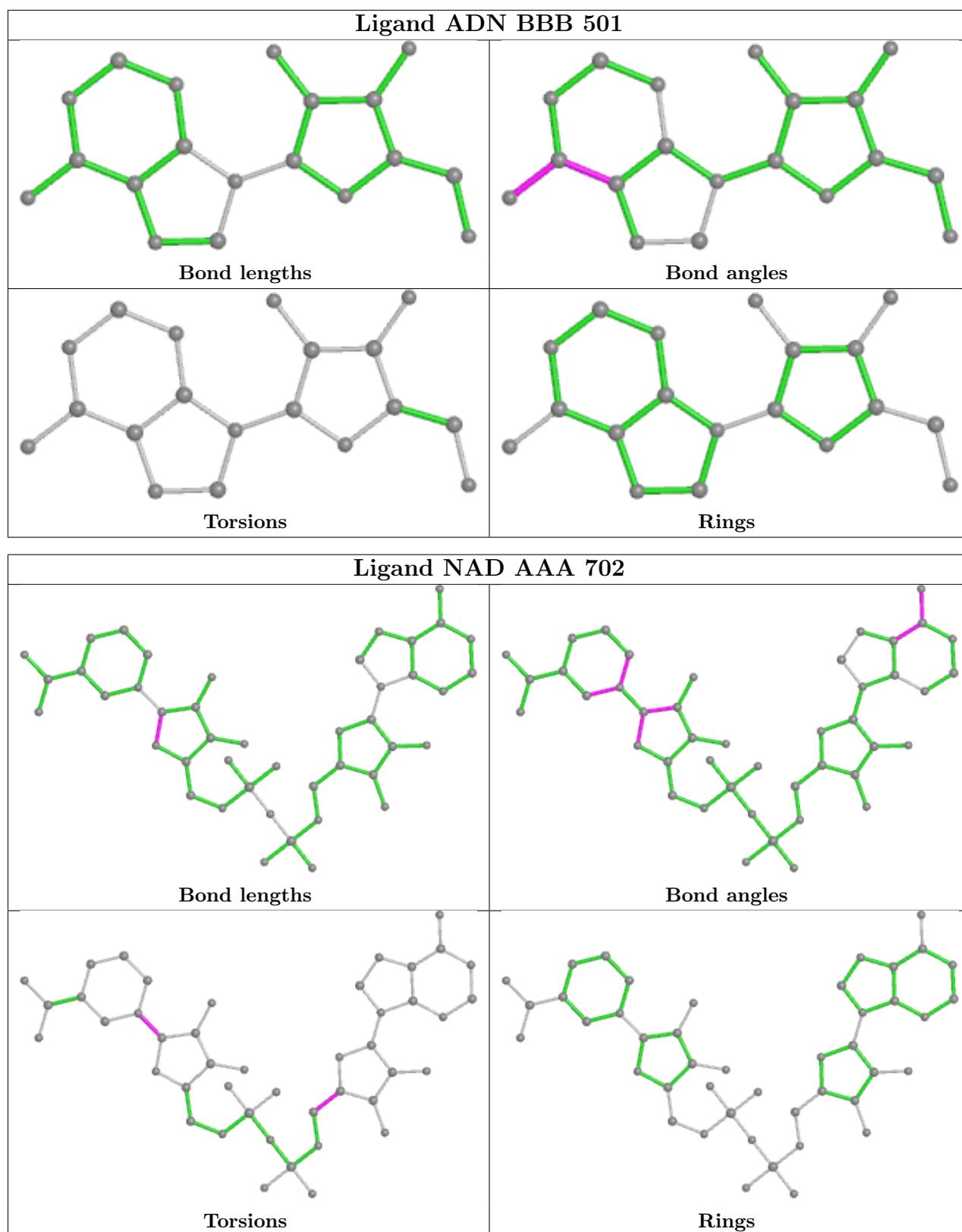
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	AAA	461/472 (97%)	-0.13	8 (1%) 70 75	22, 30, 48, 67	13 (2%)
1	BBB	461/472 (97%)	0.32	38 (8%) 11 12	20, 31, 54, 81	20 (4%)
1	CCC	461/472 (97%)	-0.13	6 (1%) 77 81	20, 28, 44, 61	13 (2%)
1	DDD	461/472 (97%)	0.14	32 (6%) 16 17	20, 31, 54, 72	14 (3%)
All	All	1844/1888 (97%)	0.05	84 (4%) 32 35	20, 30, 51, 81	60 (3%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	9	GLY	7.6
1	BBB	10	PHE	7.4
1	BBB	412	ALA	7.3
1	BBB	324[A]	PHE	6.7
1	BBB	415	ALA	5.8

