



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 12:34 PM UTC

PDB ID : 8AJV / pdb_00008ajv
Title : Crystal structure of the Q65N mutant of S-adenosyl-L-homocysteine hydrolase from *Pseudomonas aeruginosa* crystallized 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 : 1.90 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 ⓘ](#)) 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

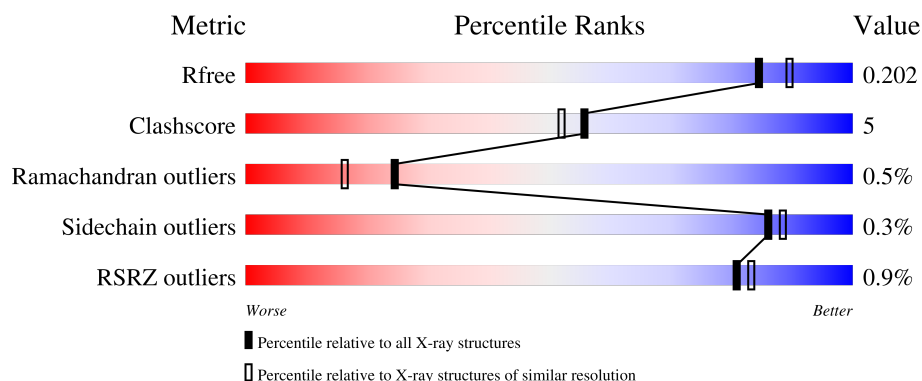
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	 87% 10% ..
1	BBB	472	 88% 9% ..
1	CCC	472	 89% 8% .
1	DDD	472	 87% 10% ..

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Mol	Chain	Length	Quality of chain
1	FFF	472	 88% 9% ..
1	GGG	472	 88% 8% ..
1	HHH	472	 88% 9% .
1	III	472	 84% 13% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PEG	CCC	505	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32384 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	35	14	0
			3642	2292	633	694	23			
1	BBB	461	Total	C	N	O	S	53	10	0
			3626	2284	630	689	23			
1	CCC	461	Total	C	N	O	S	27	9	0
			3606	2272	626	685	23			
1	DDD	461	Total	C	N	O	S	24	13	0
			3626	2283	629	691	23			
1	FFF	461	Total	C	N	O	S	4	13	0
			3636	2287	631	695	23			
1	GGG	461	Total	C	N	O	S	44	11	0
			3623	2280	627	693	23			
1	HHH	461	Total	C	N	O	S	24	8	0
			3592	2263	623	683	23			
1	III	461	Total	C	N	O	S	39	14	0
			3654	2301	636	694	23			

There are 32 discrepancies between the modelled and reference sequences:

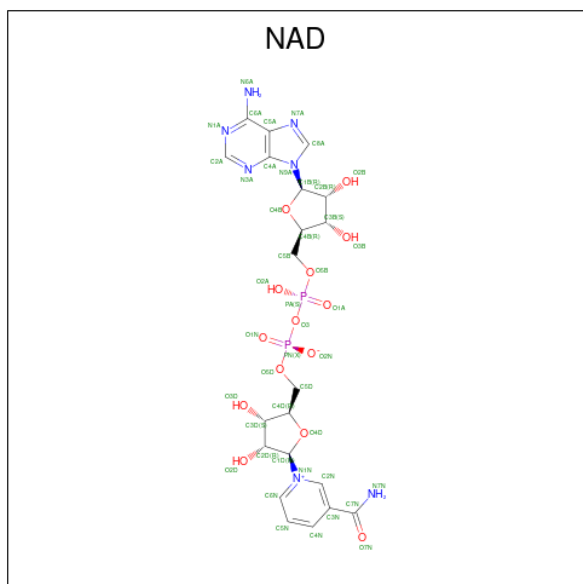
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	SER	-	expression tag	UNP Q9I685
AAA	-1	ASN	-	expression tag	UNP Q9I685
AAA	0	ALA	-	expression tag	UNP Q9I685
AAA	65	ASN	GLN	engineered mutation	UNP Q9I685
BBB	-2	SER	-	expression tag	UNP Q9I685
BBB	-1	ASN	-	expression tag	UNP Q9I685
BBB	0	ALA	-	expression tag	UNP Q9I685
BBB	65	ASN	GLN	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	65	ASN	GLN	engineered mutation	UNP Q9I685
DDD	-2	SER	-	expression tag	UNP Q9I685

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-1	ASN	-	expression tag	UNP Q9I685
DDD	0	ALA	-	expression tag	UNP Q9I685
DDD	65	ASN	GLN	engineered mutation	UNP Q9I685
FFF	-2	SER	-	expression tag	UNP Q9I685
FFF	-1	ASN	-	expression tag	UNP Q9I685
FFF	0	ALA	-	expression tag	UNP Q9I685
FFF	65	ASN	GLN	engineered mutation	UNP Q9I685
GGG	-2	SER	-	expression tag	UNP Q9I685
GGG	-1	ASN	-	expression tag	UNP Q9I685
GGG	0	ALA	-	expression tag	UNP Q9I685
GGG	65	ASN	GLN	engineered mutation	UNP Q9I685
HHH	-2	SER	-	expression tag	UNP Q9I685
HHH	-1	ASN	-	expression tag	UNP Q9I685
HHH	0	ALA	-	expression tag	UNP Q9I685
HHH	65	ASN	GLN	engineered mutation	UNP Q9I685
III	-2	SER	-	expression tag	UNP Q9I685
III	-1	ASN	-	expression tag	UNP Q9I685
III	0	ALA	-	expression tag	UNP Q9I685
III	65	ASN	GLN	engineered mutation	UNP Q9I685

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



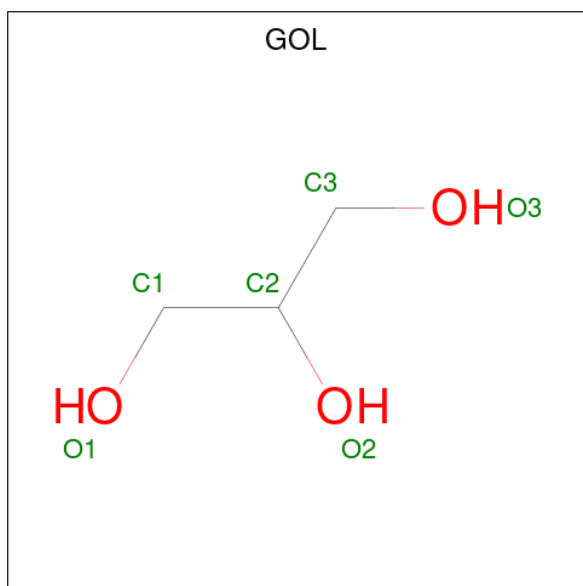
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	
			44	21	7	14	2	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	BBB	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	CCC	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	DDD	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	FFF	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	GGG	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	HHH	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	III	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



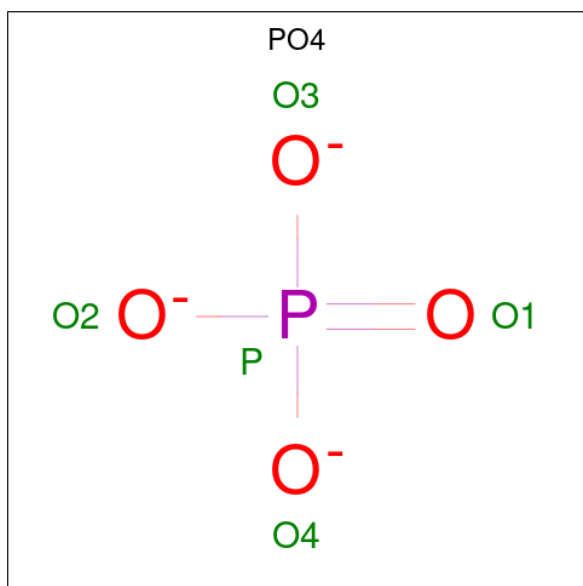
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	CCC	1	Total	C	O	0	0
			6	3	3		
3	DDD	1	Total	C	O	0	0
			6	3	3		
3	DDD	1	Total	C	O	0	0
			6	3	3		
3	DDD	1	Total	C	O	0	0
			6	3	3		
3	GGG	1	Total	C	O	0	0
			6	3	3		
3	HHH	1	Total	C	O	0	0
			6	3	3		
3	III	1	Total	C	O	0	0
			6	3	3		
3	III	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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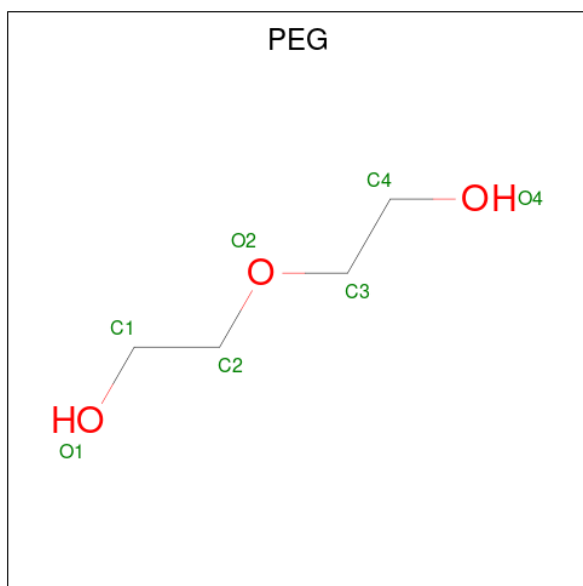
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	O	P	0	0
			5	4	1		
4	BBB	1	Total	O	P	0	0
			5	4	1		
4	BBB	1	Total	O	P	0	0
			5	4	1		
4	BBB	1	Total	O	P	0	0
			5	4	1		
4	CCC	1	Total	O	P	0	0
			5	4	1		
4	CCC	1	Total	O	P	0	0
			5	4	1		
4	DDD	1	Total	O	P	0	0
			5	4	1		
4	DDD	1	Total	O	P	0	0
			5	4	1		
4	DDD	1	Total	O	P	0	0
			5	4	1		
4	FFF	1	Total	O	P	0	0
			5	4	1		
4	FFF	1	Total	O	P	0	0
			5	4	1		
4	FFF	1	Total	O	P	0	0
			5	4	1		
4	GGG	1	Total	O	P	0	0
			5	4	1		
4	GGG	1	Total	O	P	0	0
			5	4	1		
4	GGG	1	Total	O	P	0	0
			5	4	1		
4	GGG	1	Total	O	P	0	0
			5	4	1		
4	HHH	1	Total	O	P	0	0
			5	4	1		
4	HHH	1	Total	O	P	0	0
			5	4	1		
4	III	1	Total	O	P	0	0
			5	4	1		
4	III	1	Total	O	P	0	0
			5	4	1		
4	III	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total K 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	429	Total O 429 429	0	0
7	BBB	337	Total O 337 337	0	0
7	CCC	385	Total O 385 385	0	0
7	DDD	333	Total O 333 333	0	0
7	FFF	390	Total O 390 390	0	0

