



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 02:14 PM UTC

PDB ID : 8AJT / pdb_00008ajt
Title : Crystal structure of the H323A mutant of S-adenosyl-L-homocysteine hydrolase from *Pseudomonas aeruginosa* cocrystallized with adenosine in the presence of K⁺ cations
Authors : Drozdal, P.; Wozniak, K.; Malecki, P.; Gawel, M.; Komorowska, M.; Brzezinski, 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

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>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

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

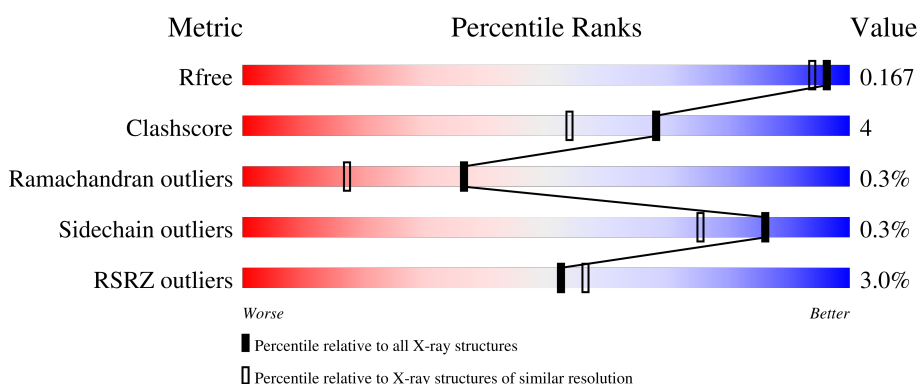
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 ≥ 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% 90% 7%
1	BBB	472	3% 89% 8%
1	CCC	472	2% 92% 6%
1	DDD	472	4% 91% 7%

2 Entry composition

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.

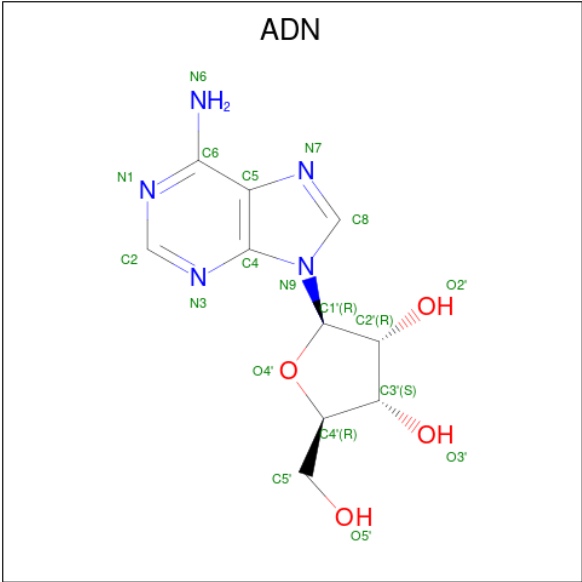
- Molecule 1 is a protein called Adenosylhomocysteinase.

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

There are 16 discrepancies between the modelled and reference sequences:

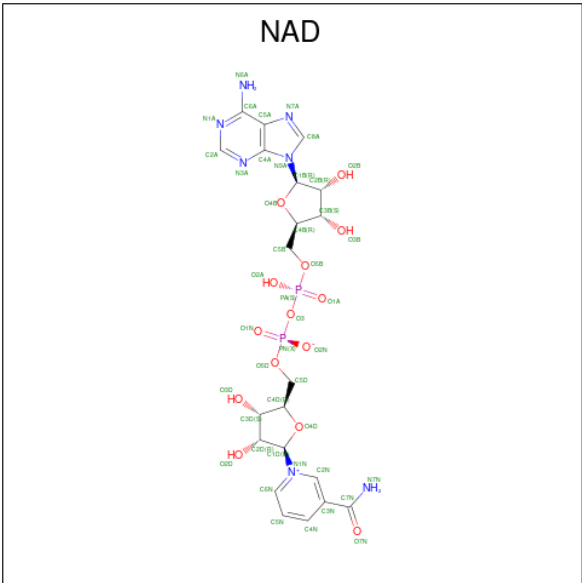
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	SER	-	expression tag	UNP Q9I685
AAA	-1	ASN	-	expression tag	UNP Q9I685
AAA	0	ALA	-	expression tag	UNP Q9I685
AAA	323	ALA	HIS	engineered mutation	UNP Q9I685
BBB	-2	SER	-	expression tag	UNP Q9I685
BBB	-1	ASN	-	expression tag	UNP Q9I685
BBB	0	ALA	-	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 (CCD ID: ADN) (formula: C₁₀H₁₃N₅O₄) (labeled as "Ligand of Interest" by depositor).



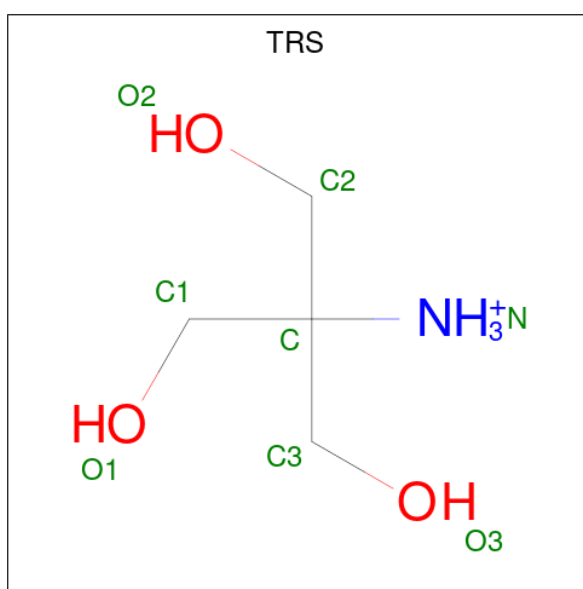
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			19	10	5	4		
2	BBB	1	Total	C	N	O	0	0
			19	10	5	4		
2	CCC	1	Total	C	N	O	0	0
			19	10	5	4		
2	DDD	1	Total	C	N	O	0	0
			19	10	5	4		

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



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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

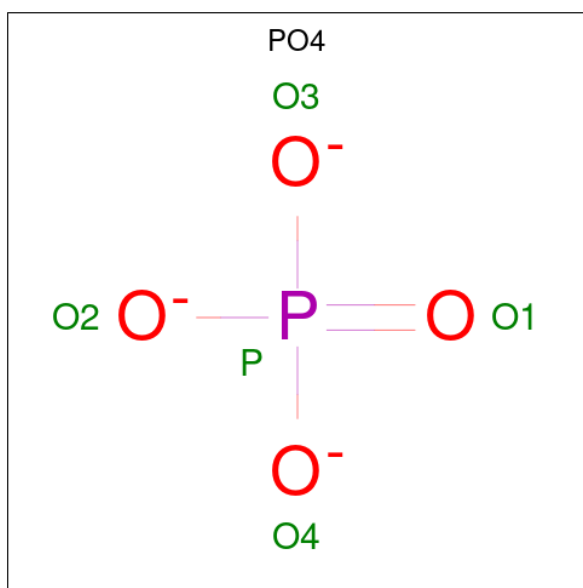


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			7	4	3		
5	CCC	1	Total	C	O	0	0
			7	4	3		
5	CCC	1	Total	C	O	0	0
			7	4	3		
5	DDD	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 9 is water.