### 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.

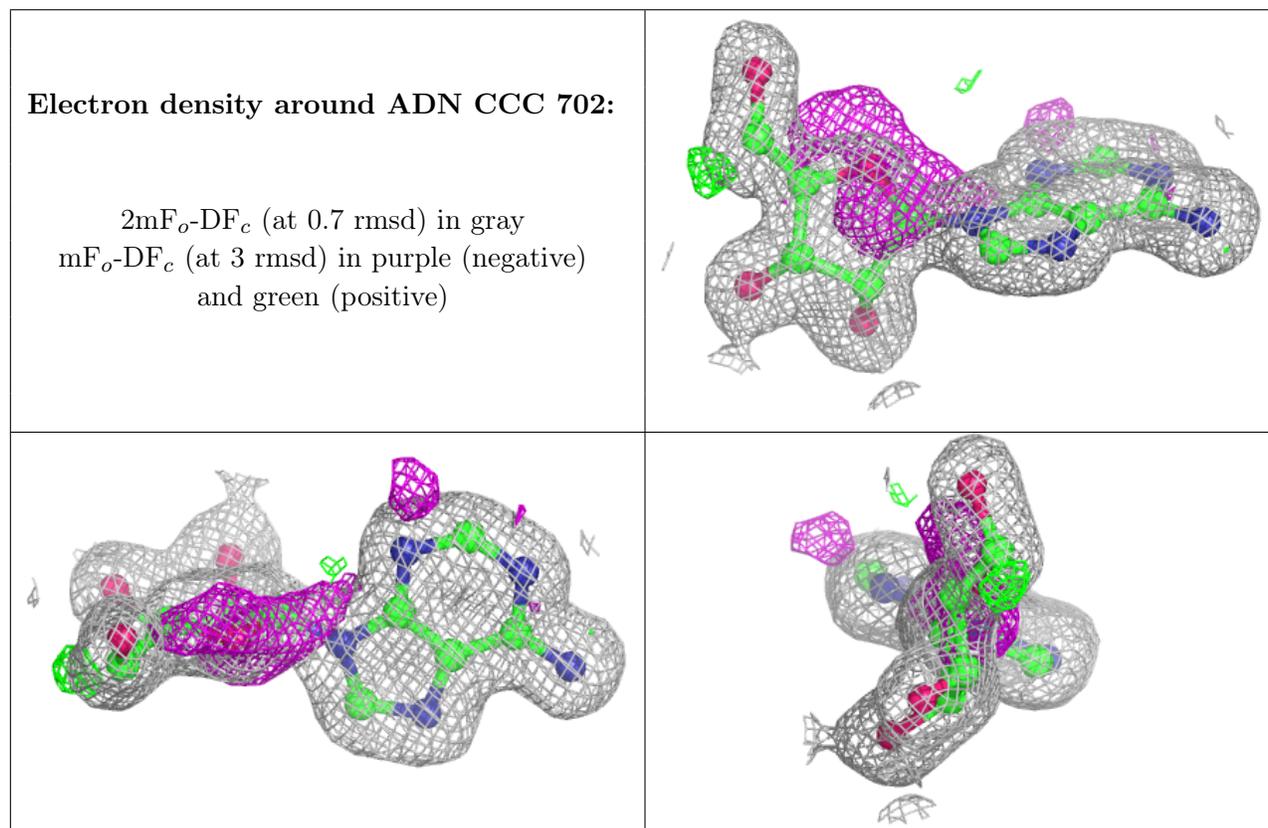
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CL	BBB	508	1/1	0.58	0.10	78,78,78,78	0
4	TRS	CCC	704[B]	8/8	0.63	0.29	55,60,66,72	2
4	TRS	CCC	704[A]	8/8	0.63	0.29	28,60,66,72	2
4	TRS	BBB	503[B]	8/8	0.72	0.25	28,38,43,44	8
4	TRS	BBB	503[A]	8/8	0.72	0.25	20,35,40,44	8
4	TRS	CCC	703[B]	8/8	0.77	0.20	28,42,54,55	2
4	TRS	CCC	703[A]	8/8	0.77	0.20	18,35,46,54	2
4	TRS	AAA	703[B]	8/8	0.78	0.23	35,45,49,58	2
4	TRS	AAA	703[A]	8/8	0.78	0.23	20,44,49,58	2
5	PEG	DDD	504	7/7	0.79	0.25	49,59,69,73	0
5	PEG	CCC	706	7/7	0.79	0.18	66,68,75,76	0
4	TRS	DDD	503[B]	8/8	0.81	0.17	35,43,49,51	2
4	TRS	DDD	503[A]	8/8	0.81	0.17	20,42,45,49	2
4	TRS	AAA	704	8/8	0.84	0.23	40,64,67,75	0
4	TRS	BBB	504	8/8	0.85	0.24	41,48,60,64	4
7	PO4	AAA	707	5/5	0.87	0.19	57,60,75,75	5
7	PO4	DDD	508	5/5	0.88	0.12	27,36,46,50	5
4	TRS	DDD	505	8/8	0.89	0.15	44,59,68,69	2
5	PEG	CCC	707	7/7	0.89	0.38	66,70,73,76	0