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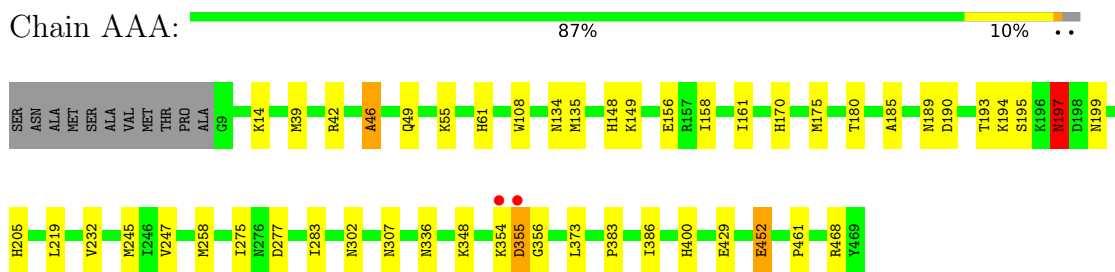
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	GGG	280	Total 280	O 280	0	0
7	HHH	337	Total 337	O 337	0	0
7	III	329	Total 329	O 329	0	0

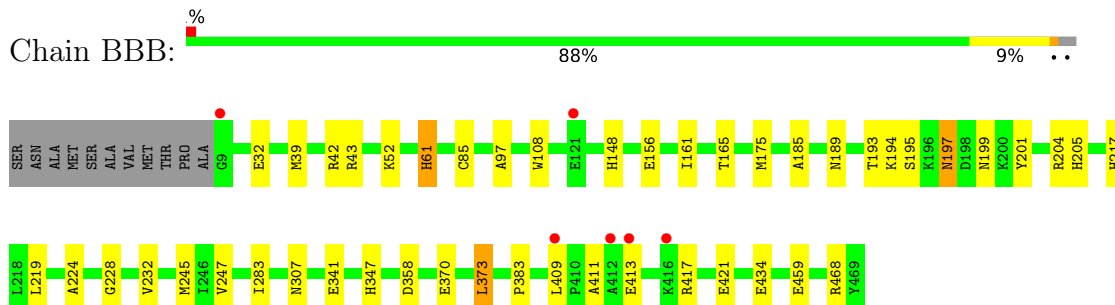
3 Residue-property plots [i](#)

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.

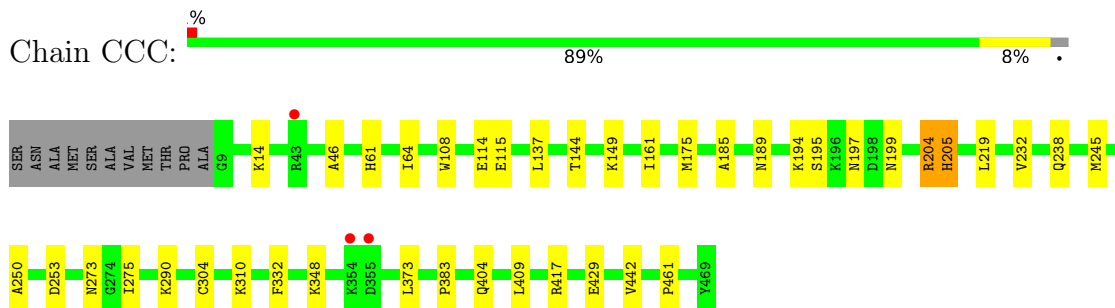
- Molecule 1: Adenosylhomocysteinase



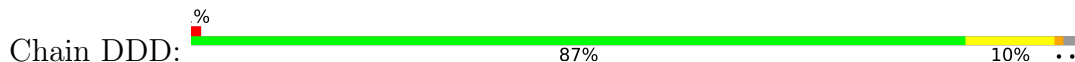
- Molecule 1: Adenosylhomocysteinase

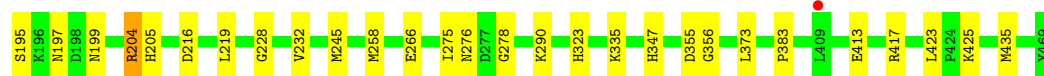


- Molecule 1: Adenosylhomocysteinase

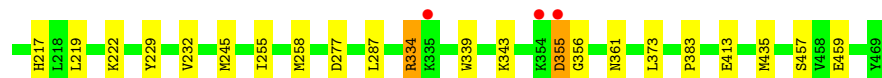
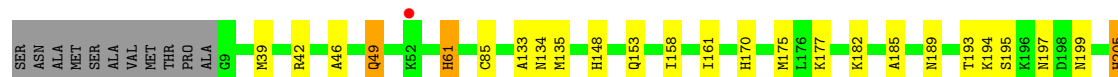
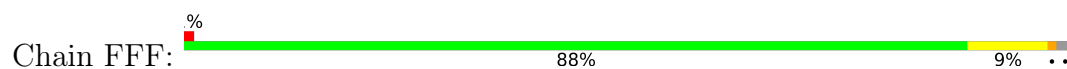


- Molecule 1: Adenosylhomocysteinase





• Molecule 1: Adenosylhomocysteinase



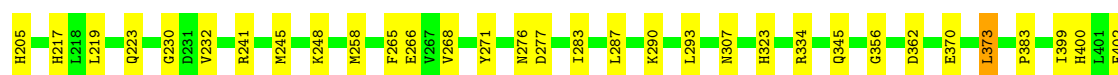
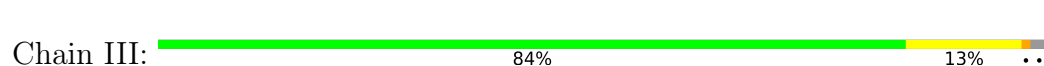
• Molecule 1: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase



E403	Q404	R405	Y406	L409	R417	K426	M435	P448	Y469
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.48Å 211.88Å 111.35Å 90.00° 105.33° 90.00°	Depositor
Resolution (Å)	95.88 – 1.90 95.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (95.88-1.90) 99.2 (95.88-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.160 , 0.194 0.167 , 0.202	Depositor DCC
R_{free} test set	1122 reflections (0.29%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.140 for l,-k,h	Xtriage
Reported twinning fraction	0.861 for H, K, L 0.139 for -L, -K, -H	Depositor
Outliers	1 of 386695 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	32384	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, PO4, GOL, K, 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	AAA	1.20	2/3711 (0.1%)	1.37	7/5015 (0.1%)
1	BBB	1.22	12/3699 (0.3%)	1.36	7/4998 (0.1%)
1	CCC	1.23	4/3681 (0.1%)	1.39	12/4975 (0.2%)
1	DDD	1.21	5/3701 (0.1%)	1.35	8/5002 (0.2%)
1	FFF	1.18	4/3705 (0.1%)	1.35	3/5008 (0.1%)
1	GGG	1.16	7/3698 (0.2%)	1.34	4/4998 (0.1%)
1	HHH	1.19	3/3664 (0.1%)	1.38	11/4952 (0.2%)
1	III	1.18	4/3729 (0.1%)	1.34	3/5039 (0.1%)
All	All	1.20	41/29588 (0.1%)	1.36	55/39987 (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	AAA	0	1
1	BBB	0	1
1	CCC	0	1
1	DDD	0	3
1	GGG	0	2
1	HHH	0	1
1	III	0	1
All	All	0	10

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	156	GLU	CD-OE2	12.30	1.48	1.25
1	DDD	156	GLU	CD-OE1	-10.42	1.05	1.25
1	FFF	205	HIS	CE1-NE2	9.76	1.42	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	HHH	417	ARG	CD-NE	9.72	1.59	1.46
1	BBB	347	HIS	CE1-NE2	7.53	1.40	1.32

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	204	ARG	CB-CG-CD	10.22	134.80	111.30
1	GGG	153	GLN	CB-CG-CD	-9.26	96.85	112.60
1	DDD	156	GLU	N-CA-CB	8.64	123.80	110.14
1	BBB	197	ASN	N-CA-CB	8.36	122.66	110.20
1	CCC	204	ARG	CB-CG-CD	7.89	129.45	111.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	452	GLU	Sidechain
1	BBB	358	ASP	Sidechain
1	CCC	114	GLU	Sidechain
1	DDD	156	GLU	Sidechain
1	DDD	355	ASP	Mainchain

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	3642	0	3641	41	0
1	BBB	3626	0	3630	24	0
1	CCC	3606	0	3620	23	0
1	DDD	3626	0	3627	34	0
1	FFF	3636	0	3627	39	0
1	GGG	3623	0	3621	29	0
1	HHH	3592	0	3599	30	0
1	III	3654	0	3656	60	0
2	AAA	44	0	26	0	0
2	BBB	44	0	26	0	0
2	CCC	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DDD	44	0	26	0	0
2	FFF	44	0	26	0	0
2	GGG	44	0	26	1	0
2	HHH	44	0	26	0	0
2	III	44	0	26	2	0
3	AAA	6	0	8	3	0
3	BBB	18	0	24	1	0
3	CCC	6	0	8	0	0
3	DDD	18	0	24	4	0
3	GGG	6	0	8	1	0
3	HHH	6	0	8	0	0
3	III	12	0	16	2	0
4	AAA	15	0	0	0	0
4	BBB	20	0	0	2	0
4	CCC	10	0	0	0	0
4	DDD	15	0	0	2	0
4	FFF	15	0	0	0	0
4	GGG	20	0	0	0	0
4	HHH	10	0	0	0	0
4	III	15	0	0	1	0
5	BBB	1	0	0	0	0
6	CCC	14	0	20	5	0
7	AAA	429	0	0	9	0
7	BBB	337	0	0	7	0
7	CCC	385	0	0	2	0
7	DDD	333	0	0	6	0
7	FFF	390	0	0	9	1
7	GGG	280	0	0	8	0
7	HHH	337	0	0	11	1
7	III	329	0	0	12	0
All	All	32384	0	29345	273	1

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 5.