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

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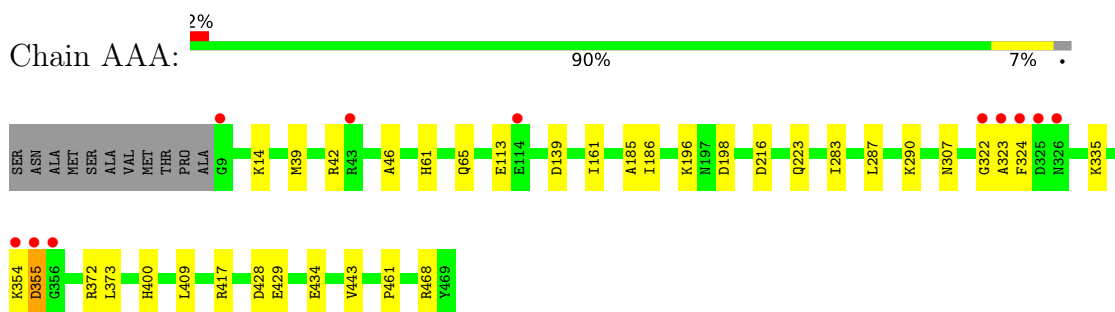
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	BBB	376	Total 376	O 376	0	0
9	CCC	430	Total 430	O 430	0	0
9	DDD	362	Total 362	O 362	0	0

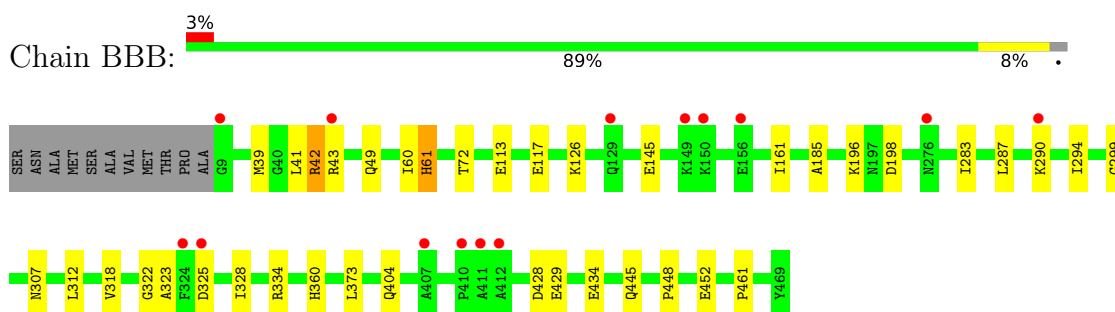
3 Residue-property plots [i](#)

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.

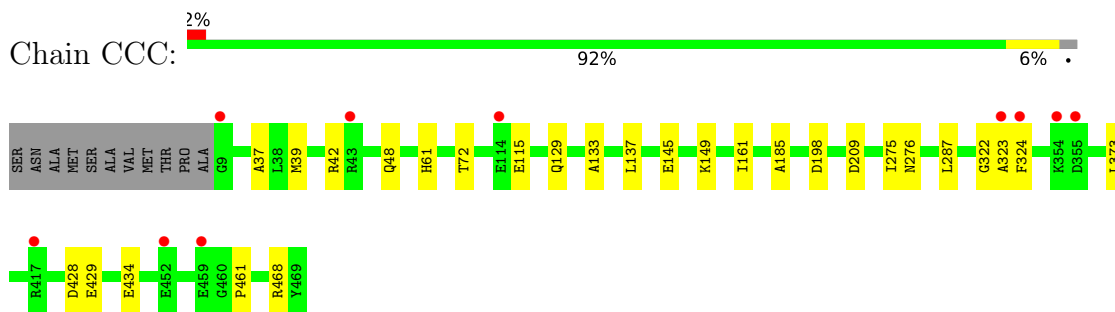
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase

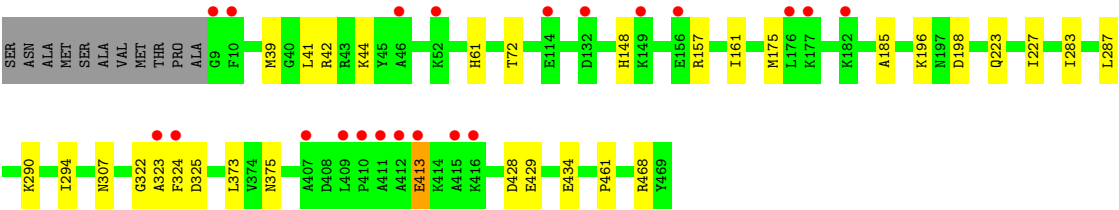


- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.152 , 0.167 0.152 , 0.167	Depositor DCC
R_{free} test set	1045 reflections (0.27%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
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	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	16457	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, K, PEG, TRS, ADN, PO4, NAD

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	1.02	1/3696 (0.0%)	1.14	4/4995 (0.1%)
1	BBB	1.03	5/3722 (0.1%)	1.12	3/5031 (0.1%)
1	CCC	1.05	4/3674 (0.1%)	1.13	4/4965 (0.1%)
1	DDD	1.01	2/3672 (0.1%)	1.13	4/4963 (0.1%)
All	All	1.03	12/14764 (0.1%)	1.13	15/19954 (0.1%)

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 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	145	GLU	CD-OE1	-10.38	1.05	1.25
1	BBB	117	GLU	CG-CD	-7.02	1.34	1.52
1	BBB	325	ASP	C-O	6.34	1.32	1.24
1	CCC	133	ALA	C-O	6.08	1.31	1.23
1	AAA	443	VAL	C-O	5.90	1.31	1.24

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	117	GLU	CB-CG-CD	11.18	131.60	112.60
1	DDD	428	ASP	CA-CB-CG	6.72	119.32	112.60
1	AAA	428	ASP	CA-CB-CG	6.71	119.31	112.60
1	BBB	428	ASP	CA-CB-CG	6.50	119.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	198	ASP	CA-CB-CG	6.37	118.97	112.60

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3631	0	3639	26	0
1	BBB	3650	0	3664	31	0
1	CCC	3608	0	3618	24	0
1	DDD	3604	0	3617	24	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	0	0
4	DDD	18	0	18	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
8	DDD	5	0	0	0	0
9	AAA	407	0	0	6	0
9	BBB	376	0	0	6	0
9	CCC	430	0	0	2	0
9	DDD	362	0	0	3	0
All	All	16457	0	14812	106	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 106 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: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
1:CCC:322[A]:GLY:O	1:CCC:373:LEU:CD2	2.10	0.99
1:DDD:148:HIS:CG	1:DDD:175:MET:HE1	2.05	0.92
1:CCC:322[B]:GLY:O	1:CCC:373:LEU:HD23	1.73	0.88

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%)	30	12
1	BBB	473/472 (100%)	457 (97%)	15 (3%)	1 (0%)	43	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CCC	467/472 (99%)	458 (98%)	8 (2%)	1 (0%)	43	22
1	DDD	467/472 (99%)	459 (98%)	7 (2%)	1 (0%)	43	22
All	All	1876/1888 (99%)	1832 (98%)	39 (2%)	5 (0%)	36	17

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 ⓘ

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%)	86	75
1	BBB	388/384 (101%)	386 (100%)	2 (0%)	81	66
1	CCC	383/384 (100%)	382 (100%)	1 (0%)	86	75
1	DDD	383/384 (100%)	383 (100%)	0	100	100
All	All	1540/1536 (100%)	1536 (100%)	4 (0%)	86	75

