



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:19 PM UTC

PDB ID : 7R3A / pdb_00007r3a
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *Methanococcus maripaludis* in complex with inosine
Authors : Saleem-Batcha, R.; Popadic, D.; Andexer, J.N.
Deposited on : 2022-02-06
Resolution : 2.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

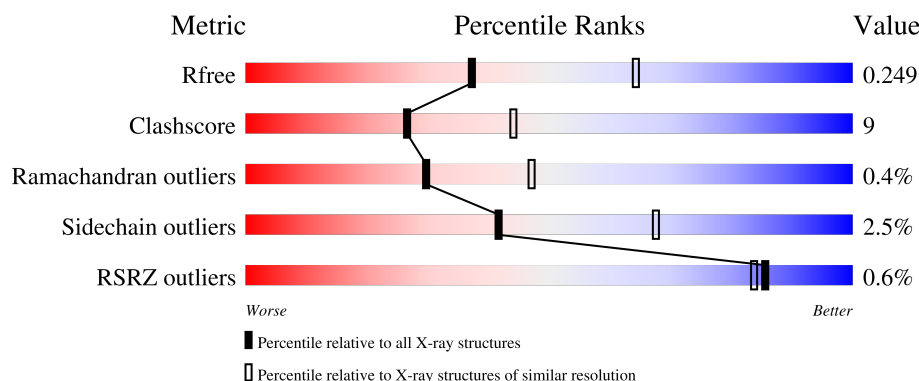
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

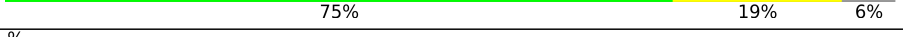
The reported resolution of this entry is 2.53 Å.

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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	A	435	
1	B	435	
1	C	435	
1	D	435	
1	E	435	

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Mol	Chain	Length	Quality of chain
1	F	435	
1	G	435	
1	H	435	