The worst 5 of 273 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:HHH:43[A]:ARG:HG3	7:HHH:637:HOH:O	1.45	1.11
1:FFF:49:GLN:OE1	7:FFF:601:HOH:O	1.89	0.90
3:GGG:506:GOL:O3	7:GGG:601:HOH:O	1.91	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:177:LYS:HG3	7:FFF:693:HOH:O	1.74	0.88
1:FFF:457:SER:OG	1:FFF:459:GLU:OE1	1.96	0.84

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:FFF:623:HOH:O	7:HHH:816:HOH:O[1_556]	1.97	0.23

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	471/472 (100%)	458 (97%)	10 (2%)	3 (1%)	21	13
1	BBB	469/472 (99%)	457 (97%)	10 (2%)	2 (0%)	30	22
1	CCC	467/472 (99%)	454 (97%)	11 (2%)	2 (0%)	30	22
1	DDD	470/472 (100%)	459 (98%)	9 (2%)	2 (0%)	30	22
1	FFF	470/472 (100%)	458 (97%)	9 (2%)	3 (1%)	21	13
1	GGG	469/472 (99%)	457 (97%)	10 (2%)	2 (0%)	30	22
1	HHH	465/472 (98%)	454 (98%)	9 (2%)	2 (0%)	30	22
1	III	472/472 (100%)	457 (97%)	13 (3%)	2 (0%)	30	22
All	All	3753/3776 (99%)	3654 (97%)	81 (2%)	18 (0%)	24	16

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	355	ASP
1	BBB	61	HIS
1	CCC	61	HIS

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Mol	Chain	Res	Type
1	DDD	373	LEU
1	FFF	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	388/385 (101%)	387 (100%)	1 (0%)	86	88
1	BBB	386/385 (100%)	385 (100%)	1 (0%)	86	88
1	CCC	385/385 (100%)	385 (100%)	0	100	100
1	DDD	387/385 (100%)	386 (100%)	1 (0%)	86	88
1	FFF	388/385 (101%)	387 (100%)	1 (0%)	86	88
1	GGG	387/385 (100%)	384 (99%)	3 (1%)	73	75
1	HHH	383/385 (100%)	382 (100%)	1 (0%)	86	88
1	III	390/385 (101%)	389 (100%)	1 (0%)	86	88
All	All	3094/3080 (100%)	3085 (100%)	9 (0%)	86	88

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	349	ILE
1	III	409	LEU
1	FFF	334	ARG
1	GGG	182	LYS
1	GGG	372	ARG

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 1 is monoatomic - leaving 46 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	CCC	501	-	46,48,48	0.76	2 (4%)	64,73,73	0.73	1 (1%)
3	GOL	AAA	502	-	5,5,5	0.10	0	5,5,5	0.30	0
4	PO4	BBB	506	-	4,4,4	1.06	0	6,6,6	0.77	0
4	PO4	FFF	501	-	4,4,4	0.61	0	6,6,6	0.77	0
4	PO4	GGG	503	-	4,4,4	1.34	1 (25%)	6,6,6	0.36	0
4	PO4	HHH	502	-	4,4,4	0.95	0	6,6,6	0.73	0
3	GOL	III	506	-	5,5,5	0.15	0	5,5,5	0.34	0
6	PEG	CCC	505	-	6,6,6	0.16	0	5,5,5	0.21	0
3	GOL	BBB	502	-	5,5,5	0.18	0	5,5,5	0.25	0
2	NAD	AAA	501	-	46,48,48	0.64	1 (2%)	64,73,73	0.73	1 (1%)
4	PO4	BBB	505	-	4,4,4	1.12	0	6,6,6	0.80	0
3	GOL	III	505	-	5,5,5	0.30	0	5,5,5	0.45	0
4	PO4	DDD	505	-	4,4,4	1.08	0	6,6,6	0.66	0
3	GOL	BBB	503	-	5,5,5	0.25	0	5,5,5	0.43	0
4	PO4	III	501	-	4,4,4	1.45	1 (25%)	6,6,6	0.75	0
4	PO4	CCC	503	-	4,4,4	0.61	0	6,6,6	0.35	0
2	NAD	DDD	501	-	46,48,48	0.97	2 (4%)	64,73,73	0.89	3 (4%)
4	PO4	BBB	508	-	4,4,4	0.76	0	6,6,6	0.57	0
2	NAD	HHH	503	-	46,48,48	0.82	2 (4%)	64,73,73	0.77	1 (1%)
4	PO4	AAA	505	-	4,4,4	0.59	0	6,6,6	0.60	0
4	PO4	GGG	501	-	4,4,4	0.80	0	6,6,6	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	DDD	502	-	5,5,5	0.13	0	5,5,5	0.34	0
3	GOL	DDD	504	-	5,5,5	0.38	0	5,5,5	0.70	0
4	PO4	GGG	504	-	4,4,4	0.38	0	6,6,6	0.46	0
4	PO4	BBB	507	-	4,4,4	0.42	0	6,6,6	0.32	0
4	PO4	III	503	-	4,4,4	1.15	0	6,6,6	0.67	0
3	GOL	GGG	506	-	5,5,5	0.18	0	5,5,5	0.38	0
4	PO4	CCC	504	-	4,4,4	0.82	0	6,6,6	0.43	0
4	PO4	III	502	-	4,4,4	1.40	1 (25%)	6,6,6	0.83	0
4	PO4	AAA	503	-	4,4,4	1.29	1 (25%)	6,6,6	0.42	0
4	PO4	FFF	502	-	4,4,4	0.96	0	6,6,6	0.63	0
3	GOL	BBB	504	-	5,5,5	0.11	0	5,5,5	0.44	0
4	PO4	AAA	504	-	4,4,4	1.21	0	6,6,6	0.52	0
3	GOL	HHH	504	-	5,5,5	0.23	0	5,5,5	0.60	0
4	PO4	FFF	503	-	4,4,4	1.42	1 (25%)	6,6,6	0.63	0
4	PO4	DDD	506	-	4,4,4	0.50	0	6,6,6	0.81	0
4	PO4	DDD	507	-	4,4,4	0.94	0	6,6,6	0.62	0
4	PO4	HHH	501	-	4,4,4	0.38	0	6,6,6	0.62	0
2	NAD	BBB	501	-	46,48,48	0.79	2 (4%)	64,73,73	0.79	1 (1%)
4	PO4	GGG	502	-	4,4,4	0.36	0	6,6,6	0.56	0
2	NAD	III	504	-	46,48,48	1.06	2 (4%)	64,73,73	0.79	1 (1%)
2	NAD	GGG	505	-	46,48,48	1.01	3 (6%)	64,73,73	0.77	1 (1%)
3	GOL	CCC	502	-	5,5,5	0.23	0	5,5,5	0.30	0
2	NAD	FFF	504	-	46,48,48	0.99	4 (8%)	64,73,73	0.85	2 (3%)
3	GOL	DDD	503	-	5,5,5	0.17	0	5,5,5	0.29	0
6	PEG	CCC	506	-	6,6,6	0.30	0	5,5,5	0.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	CCC	501	-	-	4/30/62/62	0/5/5/5
3	GOL	AAA	502	-	-	4/4/4/4	-
3	GOL	III	506	-	-	4/4/4/4	-
6	PEG	CCC	505	-	-	4/4/4/4	-
3	GOL	BBB	502	-	-	2/4/4/4	-
2	NAD	AAA	501	-	-	4/30/62/62	0/5/5/5
3	GOL	III	505	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	BBB	503	-	-	4/4/4/4	-
2	NAD	DDD	501	-	-	4/30/62/62	0/5/5/5
2	NAD	HHH	503	-	-	4/30/62/62	0/5/5/5
3	GOL	DDD	502	-	-	4/4/4/4	-
3	GOL	DDD	504	-	-	3/4/4/4	-
3	GOL	GGG	506	-	-	0/4/4/4	-
3	GOL	BBB	504	-	-	4/4/4/4	-
3	GOL	HHH	504	-	-	4/4/4/4	-
2	NAD	BBB	501	-	-	5/30/62/62	0/5/5/5
2	NAD	III	504	-	-	4/30/62/62	0/5/5/5
2	NAD	GGG	505	-	-	5/30/62/62	0/5/5/5
3	GOL	CCC	502	-	-	2/4/4/4	-
2	NAD	FFF	504	-	-	5/30/62/62	0/5/5/5
3	GOL	DDD	503	-	-	2/4/4/4	-
6	PEG	CCC	506	-	-	3/4/4/4	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	III	504	NAD	C2N-N1N	5.38	1.40	1.35
2	DDD	501	NAD	C2N-N1N	4.45	1.39	1.35
2	GGG	505	NAD	C2N-N1N	4.35	1.39	1.35
2	FFF	504	NAD	O4D-C1D	3.27	1.45	1.40
2	GGG	505	NAD	O4D-C1D	3.25	1.45	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	501	NAD	C6N-N1N-C2N	-3.52	118.89	121.88
2	CCC	501	NAD	C6N-N1N-C2N	-3.46	118.93	121.88
2	HHH	503	NAD	C6N-N1N-C2N	-3.27	119.10	121.88
2	GGG	505	NAD	C6N-N1N-C2N	-3.16	119.19	121.88
2	FFF	504	NAD	C6N-N1N-C2N	-3.03	119.30	121.88