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 ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
5	PEG	CCC	707	-	6,6,6	0.22	0	5,5,5	0.12	0
3	NAD	AAA	702	-	46,48,48	0.87	3 (6%)	64,73,73	0.70	1 (1%)
4	TRS	CCC	704[B]	-	7,7,7	0.23	0	9,9,9	0.27	0
4	TRS	BBB	503[B]	-	7,7,7	0.46	0	9,9,9	0.78	0
4	TRS	DDD	503[B]	-	7,7,7	0.48	0	9,9,9	0.58	0
7	PO4	CCC	709	-	4,4,4	1.31	1 (25%)	6,6,6	1.07	0
5	PEG	AAA	705	-	6,6,6	0.12	0	5,5,5	0.07	0
4	TRS	AAA	703[B]	-	7,7,7	0.41	0	9,9,9	0.77	0
5	PEG	DDD	504	-	6,6,6	0.17	0	5,5,5	0.04	0
2	ADN	DDD	501	-	21,21,21	0.32	0	31,31,31	0.71	1 (3%)
4	TRS	BBB	504	-	7,7,7	0.25	0	9,9,9	0.31	0
4	TRS	AAA	704	-	7,7,7	0.24	0	9,9,9	0.32	0
4	TRS	CCC	703[B]	-	7,7,7	0.52	0	9,9,9	0.89	0
4	TRS	CCC	704[A]	-	7,7,7	0.21	0	9,9,9	0.16	0
7	PO4	CCC	705	-	4,4,4	0.60	0	6,6,6	0.40	0
3	NAD	DDD	502	-	46,48,48	0.95	2 (4%)	64,73,73	0.90	3 (4%)
4	TRS	BBB	503[A]	-	7,7,7	0.44	0	9,9,9	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TRS	DDD	503[A]	-	7,7,7	0.50	0	9,9,9	0.80	0
5	PEG	CCC	706	-	6,6,6	0.11	0	5,5,5	0.06	0
4	TRS	DDD	505	-	7,7,7	0.22	0	9,9,9	0.35	0
2	ADN	BBB	501	-	21,21,21	0.35	0	31,31,31	0.58	0
3	NAD	CCC	701	-	46,48,48	0.82	2 (4%)	64,73,73	0.74	0
7	PO4	AAA	707	-	4,4,4	0.87	0	6,6,6	0.44	0
4	TRS	AAA	703[A]	-	7,7,7	0.39	0	9,9,9	0.71	0
7	PO4	DDD	508	-	4,4,4	1.41	1 (25%)	6,6,6	0.68	0
3	NAD	BBB	502	-	46,48,48	0.99	3 (6%)	64,73,73	0.91	3 (4%)
2	ADN	AAA	701	-	21,21,21	0.41	0	31,31,31	0.94	1 (3%)
4	TRS	CCC	703[A]	-	7,7,7	0.53	0	9,9,9	0.92	0
2	ADN	CCC	702	-	21,21,21	0.38	0	31,31,31	0.69	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
5	PEG	CCC	707	-	-	3/4/4/4	-
3	NAD	AAA	702	-	-	4/30/62/62	0/5/5/5
4	TRS	CCC	704[B]	-	-	3/9/9/9	-
4	TRS	BBB	503[B]	-	-	6/9/9/9	-
4	TRS	DDD	503[B]	-	-	6/9/9/9	-
5	PEG	AAA	705	-	-	0/4/4/4	-
4	TRS	AAA	703[B]	-	-	6/9/9/9	-
5	PEG	DDD	504	-	-	3/4/4/4	-
2	ADN	DDD	501	-	-	0/6/22/22	0/3/3/3
4	TRS	BBB	504	-	-	5/9/9/9	-
4	TRS	AAA	704	-	-	6/9/9/9	-
4	TRS	CCC	703[B]	-	-	4/9/9/9	-
4	TRS	CCC	704[A]	-	-	3/9/9/9	-
3	NAD	DDD	502	-	-	4/30/62/62	0/5/5/5
4	TRS	BBB	503[A]	-	-	6/9/9/9	-
4	TRS	DDD	503[A]	-	-	6/9/9/9	-
5	PEG	CCC	706	-	-	1/4/4/4	-
4	TRS	DDD	505	-	-	8/9/9/9	-
2	ADN	BBB	501	-	-	0/6/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	CCC	701	-	-	4/30/62/62	0/5/5/5
4	TRS	AAA	703[A]	-	-	6/9/9/9	-
3	NAD	BBB	502	-	-	4/30/62/62	0/5/5/5
2	ADN	AAA	701	-	-	0/6/22/22	0/3/3/3
4	TRS	CCC	703[A]	-	-	5/9/9/9	-
2	ADN	CCC	702	-	-	0/6/22/22	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DDD	502	NAD	C2N-N1N	4.06	1.39	1.35
3	CCC	701	NAD	O4D-C1D	3.51	1.45	1.40
3	BBB	502	NAD	C2N-N1N	3.36	1.38	1.35
3	AAA	702	NAD	O4D-C1D	3.28	1.45	1.40
3	BBB	502	NAD	O4D-C1D	3.12	1.45	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	502	NAD	C6N-N1N-C2N	-4.23	118.28	121.88
3	AAA	702	NAD	C6N-N1N-C2N	-3.20	119.15	121.88
3	DDD	502	NAD	C6N-N1N-C2N	-3.15	119.19	121.88
3	DDD	502	NAD	O2N-PN-O1N	2.73	125.17	112.44
3	BBB	502	NAD	O2A-PA-O1A	2.53	124.22	112.44

There are no chirality outliers.

5 of 93 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.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	CCC	707	PEG	1	0

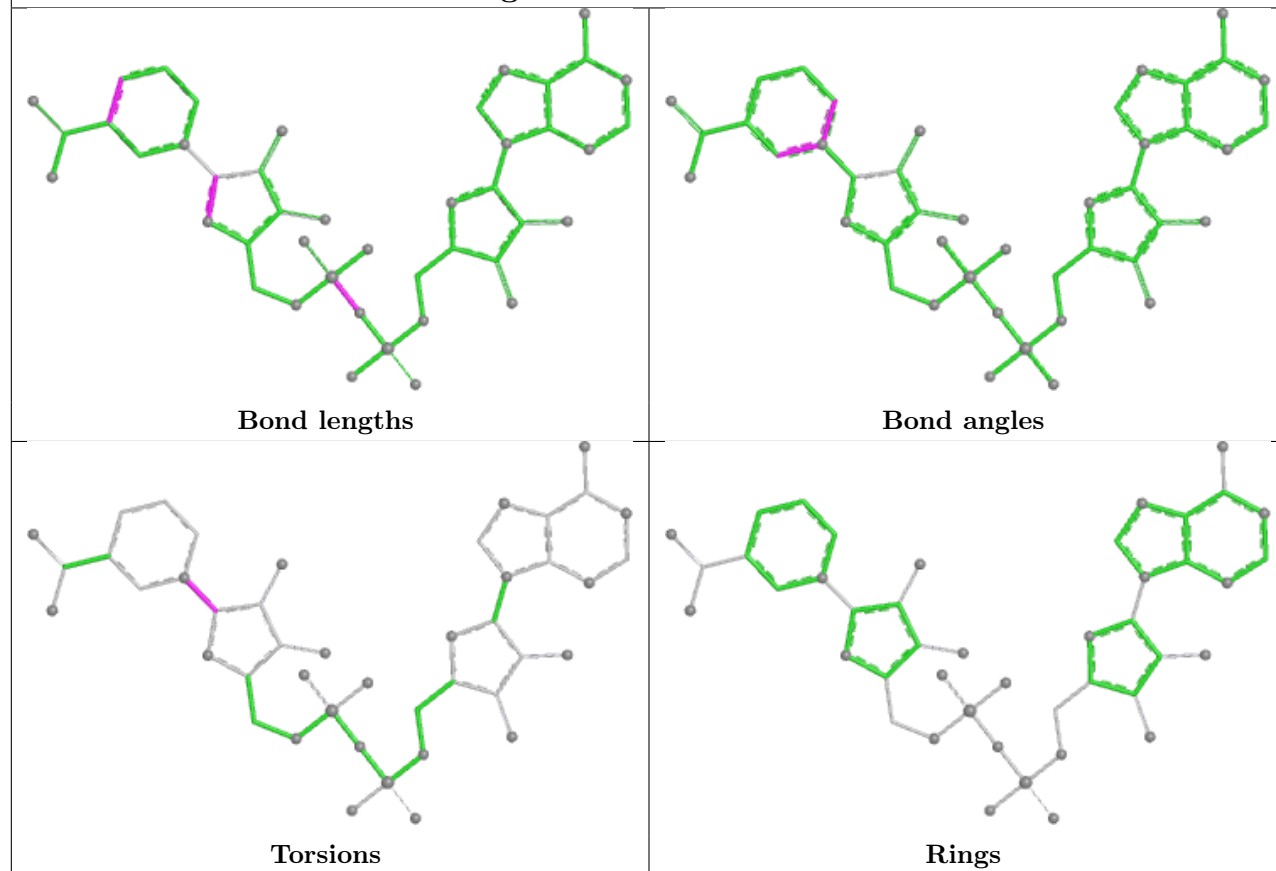
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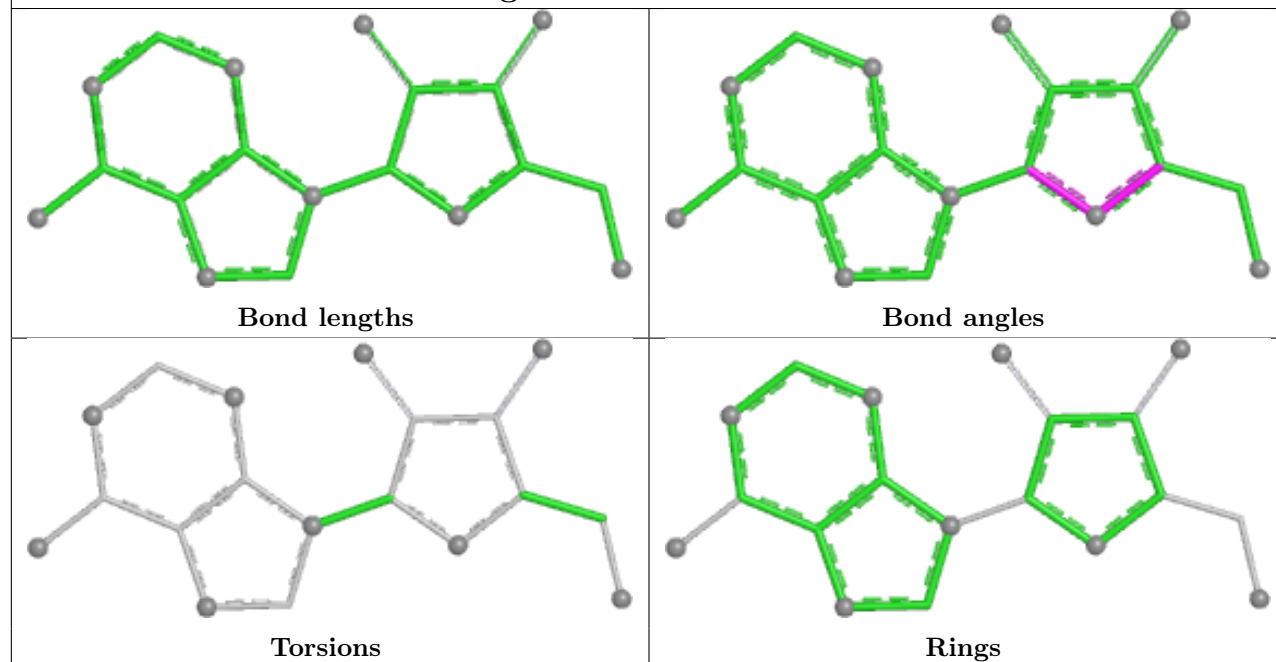
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	702	NAD	1	0
5	DDD	504	PEG	1	0
2	DDD	501	ADN	1	0
4	BBB	504	TRS	4	0
4	AAA	704	TRS	4	0
3	DDD	502	NAD	3	0
4	DDD	505	TRS	4	0
2	BBB	501	ADN	1	0
3	CCC	701	NAD	1	0
3	BBB	502	NAD	1	0
2	AAA	701	ADN	2	0
2	CCC	702	ADN	1	0