8	CL	AAA	708	1/1	0.91	0.20	46,46,46,46	1
8	CL	BBB	507	1/1	0.91	0.21	47,47,47,47	1
5	PEG	AAA	705	7/7	0.91	0.18	66,68,72,75	0
8	CL	DDD	511	1/1	0.92	0.11	49,49,49,49	1
7	PO4	CCC	709	5/5	0.93	0.26	27,56,70,73	2
2	ADN	CCC	702	19/19	0.93	0.09	20,23,36,36	0
8	CL	CCC	710	1/1	0.93	0.15	43,43,43,43	1
8	CL	DDD	510	1/1	0.93	0.07	46,46,46,46	1
7	PO4	CCC	705	5/5	0.93	0.34	48,54,75,75	0
8	CL	DDD	513	1/1	0.93	0.10	54,54,54,54	1
2	ADN	DDD	501	19/19	0.95	0.10	22,24,40,41	0
2	ADN	AAA	701	19/19	0.95	0.09	19,23,40,40	0
8	CL	DDD	509	1/1	0.95	0.18	49,49,49,49	1
2	ADN	BBB	501	19/19	0.96	0.10	21,24,33,35	0
3	NAD	DDD	502	44/44	0.97	0.07	20,22,26,27	0
8	CL	BBB	506	1/1	0.97	0.06	28,28,28,28	1
8	CL	DDD	512	1/1	0.97	0.18	62,62,62,62	1
3	NAD	AAA	702	44/44	0.97	0.06	20,23,27,29	0
6	K	DDD	507	1/1	0.98	0.07	38,38,38,38	0
3	NAD	BBB	502	44/44	0.98	0.07	19,22,25,27	0
3	NAD	CCC	701	44/44	0.98	0.06	19,21,23,26	0
6	K	DDD	506	1/1	0.99	0.09	24,24,24,24	0
6	K	AAA	706	1/1	0.99	0.09	21,21,21,21	1
6	K	BBB	505	1/1	0.99	0.10	23,23,23,23	0