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

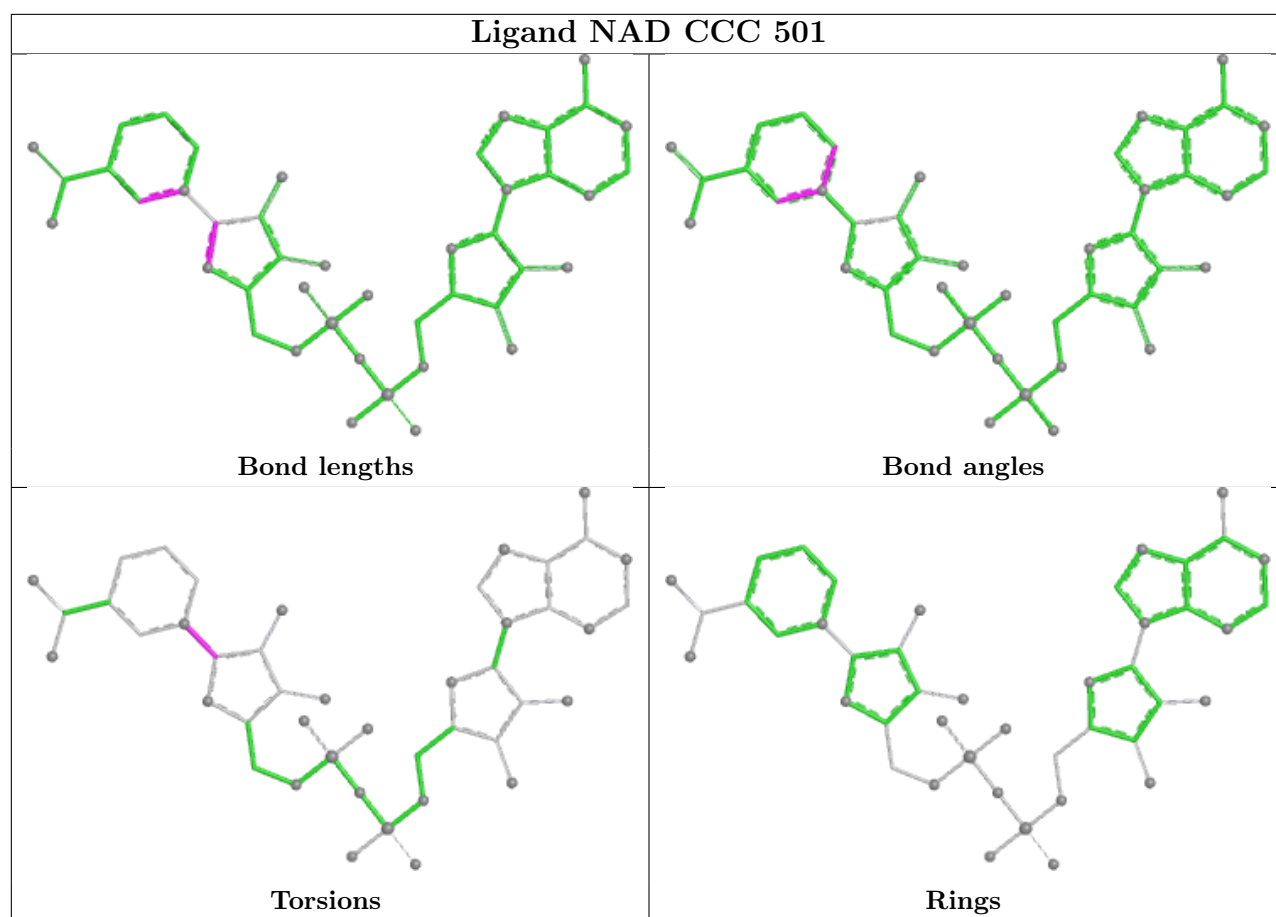
Mol	Chain	Res	Type	Atoms
2	AAA	501	NAD	O4D-C1D-N1N-C2N
2	AAA	501	NAD	O4D-C1D-N1N-C6N
2	AAA	501	NAD	C2D-C1D-N1N-C2N
2	AAA	501	NAD	C2D-C1D-N1N-C6N
2	BBB	501	NAD	O4D-C1D-N1N-C2N

There are no ring outliers.

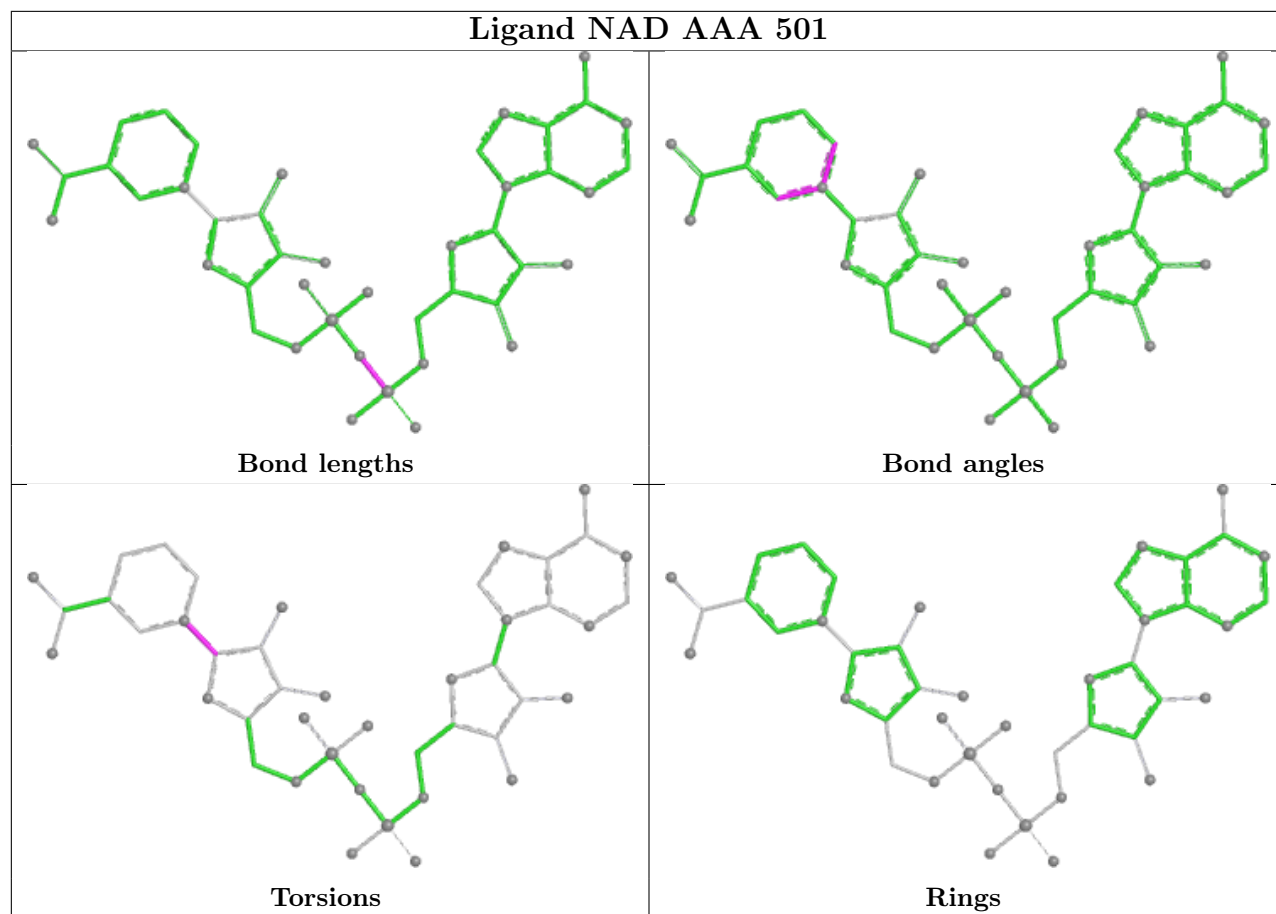
15 monomers are involved in 24 short contacts:

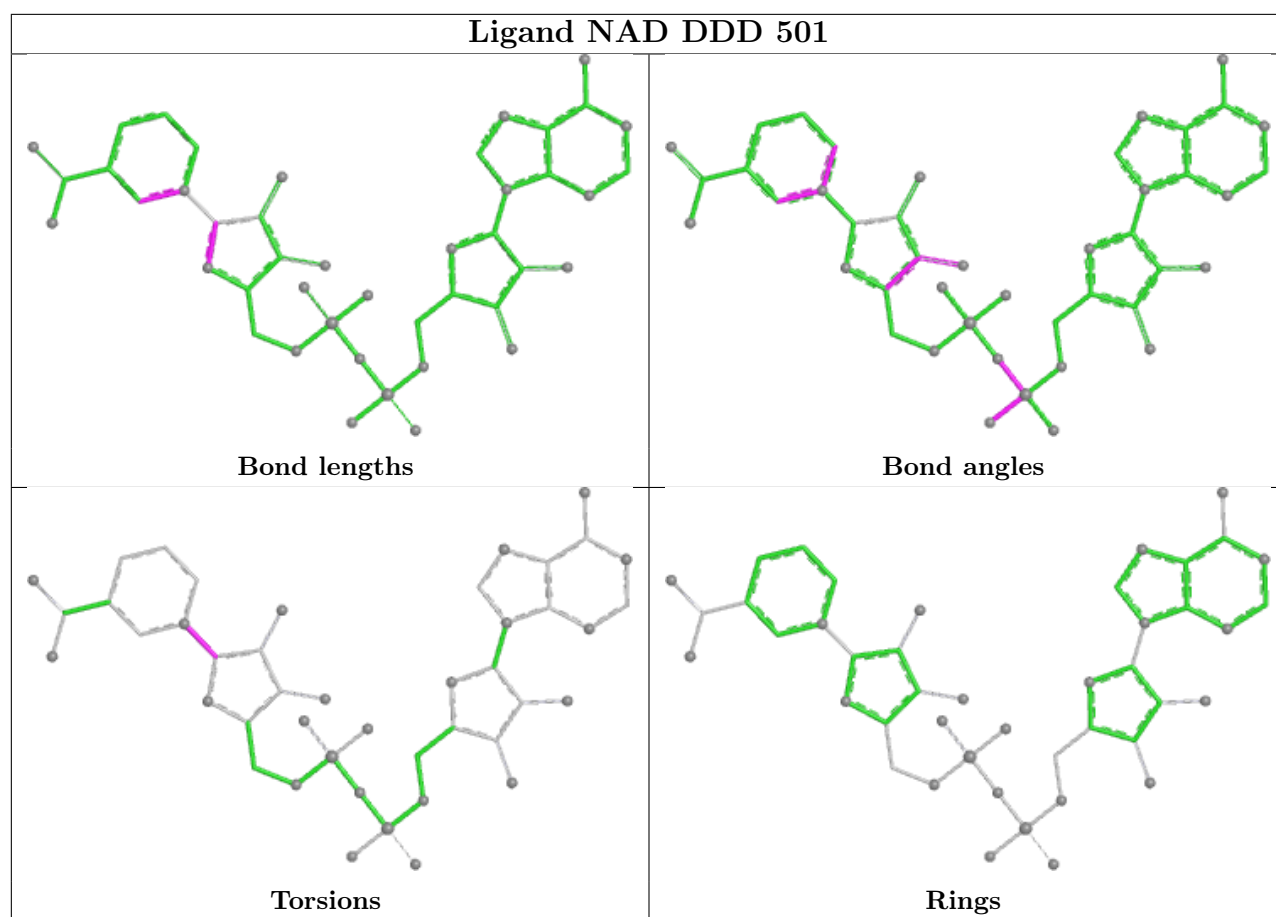
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	502	GOL	3	0
4	BBB	506	PO4	1	0
6	CCC	505	PEG	4	0
4	BBB	505	PO4	1	0
3	III	505	GOL	2	0
4	DDD	505	PO4	1	0
3	DDD	502	GOL	3	0
3	DDD	504	GOL	1	0
3	GGG	506	GOL	1	0
4	III	502	PO4	1	0
3	BBB	504	GOL	1	0
4	DDD	506	PO4	1	0
2	III	504	NAD	2	0
2	GGG	505	NAD	1	0
6	CCC	506	PEG	1	0