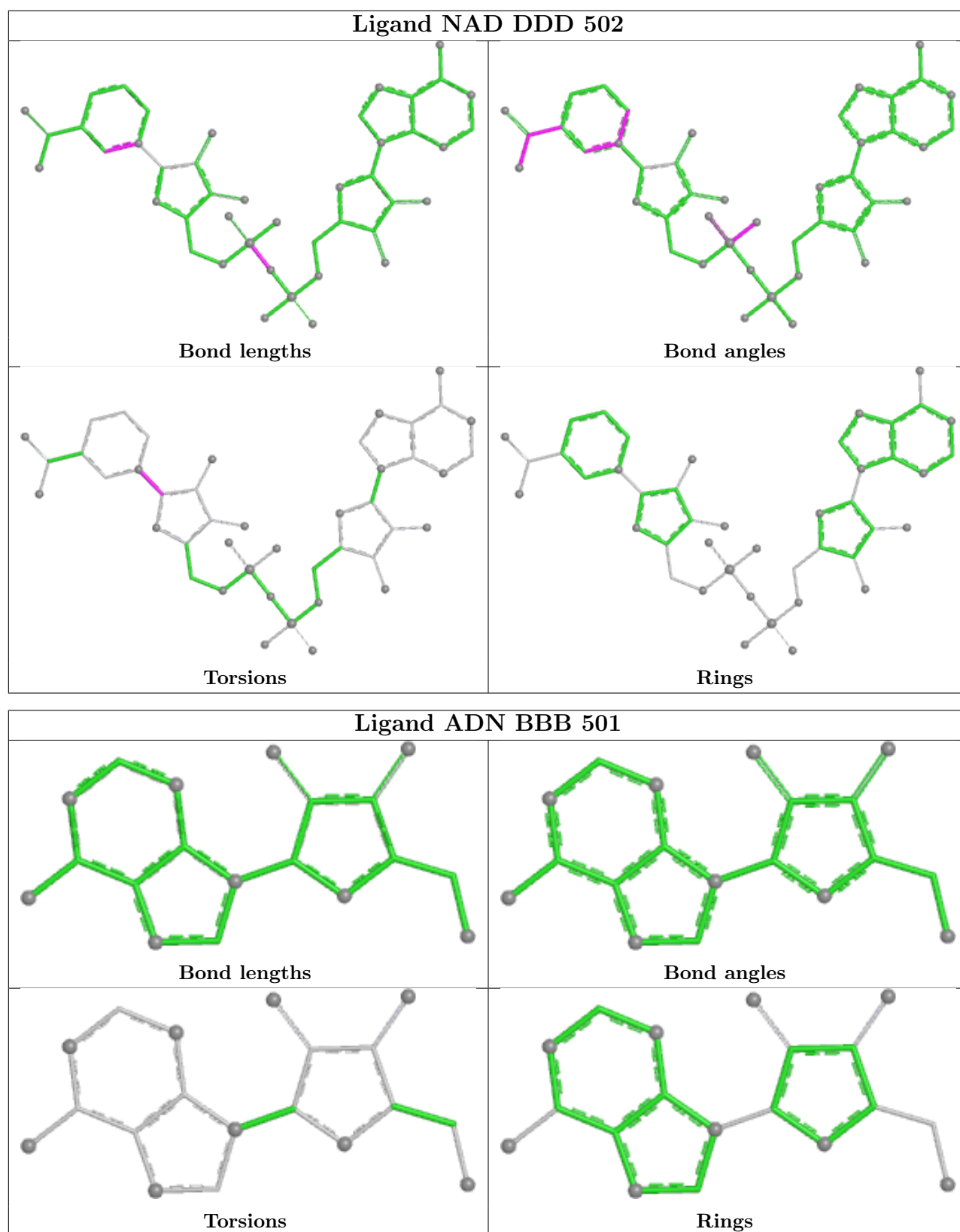
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