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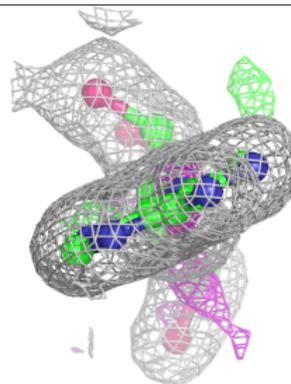
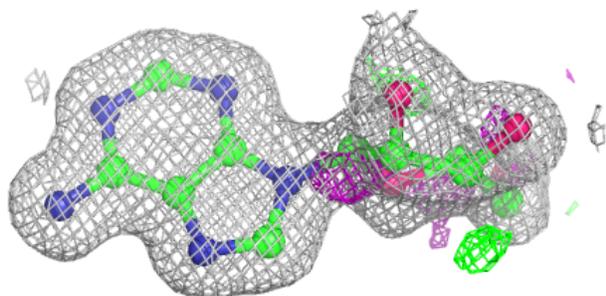
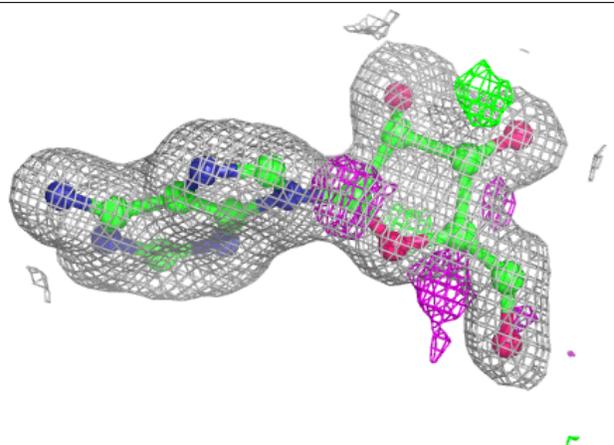
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	K	CCC	708	1/1	0.99	0.10	20,20,20,20	1

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

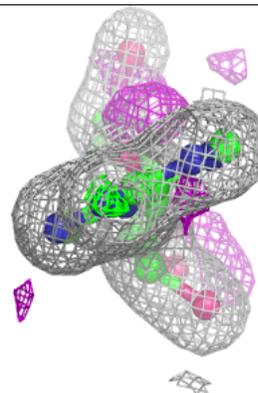
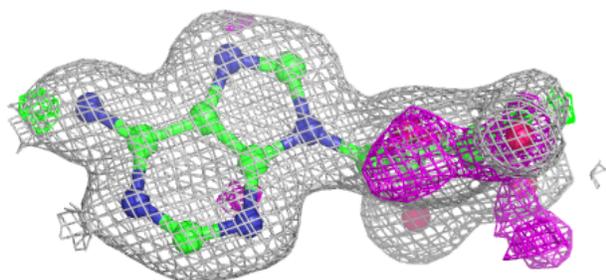
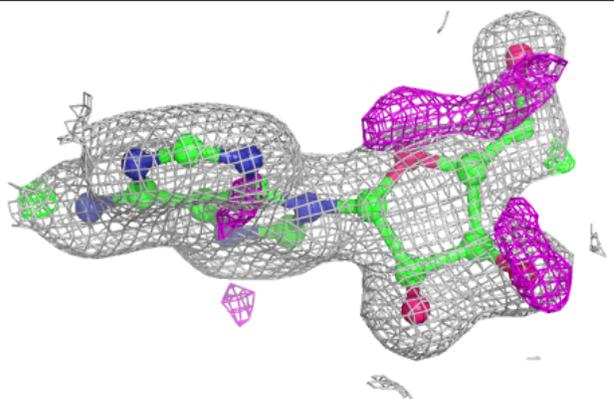