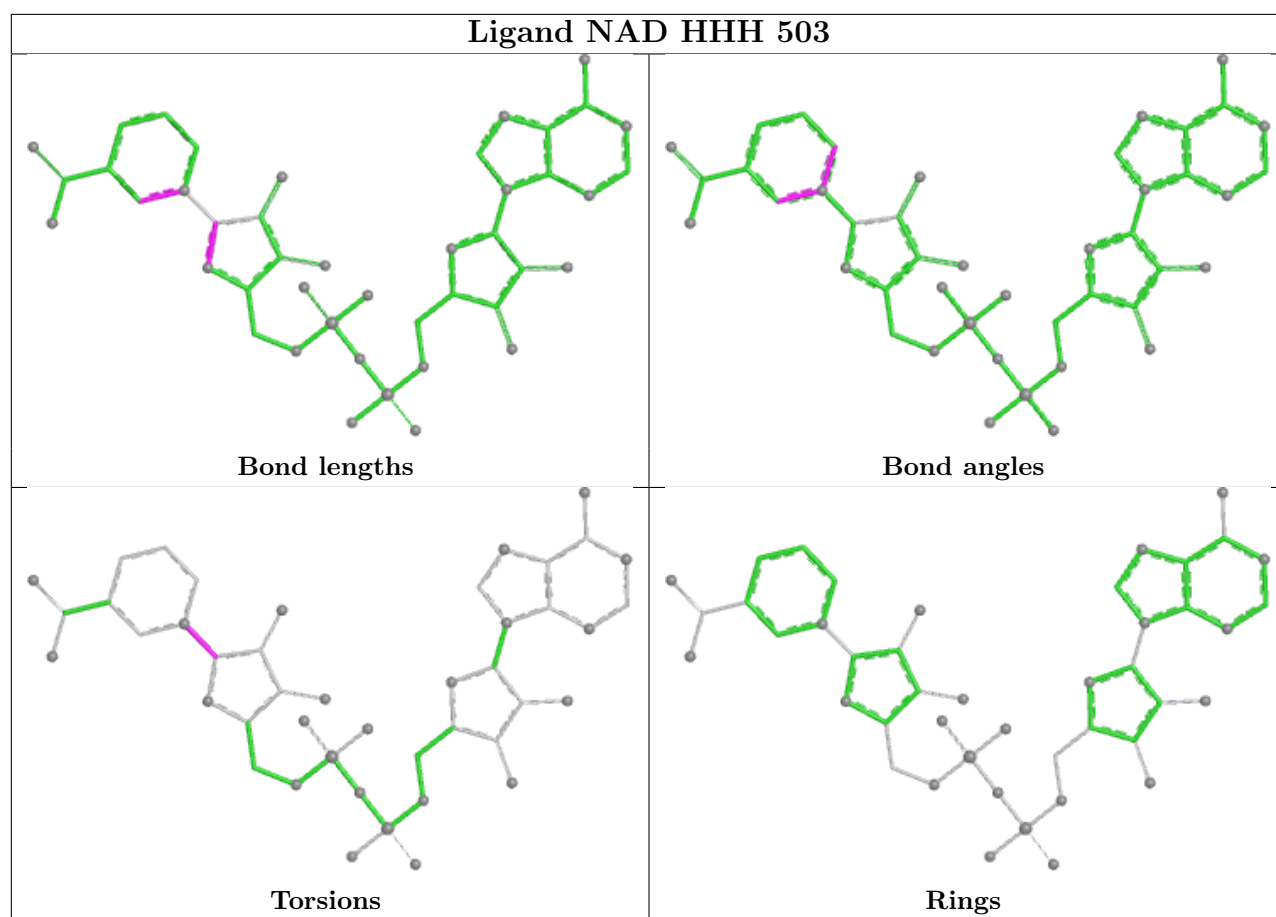
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