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
2	NOS	G	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26142 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 S-inosyl-L-homocysteine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3180	2005	539	613	23			
1	B	411	Total	C	N	O	S	0	0	0
			3180	2005	539	613	23			
1	C	411	Total	C	N	O	S	0	0	0
			3180	2005	539	613	23			
1	D	411	Total	C	N	O	S	0	0	0
			3180	2005	539	613	23			
1	E	411	Total	C	N	O	S	0	0	0
			3180	2005	539	613	23			
1	F	411	Total	C	N	O	S	0	0	0
			3180	2005	539	613	23			
1	G	411	Total	C	N	O	S	0	0	0
			3180	2005	539	613	23			
1	H	411	Total	C	N	O	S	0	0	0
			3180	2005	539	613	23			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q6LYR8
A	2	GLY	-	expression tag	UNP Q6LYR8
A	3	SER	-	expression tag	UNP Q6LYR8
A	4	SER	-	expression tag	UNP Q6LYR8
A	5	HIS	-	expression tag	UNP Q6LYR8
A	6	HIS	-	expression tag	UNP Q6LYR8
A	7	HIS	-	expression tag	UNP Q6LYR8
A	8	HIS	-	expression tag	UNP Q6LYR8
A	9	HIS	-	expression tag	UNP Q6LYR8
A	10	HIS	-	expression tag	UNP Q6LYR8
A	11	SER	-	expression tag	UNP Q6LYR8
A	12	SER	-	expression tag	UNP Q6LYR8
A	13	GLY	-	expression tag	UNP Q6LYR8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	-	expression tag	UNP Q6LYR8
A	15	VAL	-	expression tag	UNP Q6LYR8
A	16	PRO	-	expression tag	UNP Q6LYR8
A	17	ARG	-	expression tag	UNP Q6LYR8
A	18	GLY	-	expression tag	UNP Q6LYR8
A	19	SER	-	expression tag	UNP Q6LYR8
A	20	HIS	-	expression tag	UNP Q6LYR8
B	1	MET	-	initiating methionine	UNP Q6LYR8
B	2	GLY	-	expression tag	UNP Q6LYR8
B	3	SER	-	expression tag	UNP Q6LYR8
B	4	SER	-	expression tag	UNP Q6LYR8
B	5	HIS	-	expression tag	UNP Q6LYR8
B	6	HIS	-	expression tag	UNP Q6LYR8
B	7	HIS	-	expression tag	UNP Q6LYR8
B	8	HIS	-	expression tag	UNP Q6LYR8
B	9	HIS	-	expression tag	UNP Q6LYR8
B	10	HIS	-	expression tag	UNP Q6LYR8
B	11	SER	-	expression tag	UNP Q6LYR8
B	12	SER	-	expression tag	UNP Q6LYR8
B	13	GLY	-	expression tag	UNP Q6LYR8
B	14	LEU	-	expression tag	UNP Q6LYR8
B	15	VAL	-	expression tag	UNP Q6LYR8
B	16	PRO	-	expression tag	UNP Q6LYR8
B	17	ARG	-	expression tag	UNP Q6LYR8
B	18	GLY	-	expression tag	UNP Q6LYR8
B	19	SER	-	expression tag	UNP Q6LYR8
B	20	HIS	-	expression tag	UNP Q6LYR8
C	1	MET	-	initiating methionine	UNP Q6LYR8
C	2	GLY	-	expression tag	UNP Q6LYR8
C	3	SER	-	expression tag	UNP Q6LYR8
C	4	SER	-	expression tag	UNP Q6LYR8
C	5	HIS	-	expression tag	UNP Q6LYR8
C	6	HIS	-	expression tag	UNP Q6LYR8
C	7	HIS	-	expression tag	UNP Q6LYR8
C	8	HIS	-	expression tag	UNP Q6LYR8
C	9	HIS	-	expression tag	UNP Q6LYR8
C	10	HIS	-	expression tag	UNP Q6LYR8
C	11	SER	-	expression tag	UNP Q6LYR8
C	12	SER	-	expression tag	UNP Q6LYR8
C	13	GLY	-	expression tag	UNP Q6LYR8
C	14	LEU	-	expression tag	UNP Q6LYR8
C	15	VAL	-	expression tag	UNP Q6LYR8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	PRO	-	expression tag	UNP Q6LYR8
C	17	ARG	-	expression tag	UNP Q6LYR8
C	18	GLY	-	expression tag	UNP Q6LYR8
C	19	SER	-	expression tag	UNP Q6LYR8
C	20	HIS	-	expression tag	UNP Q6LYR8
D	1	MET	-	initiating methionine	UNP Q6LYR8
D	2	GLY	-	expression tag	UNP Q6LYR8
D	3	SER	-	expression tag	UNP Q6LYR8
D	4	SER	-	expression tag	UNP Q6LYR8
D	5	HIS	-	expression tag	UNP Q6LYR8
D	6	HIS	-	expression tag	UNP Q6LYR8
D	7	HIS	-	expression tag	UNP Q6LYR8
D	8	HIS	-	expression tag	UNP Q6LYR8
D	9	HIS	-	expression tag	UNP Q6LYR8
D	10	HIS	-	expression tag	UNP Q6LYR8
D	11	SER	-	expression tag	UNP Q6LYR8
D	12	SER	-	expression tag	UNP Q6LYR8
D	13	GLY	-	expression tag	UNP Q6LYR8
D	14	LEU	-	expression tag	UNP Q6LYR8
D	15	VAL	-	expression tag	UNP Q6LYR8
D	16	PRO	-	expression tag	UNP Q6LYR8
D	17	ARG	-	expression tag	UNP Q6LYR8
D	18	GLY	-	expression tag	UNP Q6LYR8
D	19	SER	-	expression tag	UNP Q6LYR8
D	20	HIS	-	expression tag	UNP Q6LYR8
E	1	MET	-	initiating methionine	UNP Q6LYR8
E	2	GLY	-	expression tag	UNP Q6LYR8
E	3	SER	-	expression tag	UNP Q6LYR8
E	4	SER	-	expression tag	UNP Q6LYR8
E	5	HIS	-	expression tag	UNP Q6LYR8
E	6	HIS	-	expression tag	UNP Q6LYR8
E	7	HIS	-	expression tag	UNP Q6LYR8
E	8	HIS	-	expression tag	UNP Q6LYR8
E	9	HIS	-	expression tag	UNP Q6LYR8
E	10	HIS	-	expression tag	UNP Q6LYR8
E	11	SER	-	expression tag	UNP Q6LYR8
E	12	SER	-	expression tag	UNP Q6LYR8
E	13	GLY	-	expression tag	UNP Q6LYR8
E	14	LEU	-	expression tag	UNP Q6LYR8
E	15	VAL	-	expression tag	UNP Q6LYR8
E	16	PRO	-	expression tag	UNP Q6LYR8
E	17	ARG	-	expression tag	UNP Q6LYR8