**Electron density around ADN DDD 501:**

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

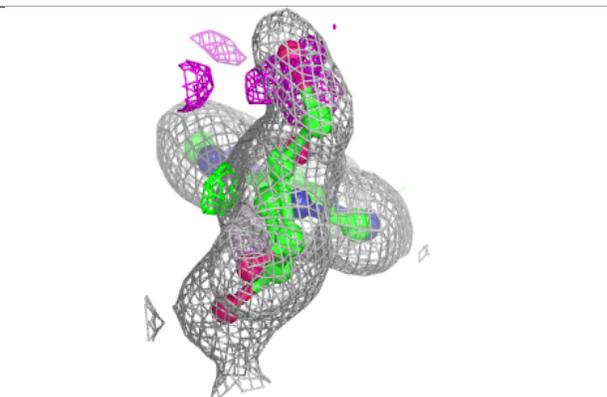
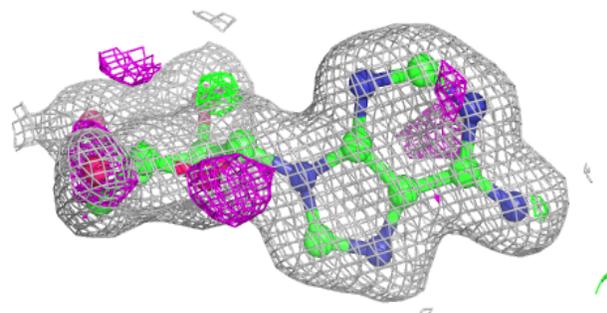
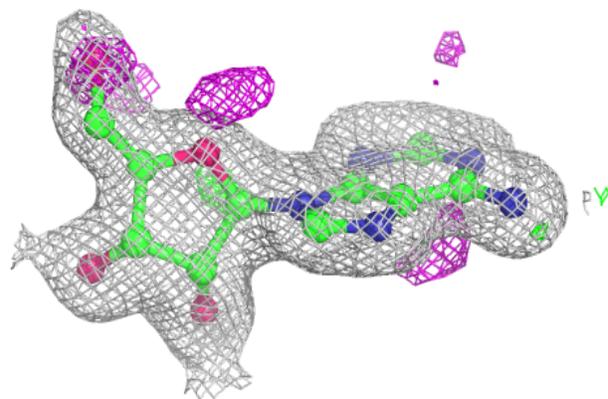
**Electron density around ADN AAA 701:**

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

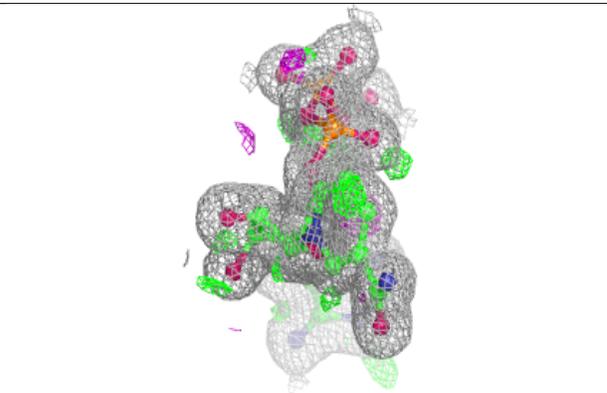
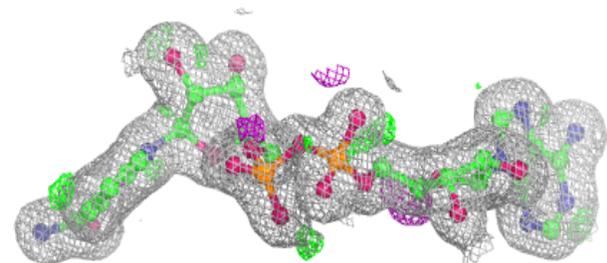
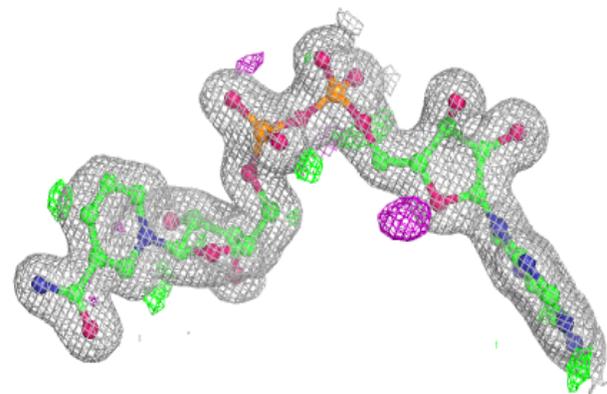