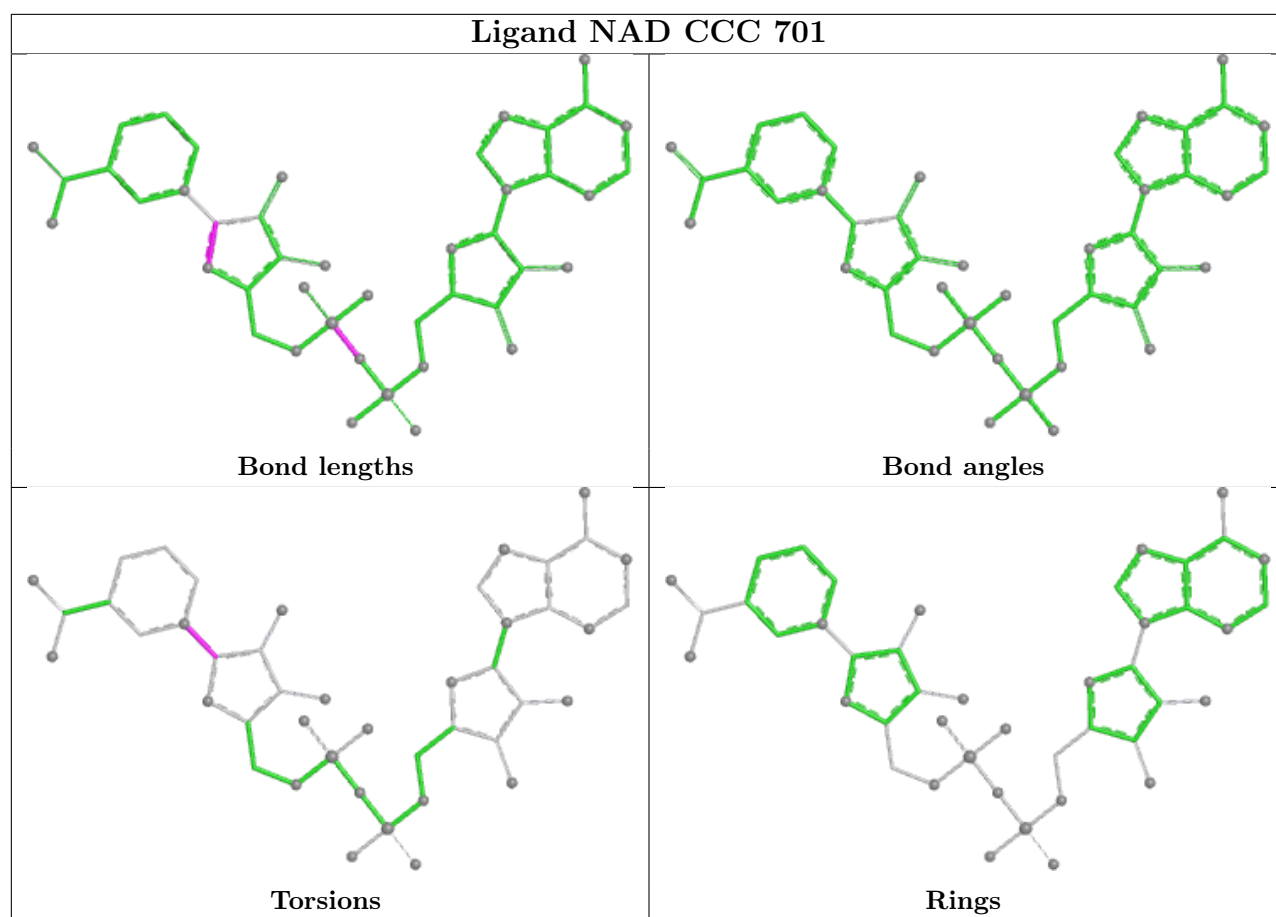
Ligand NAD AAA 702



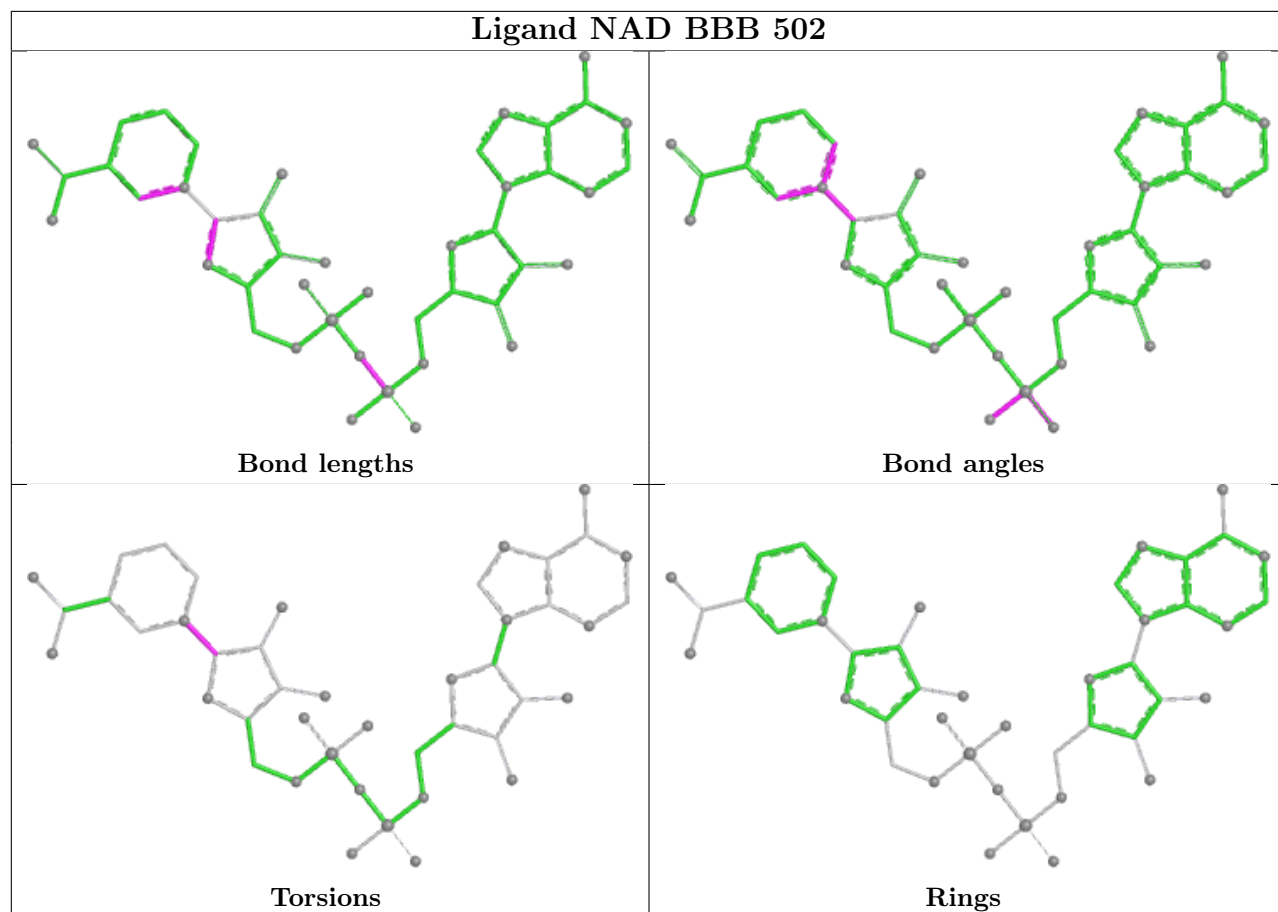
Ligand ADN DDD 501



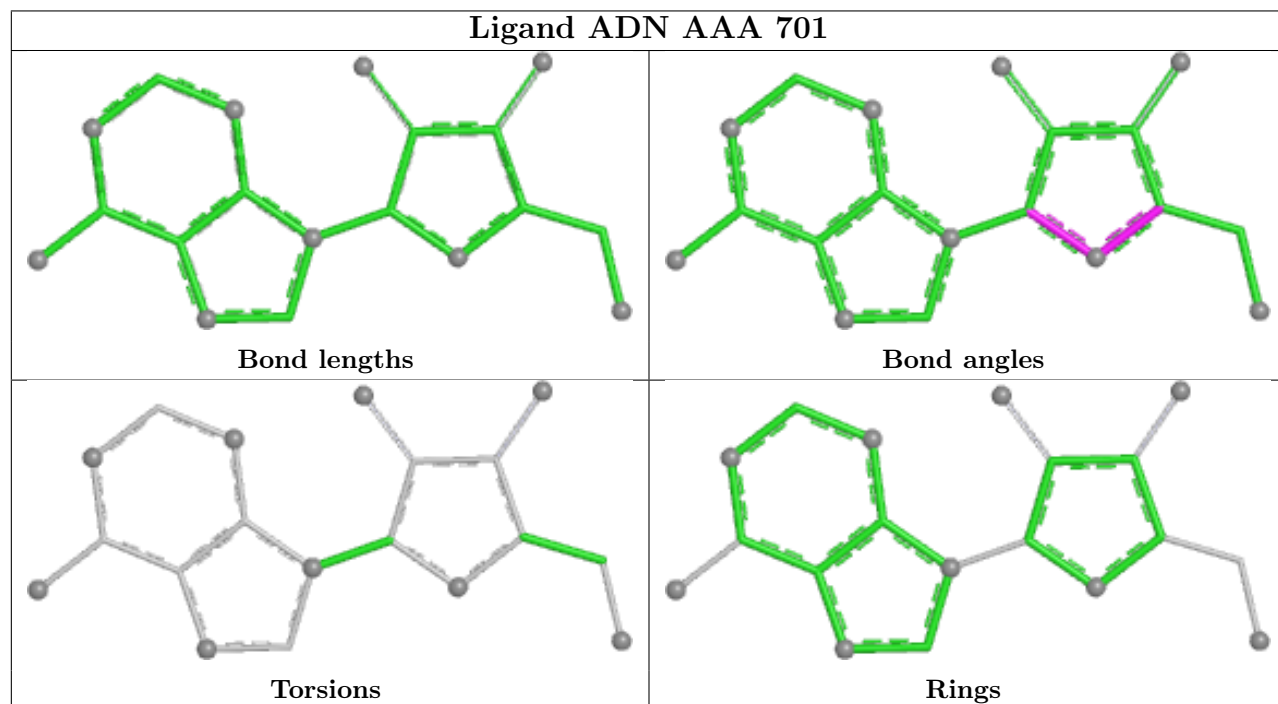


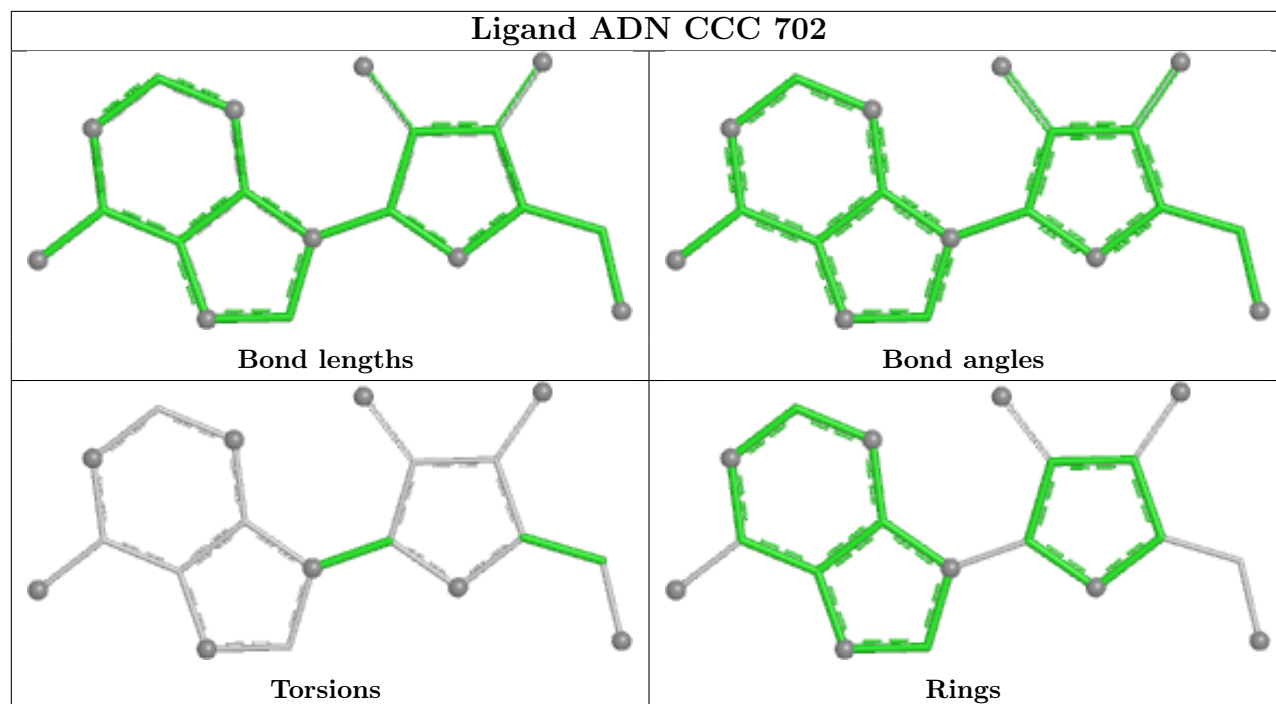


Ligand NAD BBB 502



Ligand ADN AAA 701





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, 95th 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 ²)	Q<0.9
1	AAA	461/472 (97%)	0.07	11 (2%) 59 63	12, 29, 47, 63	23 (4%)
1	BBB	461/472 (97%)	0.16	14 (3%) 52 56	12, 30, 54, 81	33 (7%)
1	CCC	461/472 (97%)	-0.00	10 (2%) 62 66	12, 27, 44, 61	21 (4%)
1	DDD	461/472 (97%)	0.18	21 (4%) 37 41	11, 31, 53, 70	22 (4%)
All	All	1844/1888 (97%)	0.10	56 (3%) 52 56	11, 29, 50, 81	99 (5%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	355	ASP	13.2
1	BBB	324[A]	PHE	9.1
1	AAA	355	ASP	8.1
1	BBB	43	ARG	6.7
1	DDD	416	LYS	6.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	DDD	504	7/7	0.75	0.25	49,59,69,73	0
7	PO4	CCC	705	5/5	0.81	0.12	48,54,75,75	0
8	CL	DDD	512	1/1	0.84	0.40	62,62,62,62	1
4	TRS	DDD	505	8/8	0.85	0.23	44,59,68,69	2
4	TRS	BBB	503[A]	8/8	0.85	0.23	20,35,40,44	8
4	TRS	BBB	503[B]	8/8	0.85	0.23	28,38,43,44	8
8	CL	AAA	708	1/1	0.85	0.18	46,46,46,46	1
4	TRS	BBB	504	8/8	0.85	0.27	41,48,60,64	4
5	PEG	AAA	705	7/7	0.86	0.17	66,68,72,75	0
7	PO4	CCC	709	5/5	0.86	0.10	27,56,70,73	2
4	TRS	AAA	704	8/8	0.86	0.16	40,64,67,75	0