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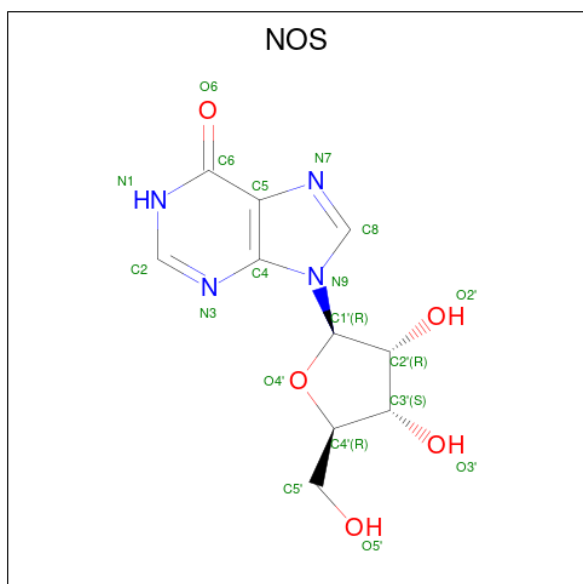
Chain	Residue	Modelled	Actual	Comment	Reference
E	18	GLY	-	expression tag	UNP Q6LYR8
E	19	SER	-	expression tag	UNP Q6LYR8
E	20	HIS	-	expression tag	UNP Q6LYR8
F	1	MET	-	initiating methionine	UNP Q6LYR8
F	2	GLY	-	expression tag	UNP Q6LYR8
F	3	SER	-	expression tag	UNP Q6LYR8
F	4	SER	-	expression tag	UNP Q6LYR8
F	5	HIS	-	expression tag	UNP Q6LYR8
F	6	HIS	-	expression tag	UNP Q6LYR8
F	7	HIS	-	expression tag	UNP Q6LYR8
F	8	HIS	-	expression tag	UNP Q6LYR8
F	9	HIS	-	expression tag	UNP Q6LYR8
F	10	HIS	-	expression tag	UNP Q6LYR8
F	11	SER	-	expression tag	UNP Q6LYR8
F	12	SER	-	expression tag	UNP Q6LYR8
F	13	GLY	-	expression tag	UNP Q6LYR8
F	14	LEU	-	expression tag	UNP Q6LYR8
F	15	VAL	-	expression tag	UNP Q6LYR8
F	16	PRO	-	expression tag	UNP Q6LYR8
F	17	ARG	-	expression tag	UNP Q6LYR8
F	18	GLY	-	expression tag	UNP Q6LYR8
F	19	SER	-	expression tag	UNP Q6LYR8
F	20	HIS	-	expression tag	UNP Q6LYR8
G	1	MET	-	initiating methionine	UNP Q6LYR8
G	2	GLY	-	expression tag	UNP Q6LYR8
G	3	SER	-	expression tag	UNP Q6LYR8
G	4	SER	-	expression tag	UNP Q6LYR8
G	5	HIS	-	expression tag	UNP Q6LYR8
G	6	HIS	-	expression tag	UNP Q6LYR8
G	7	HIS	-	expression tag	UNP Q6LYR8
G	8	HIS	-	expression tag	UNP Q6LYR8
G	9	HIS	-	expression tag	UNP Q6LYR8
G	10	HIS	-	expression tag	UNP Q6LYR8
G	11	SER	-	expression tag	UNP Q6LYR8
G	12	SER	-	expression tag	UNP Q6LYR8
G	13	GLY	-	expression tag	UNP Q6LYR8
G	14	LEU	-	expression tag	UNP Q6LYR8
G	15	VAL	-	expression tag	UNP Q6LYR8
G	16	PRO	-	expression tag	UNP Q6LYR8
G	17	ARG	-	expression tag	UNP Q6LYR8
G	18	GLY	-	expression tag	UNP Q6LYR8
G	19	SER	-	expression tag	UNP Q6LYR8

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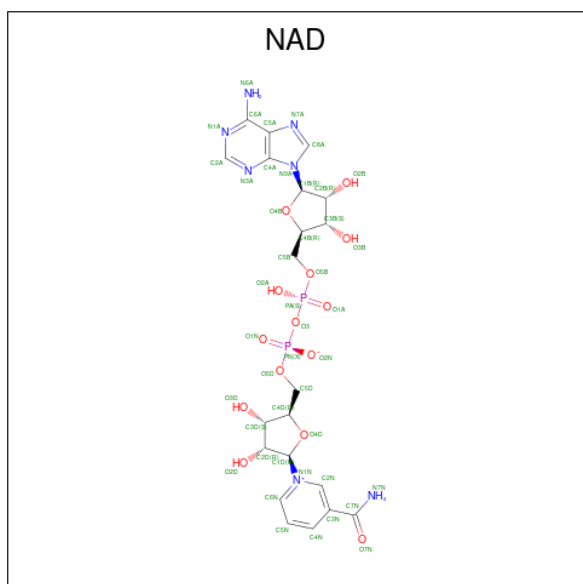
Chain	Residue	Modelled	Actual	Comment	Reference
G	20	HIS	-	expression tag	UNP Q6LYR8
H	1	MET	-	initiating methionine	UNP Q6LYR8
H	2	GLY	-	expression tag	UNP Q6LYR8
H	3	SER	-	expression tag	UNP Q6LYR8
H	4	SER	-	expression tag	UNP Q6LYR8
H	5	HIS	-	expression tag	UNP Q6LYR8
H	6	HIS	-	expression tag	UNP Q6LYR8
H	7	HIS	-	expression tag	UNP Q6LYR8
H	8	HIS	-	expression tag	UNP Q6LYR8
H	9	HIS	-	expression tag	UNP Q6LYR8
H	10	HIS	-	expression tag	UNP Q6LYR8
H	11	SER	-	expression tag	UNP Q6LYR8
H	12	SER	-	expression tag	UNP Q6LYR8
H	13	GLY	-	expression tag	UNP Q6LYR8
H	14	LEU	-	expression tag	UNP Q6LYR8
H	15	VAL	-	expression tag	UNP Q6LYR8
H	16	PRO	-	expression tag	UNP Q6LYR8
H	17	ARG	-	expression tag	UNP Q6LYR8
H	18	GLY	-	expression tag	UNP Q6LYR8
H	19	SER	-	expression tag	UNP Q6LYR8
H	20	HIS	-	expression tag	UNP Q6LYR8