**Electron density around ADN BBB 501:**

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

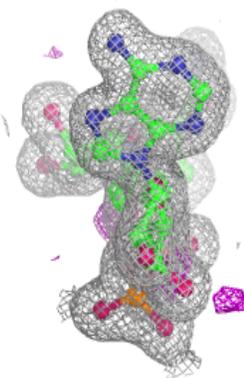
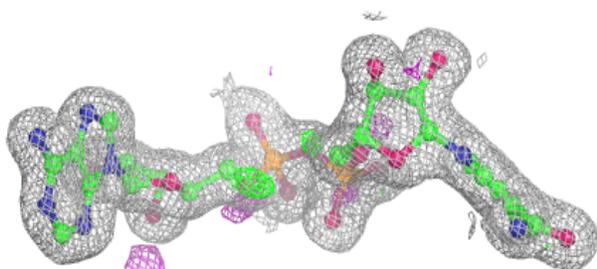
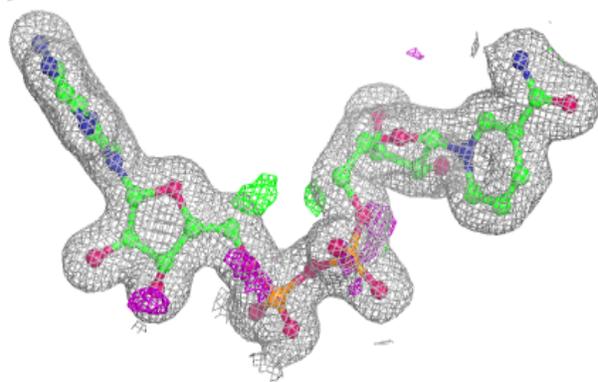
**Electron density around NAD DDD 502:**

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

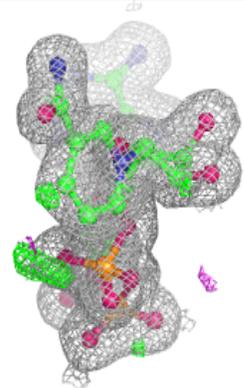
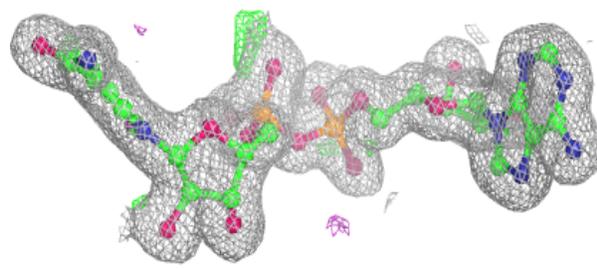
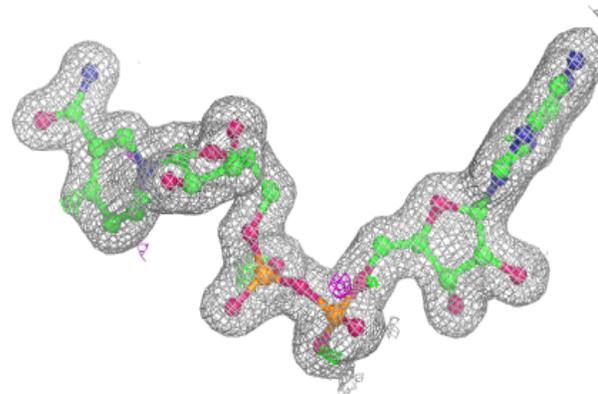