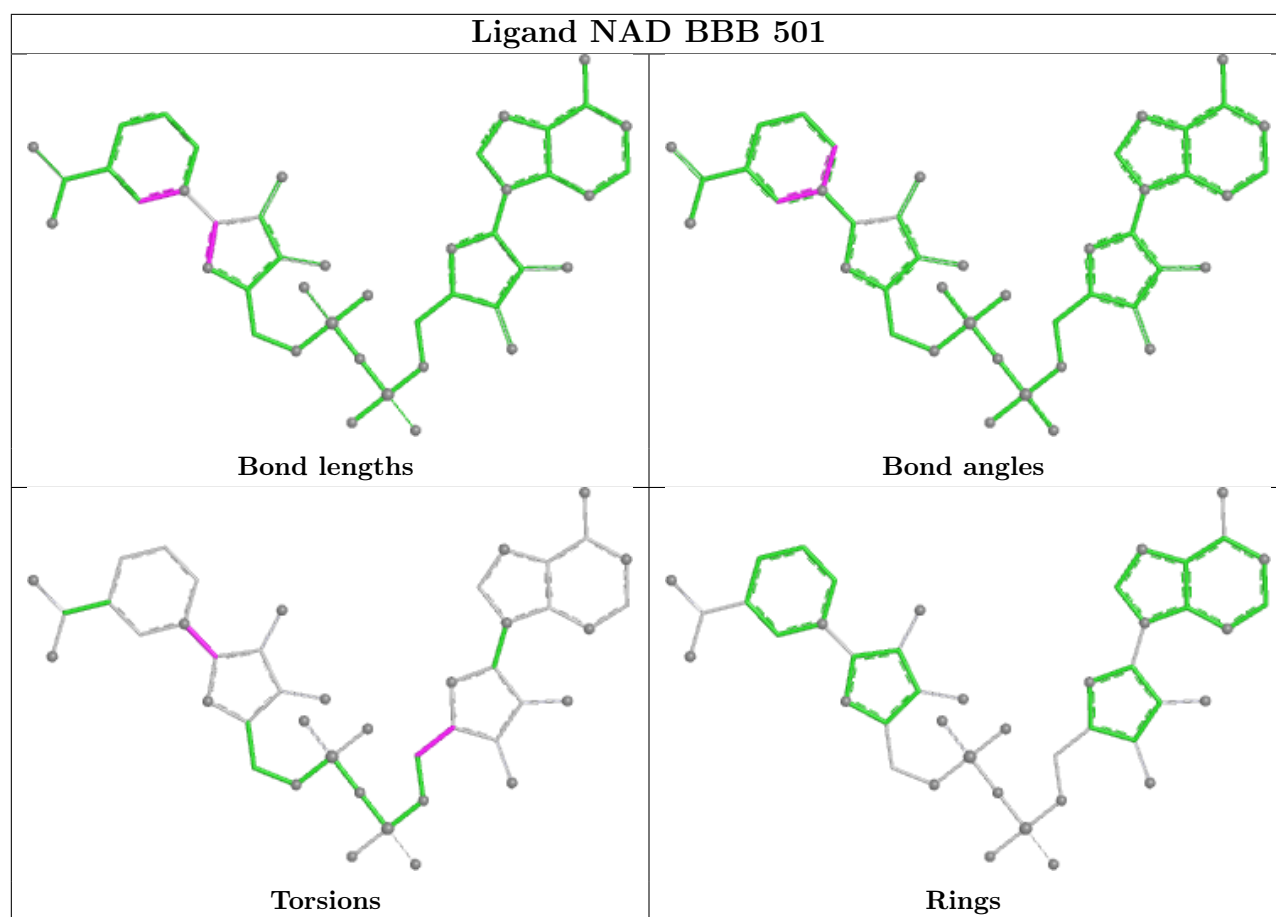


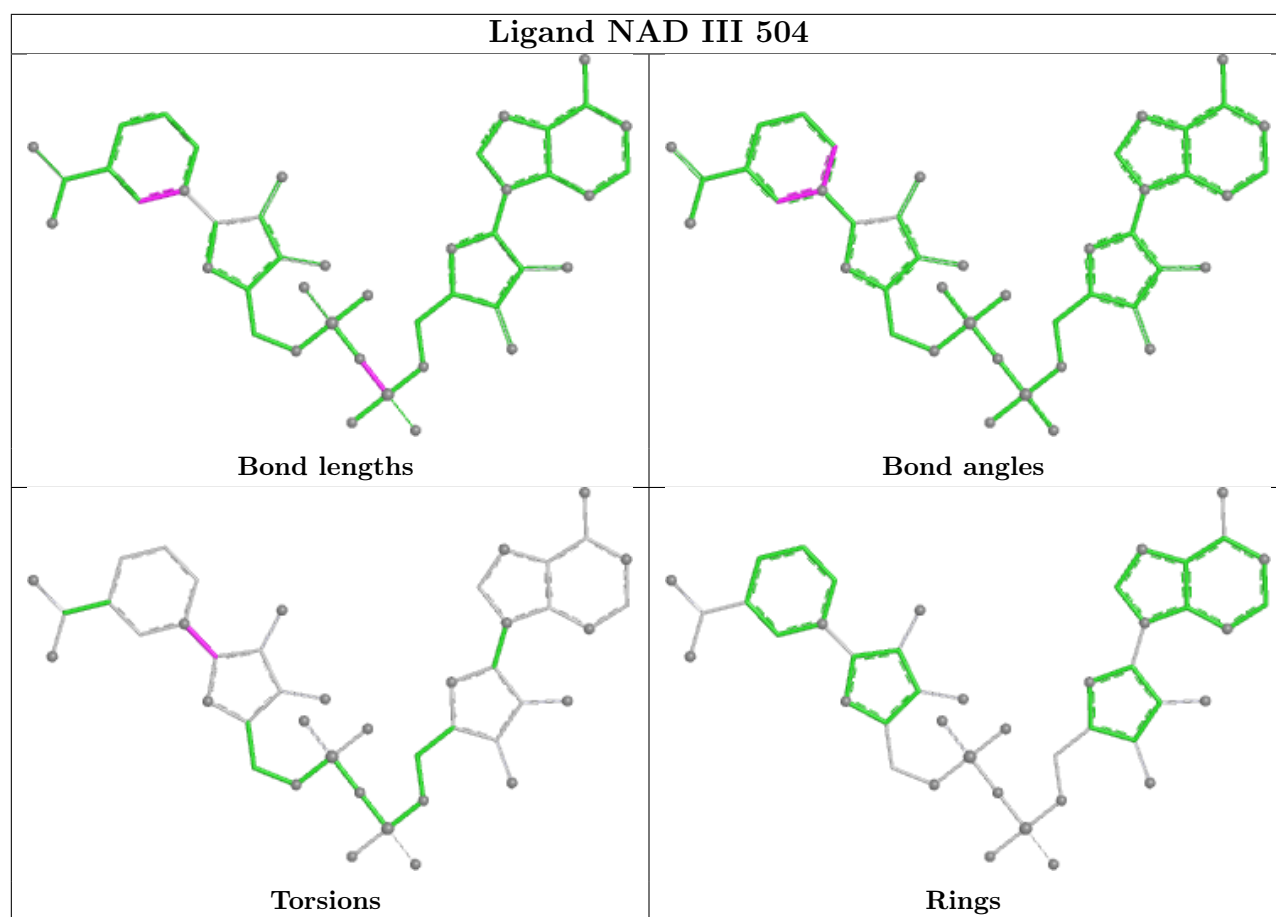
Ligand NAD AAA 501

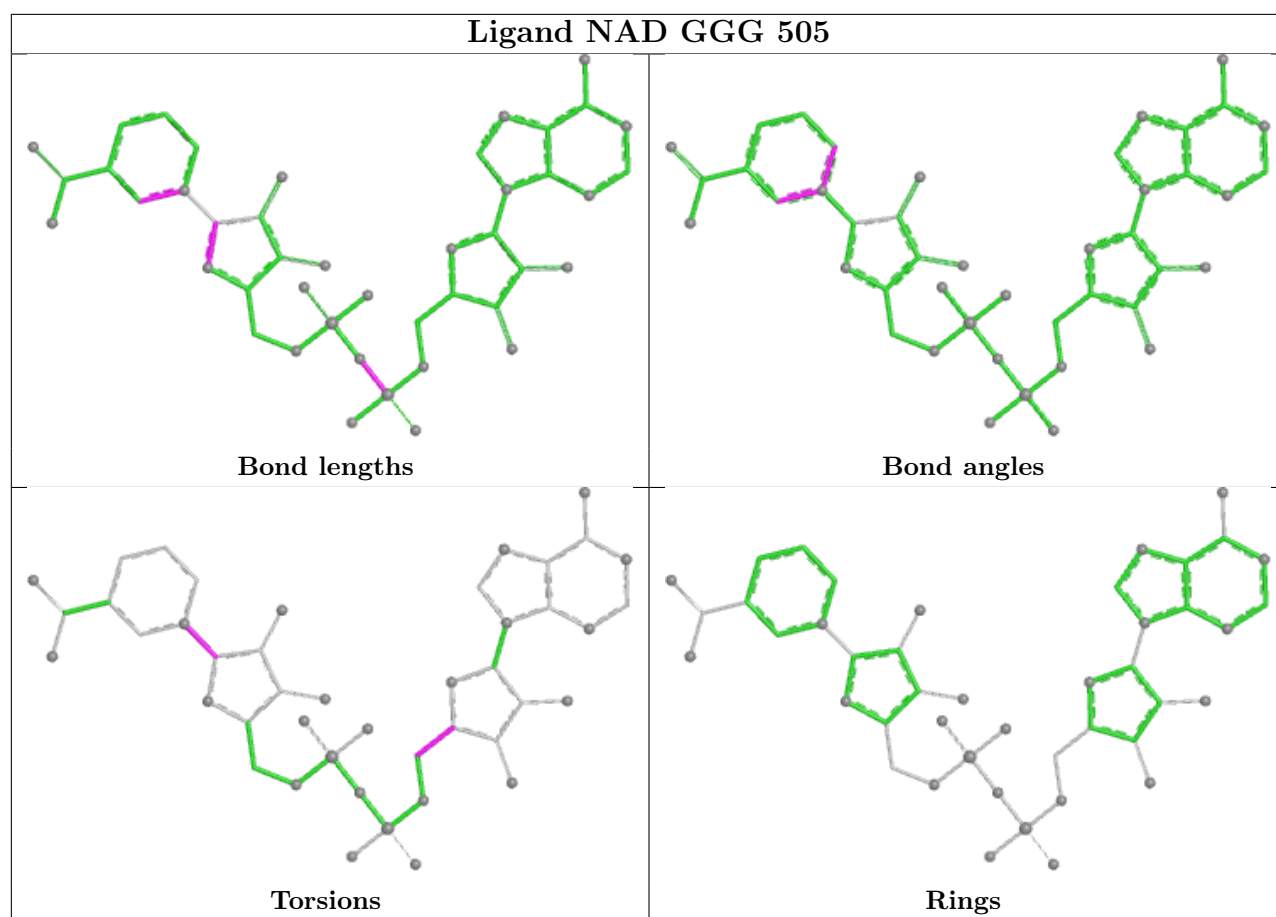


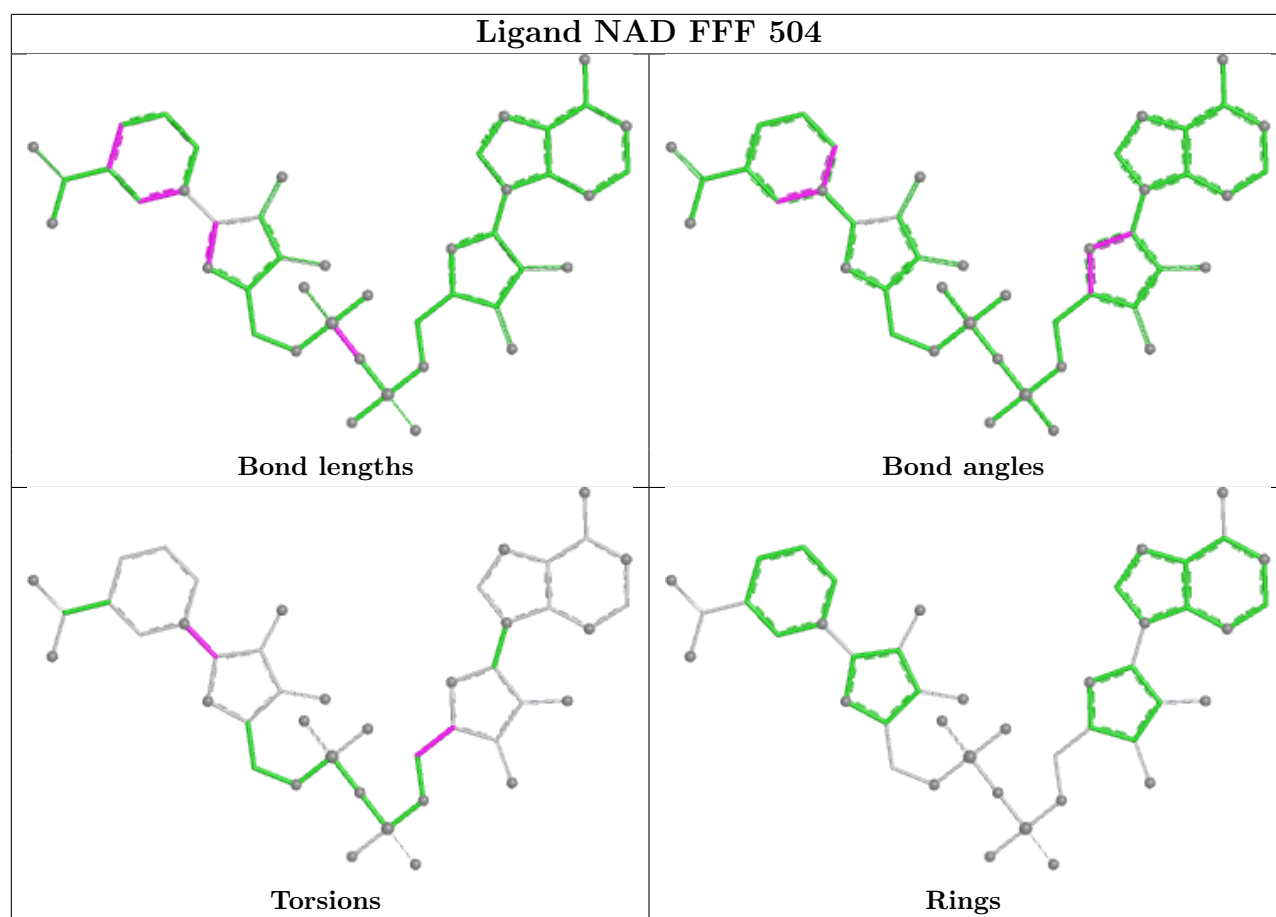












5.7 Other polymers [i](#)

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%)	-1.00	2 (0%) 88 90	15, 34, 46, 63	35 (7%)
1	BBB	461/472 (97%)	-0.80	6 (1%) 75 78	12, 37, 57, 72	48 (10%)
1	CCC	461/472 (97%)	-1.06	3 (0%) 84 86	15, 32, 44, 60	25 (5%)
1	DDD	461/472 (97%)	-0.83	4 (0%) 81 83	13, 37, 57, 88	32 (6%)
1	FFF	461/472 (97%)	-0.91	4 (0%) 81 83	15, 35, 50, 66	24 (5%)
1	GGG	461/472 (97%)	-0.61	11 (2%) 59 63	14, 43, 64, 98	39 (8%)
1	HHH	461/472 (97%)	-0.85	1 (0%) 91 92	16, 37, 49, 67	23 (4%)
1	III	461/472 (97%)	-0.92	1 (0%) 91 92	13, 37, 58, 78	31 (6%)
All	All	3688/3776 (97%)	-0.87	32 (0%) 81 83	12, 36, 56, 98	257 (6%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	412	ALA	7.4
1	GGG	413	GLU	7.3
1	BBB	413	GLU	5.9
1	BBB	9	GLY	5.2
1	GGG	416	LYS	4.9