- Molecule 2 is INOSINE (CCD ID: NOS) (formula: $C_{10}H_{12}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



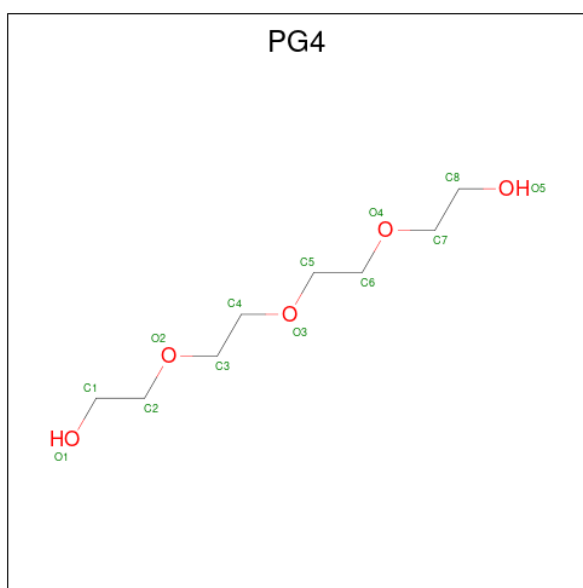
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			13	8	5		
4	H	1	Total	C	O	0	0
			13	8	5		

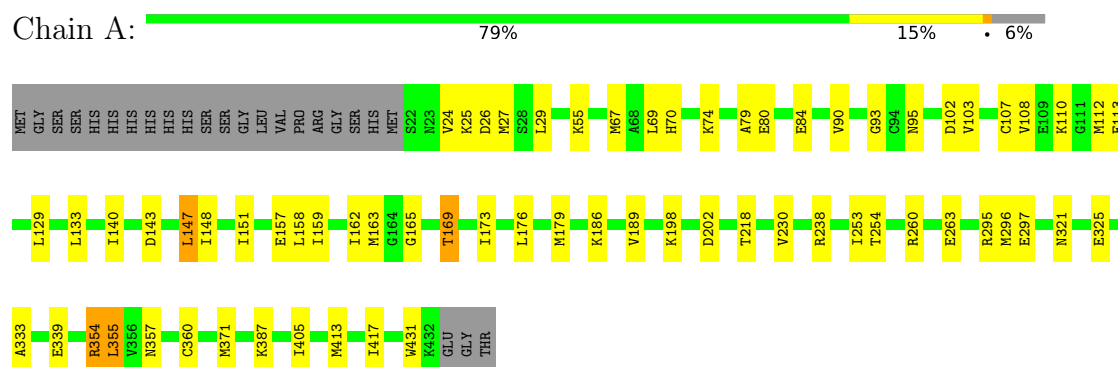
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	16	Total	O	0	0
			16	16		
5	C	21	Total	O	0	0
			21	21		
5	D	15	Total	O	0	0
			15	15		
5	E	18	Total	O	0	0
			18	18		
5	F	8	Total	O	0	0
			8	8		
5	G	3	Total	O	0	0
			3	3		
5	H	3	Total	O	0	0
			3	3		