7	PO4	AAA	707	5/5	0.86	0.13	57,60,75,75	5
4	TRS	AAA	703[A]	8/8	0.87	0.20	20,44,49,58	2
4	TRS	AAA	703[B]	8/8	0.87	0.20	35,45,49,58	2
8	CL	BBB	508	1/1	0.87	0.20	78,78,78,78	0
5	PEG	CCC	707	7/7	0.87	0.15	66,70,73,76	0
4	TRS	DDD	503[A]	8/8	0.88	0.17	20,42,45,49	2
4	TRS	DDD	503[B]	8/8	0.88	0.17	35,43,49,51	2
4	TRS	CCC	704[A]	8/8	0.88	0.14	28,60,66,72	2
4	TRS	CCC	704[B]	8/8	0.88	0.14	55,60,66,72	2
5	PEG	CCC	706	7/7	0.89	0.14	66,68,75,76	0
8	CL	BBB	507	1/1	0.89	0.17	47,47,47,47	1
4	TRS	CCC	703[A]	8/8	0.89	0.18	18,35,46,54	2
8	CL	DDD	509	1/1	0.89	0.20	49,49,49,49	1
8	CL	DDD	511	1/1	0.89	0.13	49,49,49,49	1
4	TRS	CCC	703[B]	8/8	0.89	0.18	28,42,54,55	2
8	CL	DDD	513	1/1	0.89	0.27	54,54,54,54	1
8	CL	CCC	710	1/1	0.90	0.15	43,43,43,43	1
7	PO4	DDD	508	5/5	0.91	0.12	27,36,46,50	5
8	CL	DDD	510	1/1	0.93	0.12	46,46,46,46	1
2	ADN	CCC	702	19/19	0.94	0.08	20,23,36,36	0
2	ADN	DDD	501	19/19	0.95	0.08	22,24,40,41	0
6	K	DDD	507	1/1	0.96	0.11	38,38,38,38	0
2	ADN	AAA	701	19/19	0.96	0.08	19,23,40,40	0
2	ADN	BBB	501	19/19	0.97	0.06	21,24,33,35	0
8	CL	BBB	506	1/1	0.97	0.07	28,28,28,28	1
3	NAD	BBB	502	44/44	0.98	0.05	19,22,25,27	0
3	NAD	CCC	701	44/44	0.98	0.05	19,21,23,26	0
3	NAD	DDD	502	44/44	0.98	0.06	20,22,26,27	0
3	NAD	AAA	702	44/44	0.98	0.05	20,23,27,29	0
6	K	BBB	505	1/1	0.98	0.06	23,23,23,23	0
6	K	AAA	706	1/1	0.99	0.06	21,21,21,21	1
6	K	CCC	708	1/1	0.99	0.04	20,20,20,20	1