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 ⓘ

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(Å ²)	Q<0.9
3	GOL	DDD	503	6/6	0.94	0.09	41,46,47,53	0
3	GOL	GGG	506	6/6	0.94	0.11	36,40,45,45	6
3	GOL	III	505	6/6	0.94	0.10	34,48,51,58	0
6	PEG	CCC	506	7/7	0.95	0.08	45,47,49,58	0
3	GOL	CCC	502	6/6	0.96	0.07	42,49,51,52	0
3	GOL	BBB	504	6/6	0.96	0.10	35,39,46,52	0
3	GOL	DDD	504	6/6	0.96	0.09	41,48,51,51	0
3	GOL	DDD	502	6/6	0.97	0.07	34,41,45,46	0
3	GOL	BBB	502	6/6	0.97	0.07	34,39,43,43	0
6	PEG	CCC	505	7/7	0.97	0.08	31,34,42,46	3
3	GOL	BBB	503	6/6	0.97	0.07	37,38,42,45	1
4	PO4	AAA	505	5/5	0.98	0.06	29,33,35,35	5
4	PO4	BBB	507	5/5	0.98	0.10	36,38,41,45	1
4	PO4	GGG	501	5/5	0.98	0.05	40,40,43,43	5
4	PO4	III	501	5/5	0.98	0.05	30,38,39,40	5
4	PO4	III	503	5/5	0.98	0.06	32,33,34,40	5
3	GOL	AAA	502	6/6	0.98	0.07	36,38,42,47	0
3	GOL	III	506	6/6	0.98	0.06	37,41,43,47	0
4	PO4	AAA	504	5/5	0.99	0.06	30,35,36,39	0
2	NAD	HHH	503	44/44	0.99	0.04	29,35,41,50	0
4	PO4	BBB	505	5/5	0.99	0.08	37,37,41,43	1
4	PO4	BBB	506	5/5	0.99	0.04	31,31,33,35	5
2	NAD	AAA	501	44/44	0.99	0.03	25,32,36,39	0
4	PO4	BBB	508	5/5	0.99	0.05	35,36,37,37	5
4	PO4	CCC	503	5/5	0.99	0.04	30,32,35,37	5
4	PO4	CCC	504	5/5	0.99	0.05	33,34,35,35	0
4	PO4	DDD	505	5/5	0.99	0.10	36,40,41,41	0
4	PO4	DDD	506	5/5	0.99	0.07	36,38,39,40	0
4	PO4	DDD	507	5/5	0.99	0.07	32,32,35,36	5
4	PO4	FFF	501	5/5	0.99	0.07	33,35,39,42	0
4	PO4	FFF	502	5/5	0.99	0.03	31,32,36,37	0
4	PO4	FFF	503	5/5	0.99	0.05	30,31,34,35	5
2	NAD	BBB	501	44/44	0.99	0.03	25,29,33,34	0
4	PO4	GGG	502	5/5	0.99	0.05	30,33,34,34	5
4	PO4	GGG	503	5/5	0.99	0.05	36,36,37,42	5
4	PO4	GGG	504	5/5	0.99	0.04	33,34,38,38	5
4	PO4	HHH	501	5/5	0.99	0.10	35,36,42,45	0

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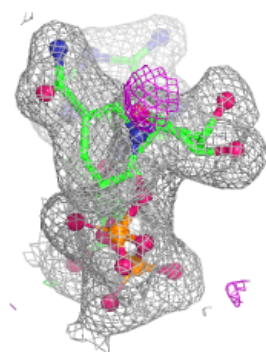
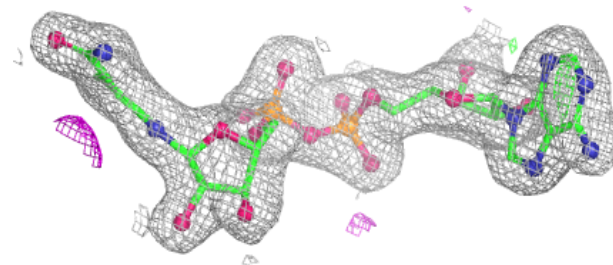
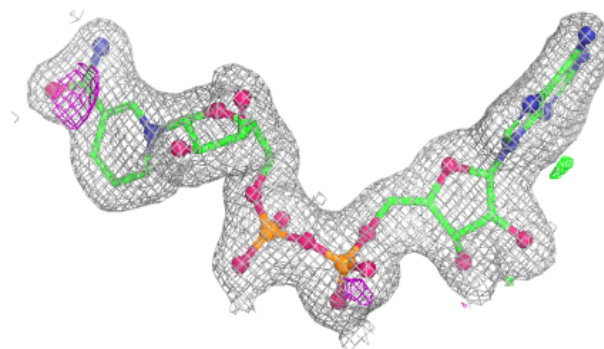
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	HHH	502	5/5	0.99	0.07	34,35,36,41	0
2	NAD	DDD	501	44/44	0.99	0.03	24,30,34,38	0
3	GOL	HHH	504	6/6	0.99	0.05	27,36,38,40	6
5	K	BBB	509	1/1	0.99	0.05	36,36,36,36	0
2	NAD	FFF	504	44/44	0.99	0.04	27,31,38,43	0
2	NAD	GGG	505	44/44	0.99	0.03	26,32,36,40	0
2	NAD	CCC	501	44/44	1.00	0.03	26,30,32,33	0
2	NAD	III	504	44/44	1.00	0.03	23,30,34,38	0
4	PO4	AAA	503	5/5	1.00	0.07	31,33,38,42	0
4	PO4	III	502	5/5	1.00	0.07	32,34,36,36	0

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

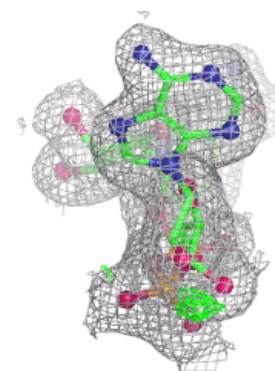
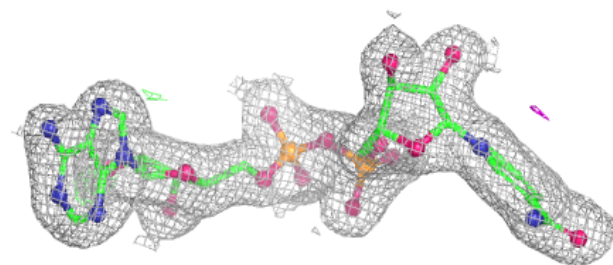
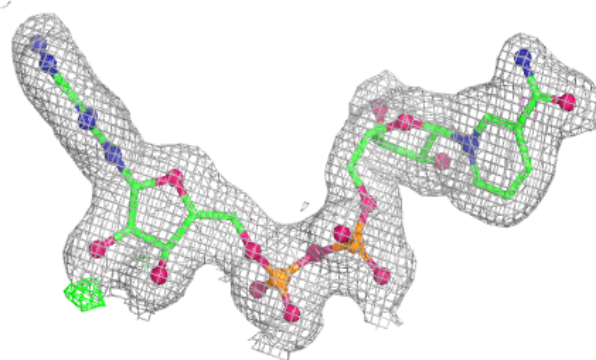
Electron density around NAD HHH 503:

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

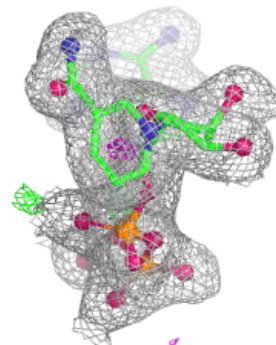
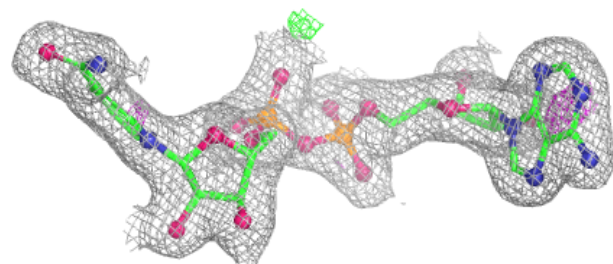
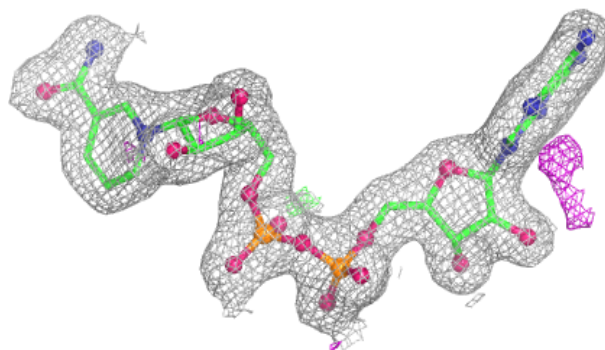


Electron density around NAD AAA 501:

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

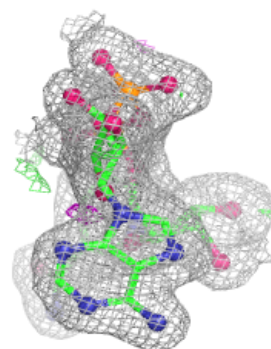
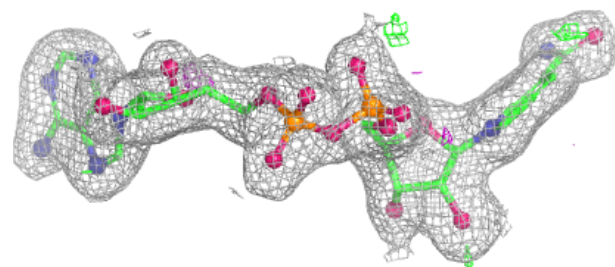
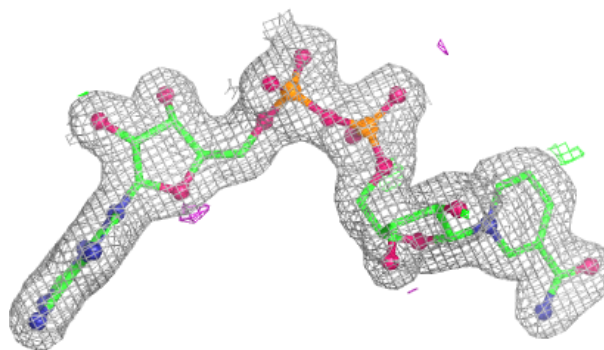
**Electron density around NAD BBB 501:**