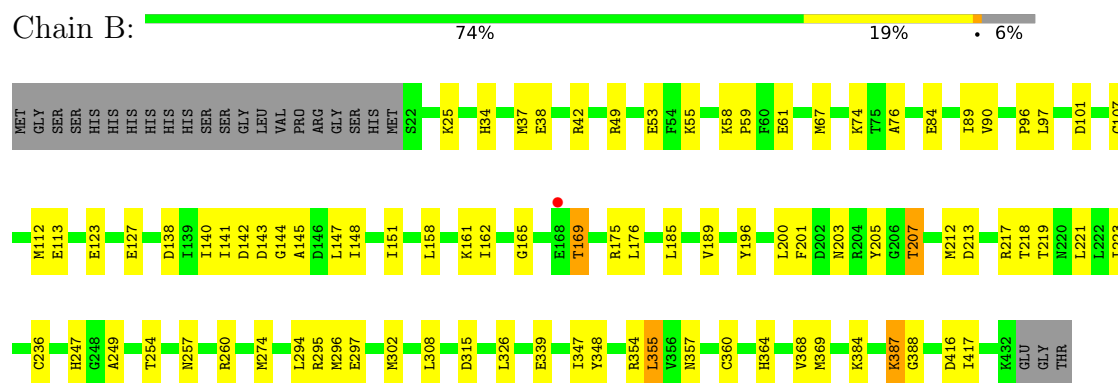
3 Residue-property plots [i](#)

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.

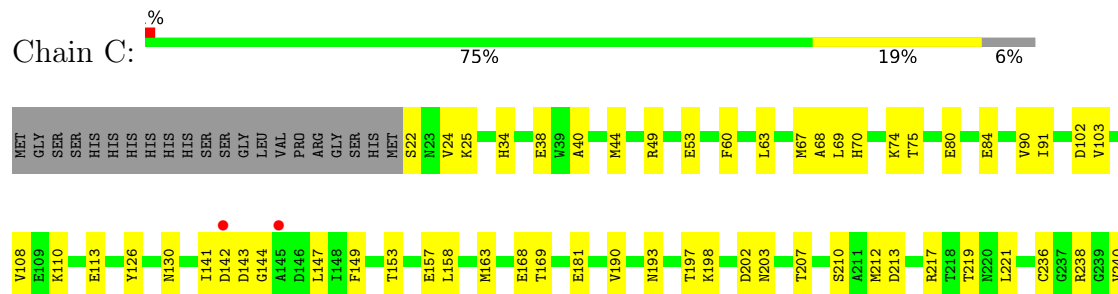
• Molecule 1: S-inosyl-L-homocysteine hydrolase

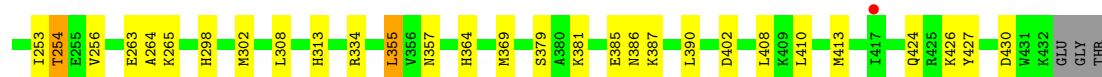


• Molecule 1: S-inosyl-L-homocysteine hydrolase



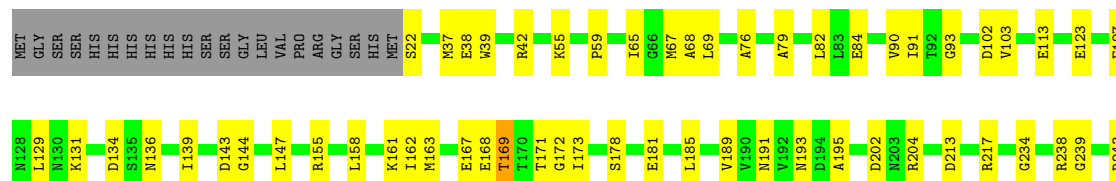
• Molecule 1: S-inosyl-L-homocysteine hydrolase





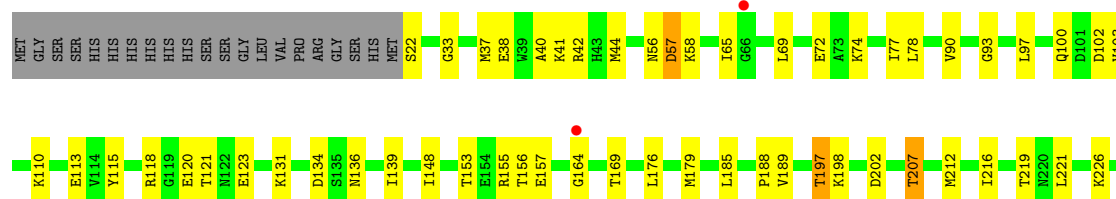
• Molecule 1: S-inosyl-L-homocysteine hydrolase