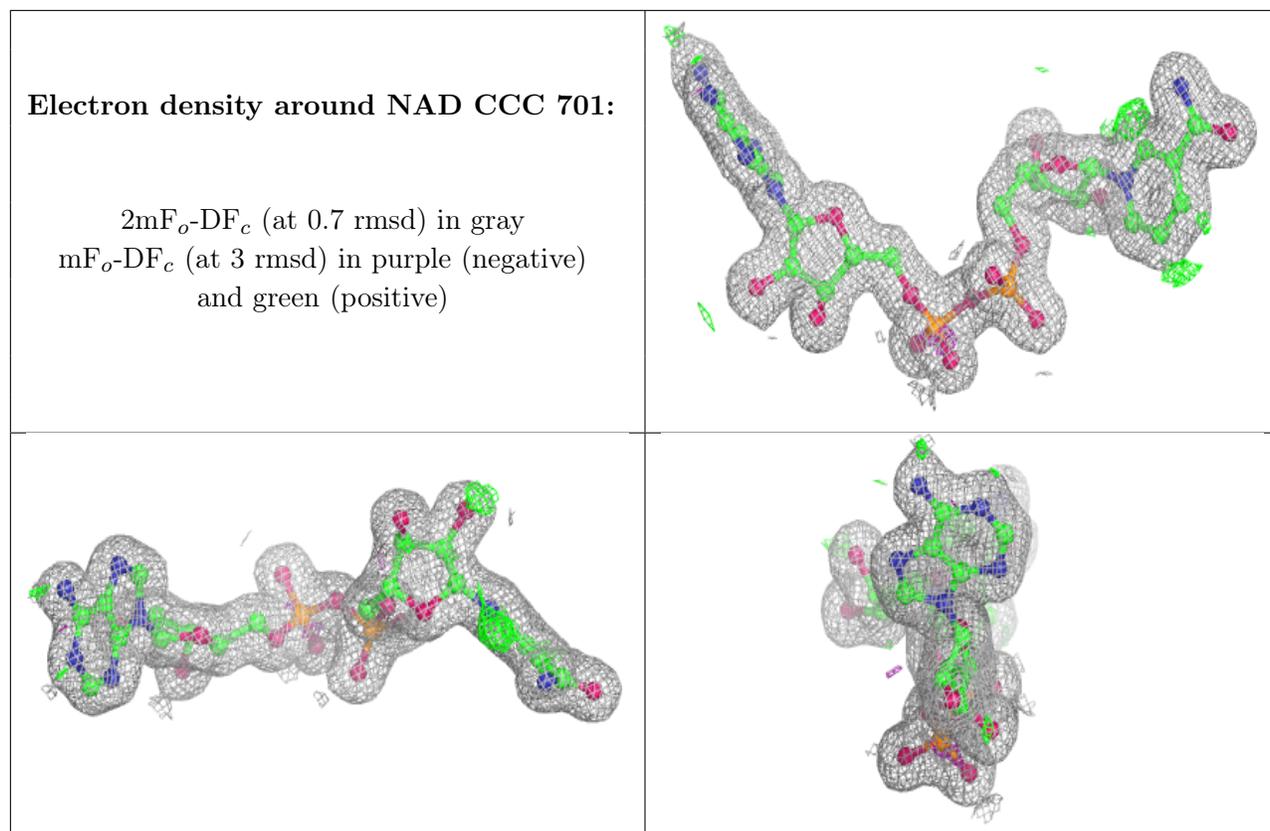
**Electron density around NAD AAA 702:**

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

**Electron density around NAD BBB 502:**

$2mF_o-DF_c$  (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.