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



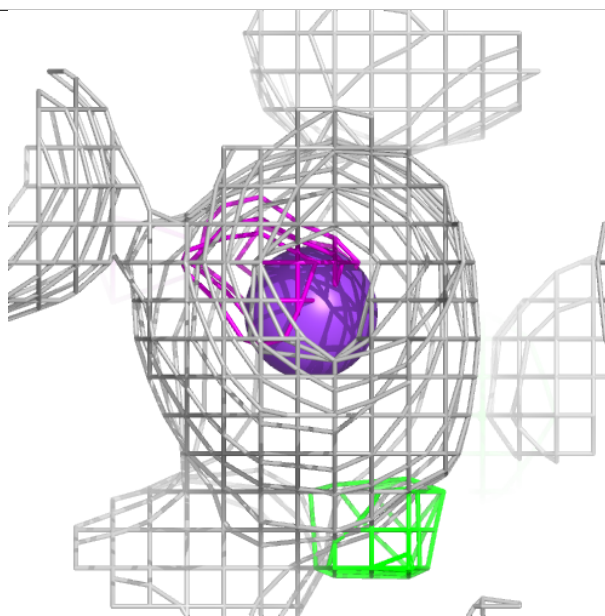
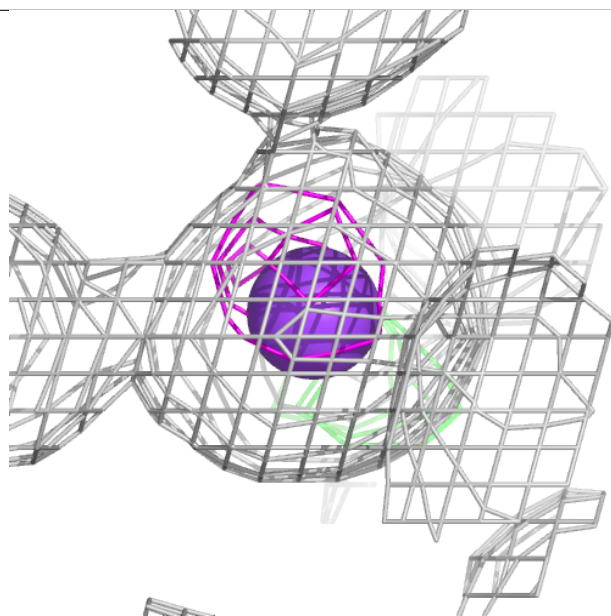
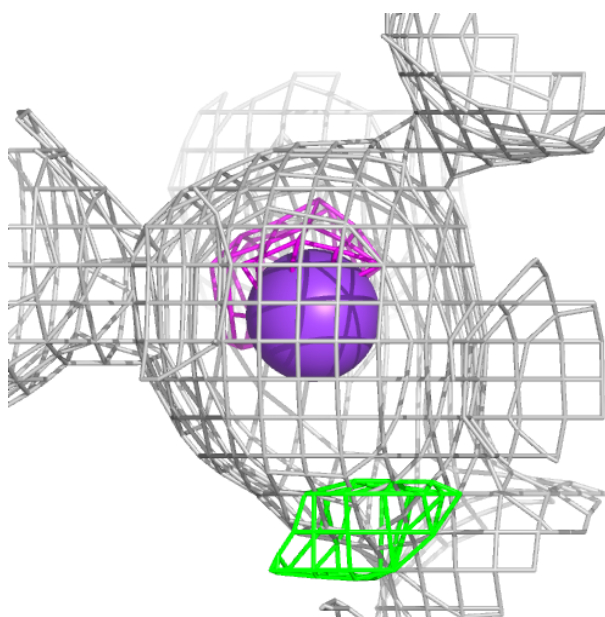
Electron density around NAD DDD 501:

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



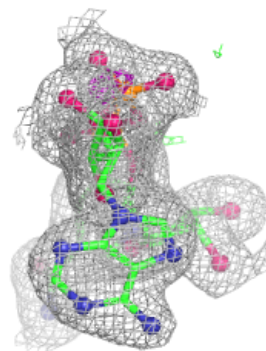
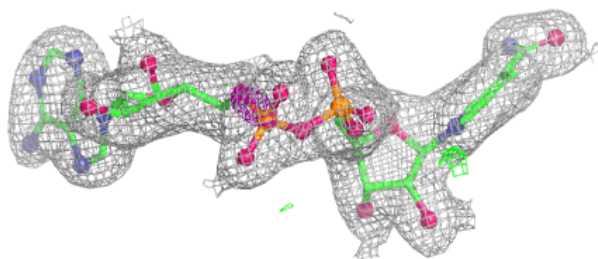
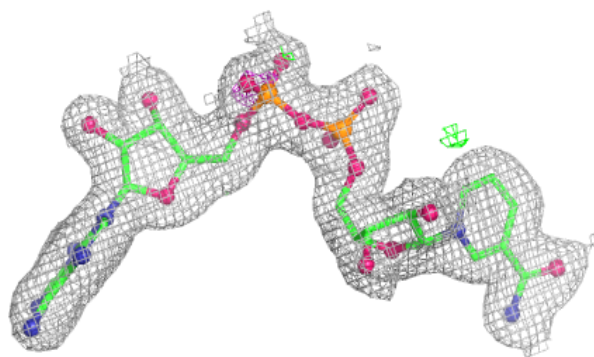
Electron density around K BBB 509:

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

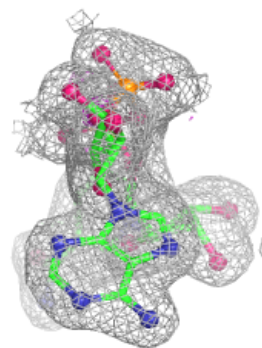
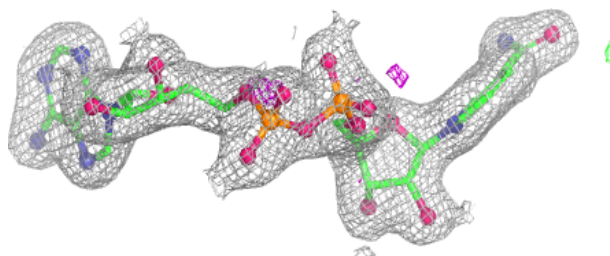
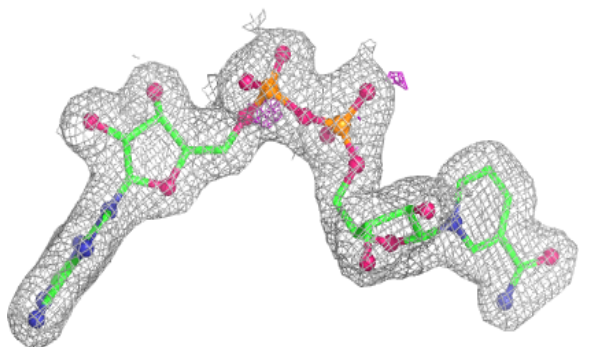


Electron density around NAD FFF 504:

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

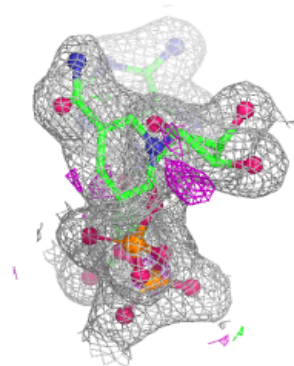
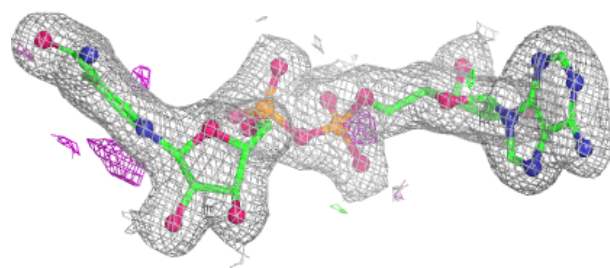
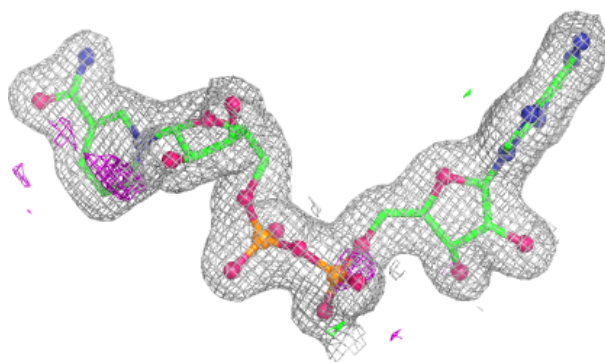
**Electron density around NAD GGG 505:**

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

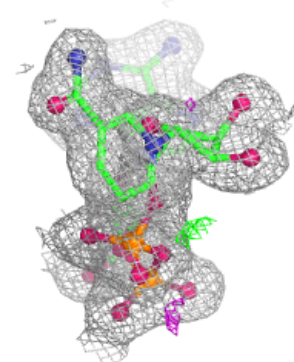
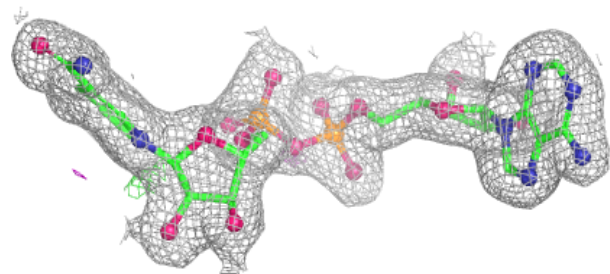
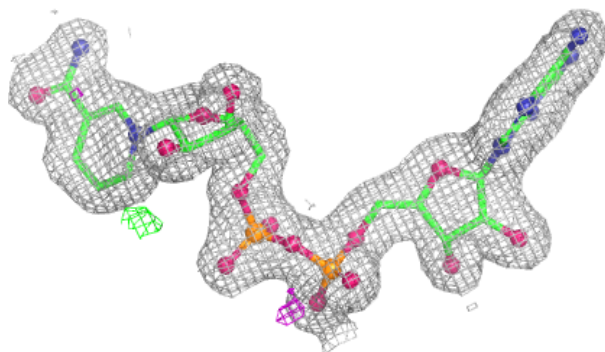


Electron density around NAD CCC 501:

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

**Electron density around NAD III 504:**

$2mF_o-DF_c$ (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.