Chain D: 75% 19% 6%



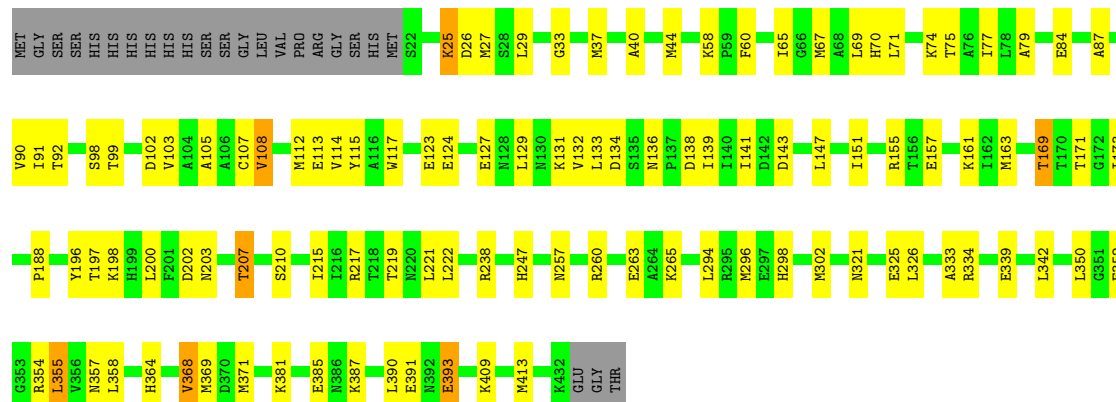
• Molecule 1: S-inosyl-L-homocysteine hydrolase