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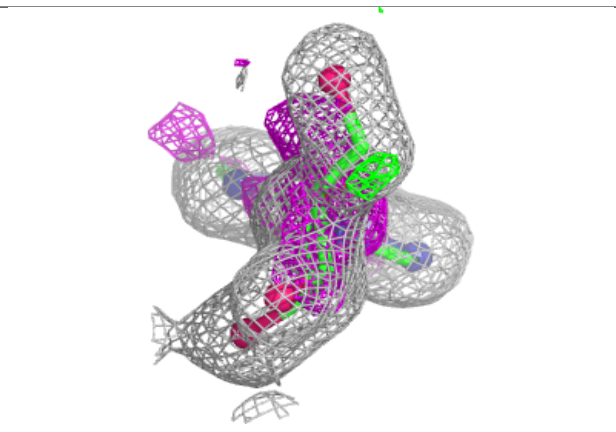
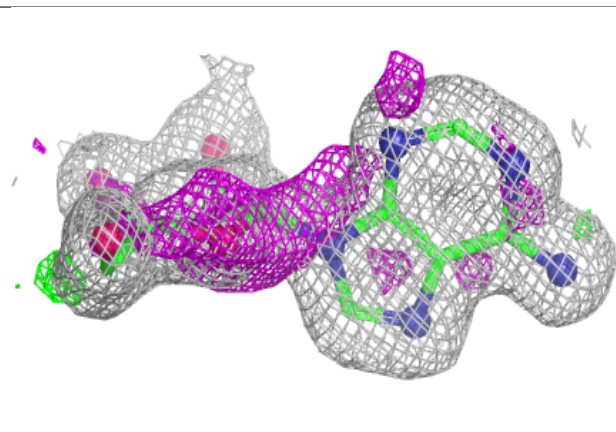
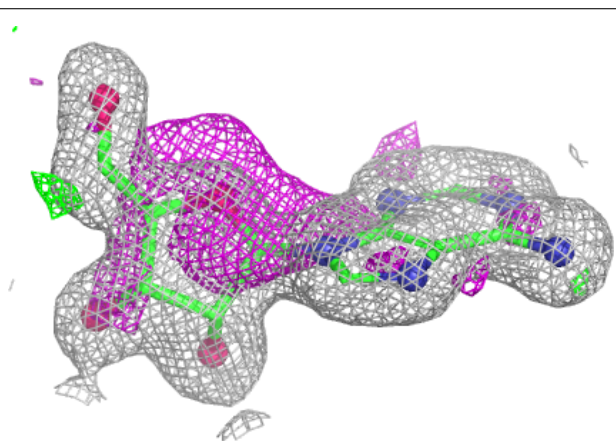
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	K	DDD	506	1/1	0.99	0.05	24,24,24,24	0

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.

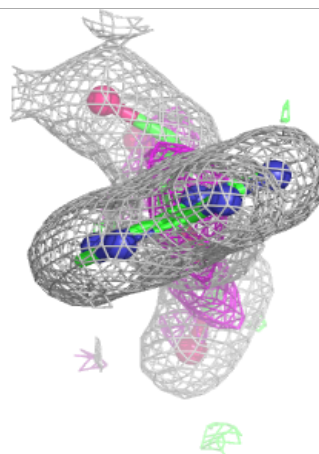
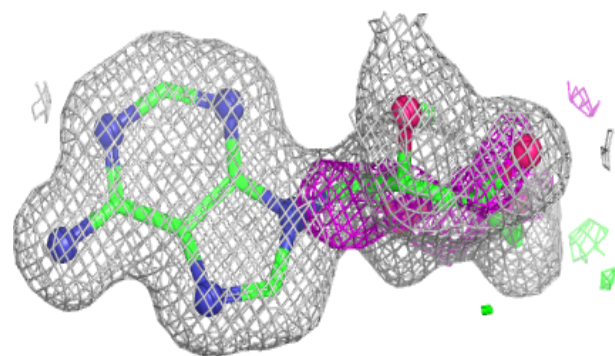
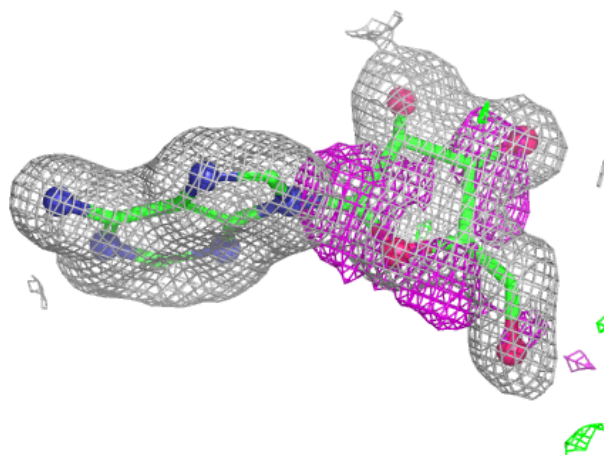
Electron density around ADN CCC 702:

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



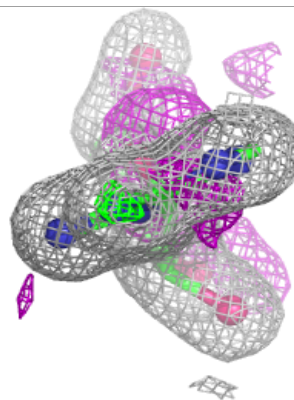
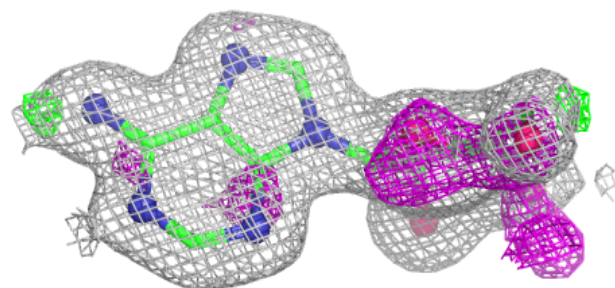
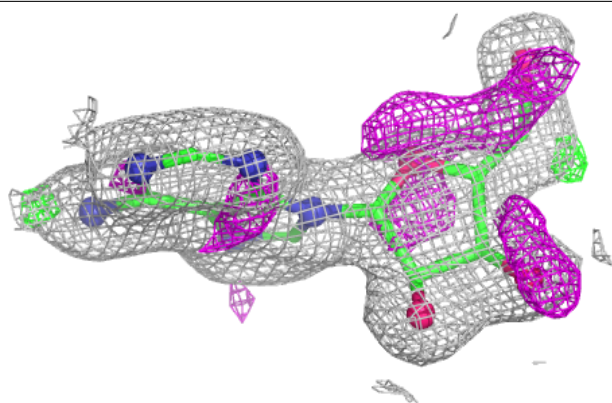
Electron density around ADN DDD 501:

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

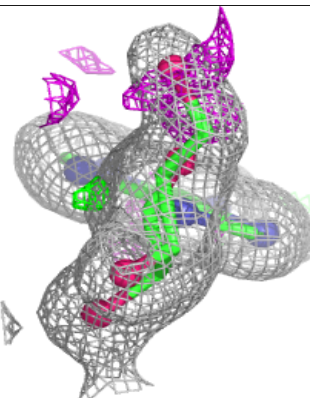
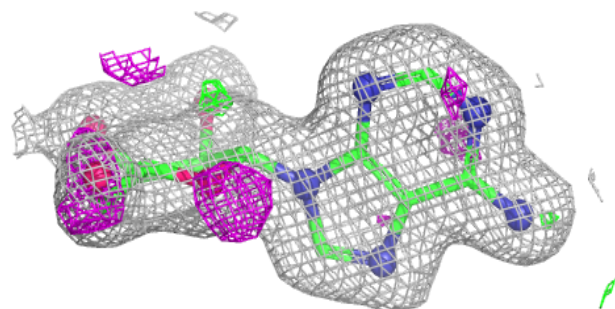
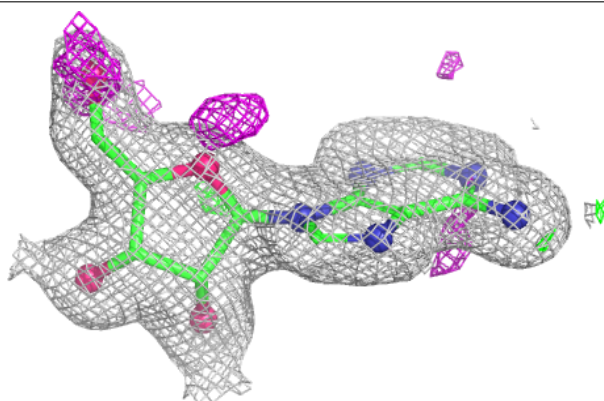


Electron density around ADN AAA 701:

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

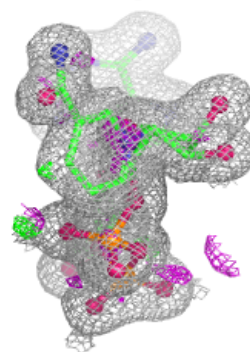
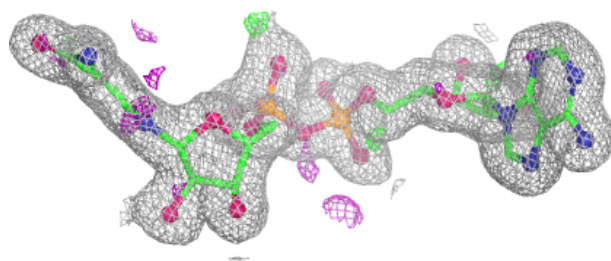
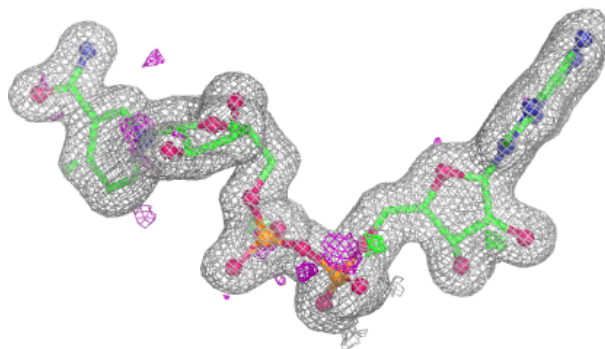
**Electron density around ADN BBB 501:**

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

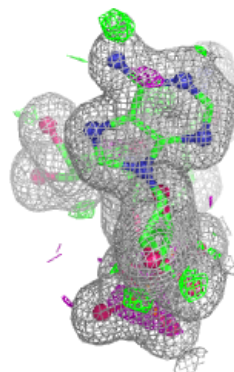
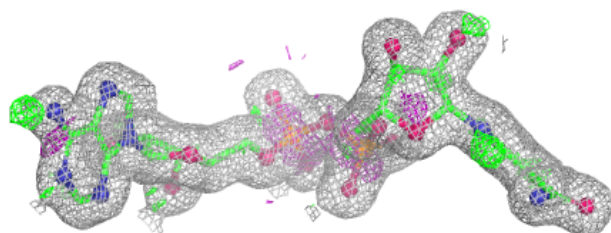
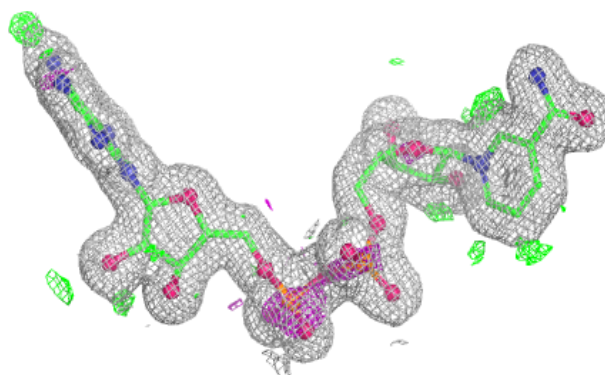


Electron density around NAD BBB 502:

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

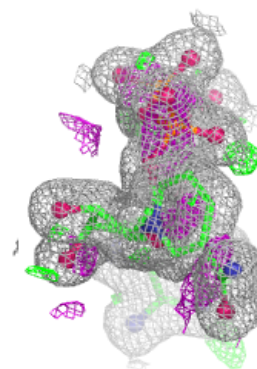
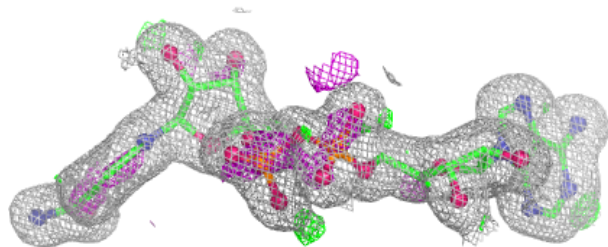
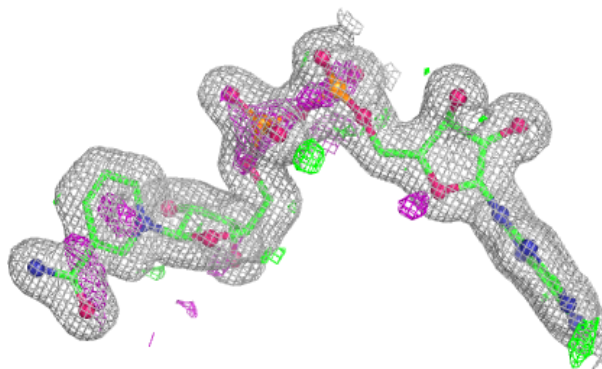
**Electron density around NAD CCC 701:**

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

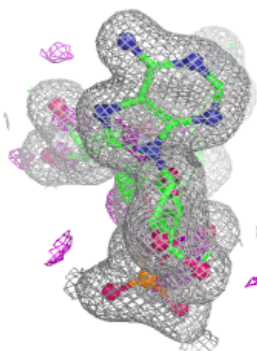
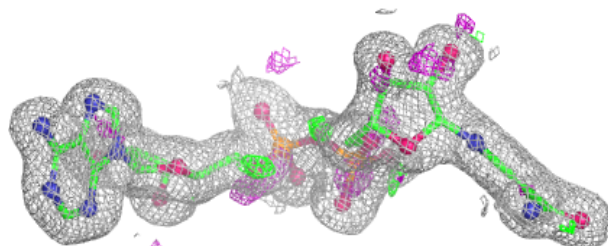
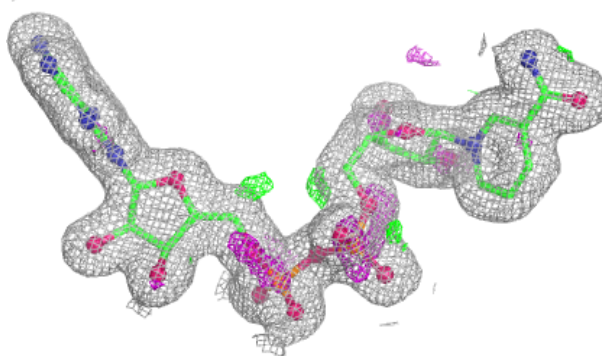


Electron density around NAD DDD 502:

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

**Electron density around NAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.