Chain E: 74% 19% 6%

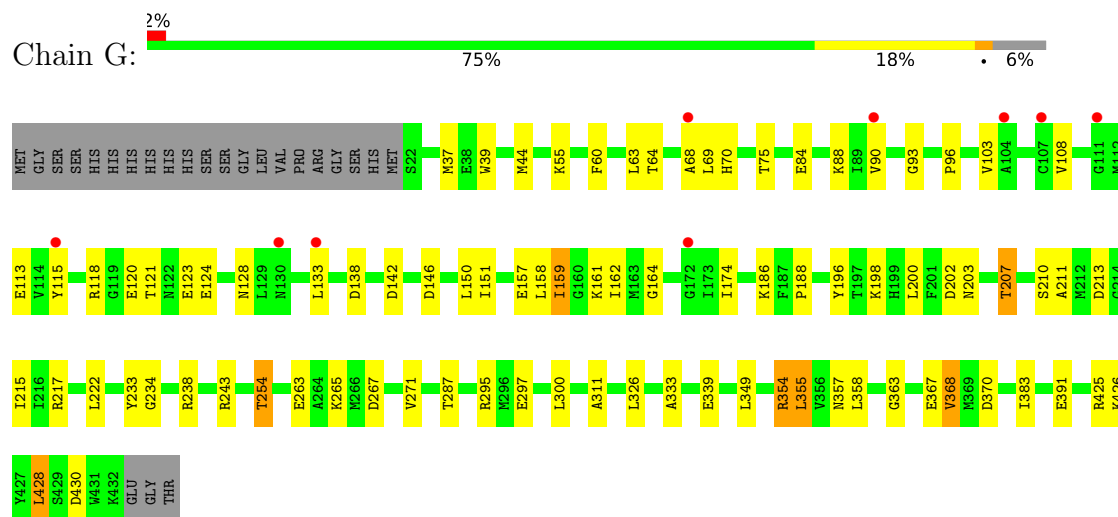


• Molecule 1: S-inosyl-L-homocysteine hydrolase

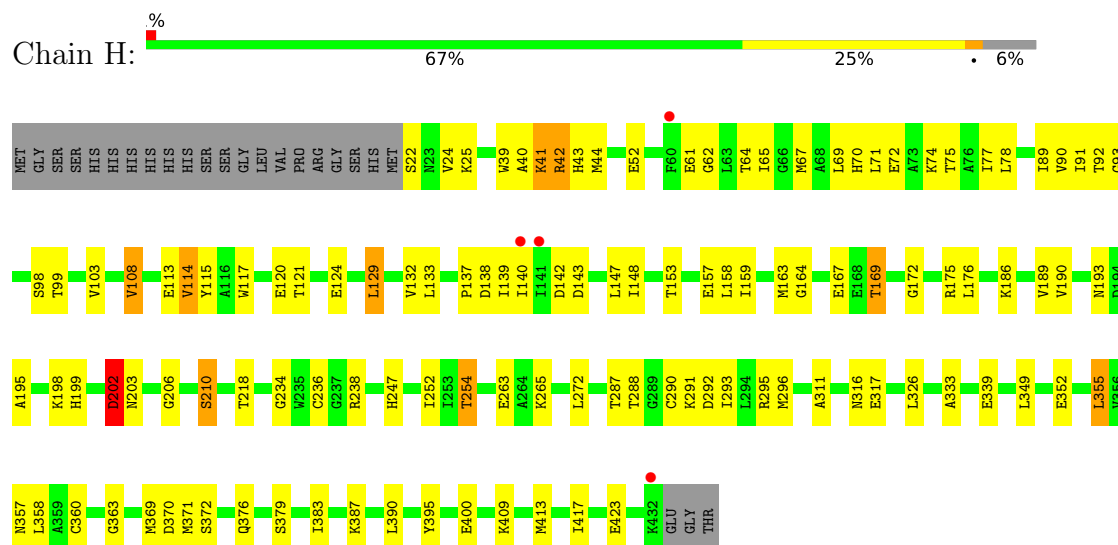
Chain F: 70% 23% 6%



• Molecule 1: S-inosyl-L-homocysteine hydrolase



• Molecule 1: S-inosyl-L-homocysteine hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.78Å 328.87Å 85.09Å 90.00° 107.23° 90.00°	Depositor
Resolution (Å)	47.86 – 2.53 47.86 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.86-2.53) 97.4 (47.86-2.53)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.188 , 0.243 0.200 , 0.249	Depositor DCC
R_{free} test set	5569 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.794	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26142	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: NOS, PG4, 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	A	0.19	0/3231	0.41	0/4353
1	B	0.16	0/3231	0.41	0/4353
1	C	0.20	0/3231	0.42	0/4353
1	D	0.18	0/3231	0.41	0/4353
1	E	0.19	0/3231	0.45	0/4353
1	F	0.19	0/3231	0.43	0/4353
1	G	0.14	0/3231	0.42	0/4353
1	H	0.23	0/3231	0.51	1/4353 (0.0%)
All	All	0.19	0/25848	0.43	1/34824 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	202	ASP	CA-CB-CG	7.19	119.79	112.60

There are no chirality outliers.

There are no planarity outliers.

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	A	3180	0	3178	50	0
1	B	3180	0	3178	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3180	0	3178	60	0
1	D	3180	0	3178	52	0
1	E	3180	0	3178	55	0
1	F	3180	0	3178	66	0
1	G	3180	0	3178	64	0
1	H	3180	0	3178	86	0
2	A	19	0	11	3	0
2	B	19	0	11	1	0
2	C	19	0	11	4	0
2	D	19	0	11	2	0
2	E	19	0	11	0	0
2	F	19	0	11	4	0
2	G	19	0	11	7	0
2	H	19	0	11	3	0
3	A	44	0	26	3	0
3	B	44	0	26	2	0
3	C	44	0	26	3	0
3	D	44	0	26	3	0
3	E	44	0	26	2	0
3	F	44	0	26	2	0
3	G	44	0	26	7	0
3	H	44	0	26	4	0
4	A	13	0	18	1	0
4	B	13	0	18	3	0
4	C	13	0	18	0	0
4	D	13	0	18	4	0
4	E	13	0	18	0	0
4	F	13	0	18	4	0
4	G	13	0	18	0	0
4	H	13	0	18	0	0
5	A	10	0	0	0	0
5	B	16	0	0	0	0
5	C	21	0	0	1	0
5	D	15	0	0	0	0
5	E	18	0	0	1	0
5	F	8	0	0	0	0
5	G	3	0	0	0	0
5	H	3	0	0	0	0
All	All	26142	0	25864	482	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 9.

All (482) 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:H:288:THR:HG23	1:H:290:CYS:H	1.29	0.97
1:C:207:THR:HG22	1:C:364:HIS:HE2	1.25	0.97
1:C:207:THR:HG22	1:C:364:HIS:NE2	1.80	0.95
1:B:58:LYS:O	1:B:61:GLU:HG3	1.70	0.92
1:E:254:THR:HG22	3:E:503:NAD:H2A	1.60	0.84
1:E:357:ASN:HD21	3:E:503:NAD:H72N	1.25	0.83
1:A:295:ARG:HH11	1:A:297:GLU:HG2	1.43	0.83
1:C:67:MET:HG2	1:C:141:ILE:HB	1.61	0.80
1:D:357:ASN:HD21	3:D:502:NAD:H72N	1.29	0.80
1:H:41:LYS:HB3	1:H:77:ILE:HD12	1.62	0.79
1:A:254:THR:HG22	3:A:502:NAD:H2A	1.63	0.79
1:B:67:MET:HG2	1:B:141:ILE:HB	1.65	0.77
1:C:254:THR:HG22	3:C:502:NAD:H2A	1.68	0.75
1:H:67:MET:HE3	1:H:91:ILE:HD12	1.66	0.75
1:H:357:ASN:HD21	3:H:503:NAD:H72N	1.34	0.75
1:C:207:THR:HG22	1:C:364:HIS:CE1	2.21	0.75
1:D:257:ASN:HD21	4:D:503:PG4:H42	1.51	0.74
1:B:315:ASP:OD2	1:B:354:ARG:NH1	2.20	0.74
1:B:274:MET:HE3	1:B:294:LEU:HD21	1.70	0.74
1:F:357:ASN:HD21	3:F:503:NAD:H72N	1.34	0.73
1:H:39:TRP:HA	1:H:42:ARG:HD2	1.70	0.73
1:H:193:ASN:HA	1:H:198:LYS:HD2	1.69	0.73
1:F:26:ASP:HB3	1:F:29:LEU:HG	1.70	0.72
2:G:502:NOS:H8	3:G:503:NAD:N7N	2.04	0.72
1:G:300:LEU:HD22	1:G:326:LEU:HD11	1.71	0.72
1:C:357:ASN:HD21	3:C:502:NAD:H72N	1.35	0.72
1:F:133:LEU:HD22	1:F:151:ILE:HD11	1.71	0.72
1:B:254:THR:HG22	3:B:502:NAD:H2A	1.72	0.71
1:D:287:THR:HG22	1:D:311:ALA:HB3	1.72	0.71
1:G:55:LYS:HZ1	1:G:84:GLU:HB2	1.54	0.71
1:G:254:THR:HG22	3:G:503:NAD:H2A	1.72	0.71
1:D:37:MET:HE3	1:D:76:ALA:HB1	1.73	0.70
1:G:157:GLU:HG2	1:G:158:LEU:HD12	1.72	0.70
1:G:295:ARG:NH2	1:G:297:GLU:OE2	2.25	0.70
1:C:190:VAL:HG21	1:C:379:SER:HB3	1.73	0.69
1:A:107:CYS:HB3	1:A:112:MET:HE2	1.74	0.69
1:G:164:GLY:HA3	1:G:383:ILE:HD12	1.74	0.68
1:F:215:ILE:O	1:F:219:THR:HG22	1.94	0.68
1:B:357:ASN:HD21	3:B:502:NAD:H72N	1.40	0.67
1:D:67:MET:HE3	1:D:82:LEU:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:THR:HG21	1:B:360:CYS:HB3	1.77	0.66
1:H:254:THR:HG22	3:H:503:NAD:H2A	1.75	0.66
1:E:41:LYS:HB2	1:E:77:ILE:HD12	1.76	0.66
1:F:257:ASN:HD21	4:F:501:PG4:H32	1.60	0.65
1:E:238:ARG:HH22	1:E:263:GLU:CD	2.05	0.65
1:C:67:MET:HE3	1:C:91:ILE:HD12	1.80	0.64
1:E:134:ASP:OD1	1:E:155:ARG:NH2	2.31	0.64
1:A:357:ASN:HD21	3:A:502:NAD:H72N	1.44	0.63
1:A:176:LEU:HD13	1:A:189:VAL:HG11	1.81	0.63
1:A:218:THR:HG21	1:A:360:CYS:HB3	1.80	0.63
1:B:144:GLY:O	1:B:175:ARG:NH1	2.32	0.63
1:D:39:TRP:HA	1:D:42:ARG:HE	1.64	0.63
1:D:238:ARG:HH22	1:D:263:GLU:CD	2.07	0.62
1:A:260:ARG:HE	4:A:503:PG4:H52	1.63	0.62
1:H:90:VAL:HG13	1:H:113:GLU:HB3	1.82	0.62
1:H:218:THR:HG21	1:H:360:CYS:HB3	1.81	0.62
1:F:67:MET:HG2	1:F:141:ILE:HB	1.82	0.62
1:H:210:SER:HB3	1:H:357:ASN:HB2	1.82	0.61
1:C:49:ARG:HD2	1:C:408:LEU:HD21	1.82	0.61
1:D:167:GLU:OE1	1:D:169:THR:N	2.30	0.61
1:B:58:LYS:O	1:B:61:GLU:CG	2.47	0.61
1:G:96:PRO:HG2	1:G:354:ARG:NH1	2.16	0.61
1:C:34:HIS:CE1	1:C:110:LYS:HE2	2.36	0.60
1:H:288:THR:HG23	1:H:290:CYS:N	2.09	0.60
1:H:64:THR:OG1	1:H:137:PRO:HA	2.02	0.60
1:G:120:GLU:HB2	1:G:124:GLU:HB2	1.84	0.60
1:C:202:ASP:OD2	1:C:369:MET:HE1	2.02	0.60
1:H:288:THR:HG21	1:H:293:ILE:HG13	1.83	0.59
1:C:80:GLU:O	1:C:84:GLU:HG2	2.02	0.59
1:F:71:LEU:HB3	1:F:99:THR:HG22	1.85	0.59
1:A:95:ASN:HD21	1:A:354:ARG:HG2	1.68	0.59
1:C:238:ARG:HH22	1:C:263:GLU:CD	2.11	0.59
1:G:96:PRO:HG2	1:G:354:ARG:HH11	1.66	0.59
1:H:71:LEU:HB3	1:H:99:THR:HG23	1.84	0.59
1:D:254:THR:HG22	3:D:502:NAD:H2A	1.83	0.59
1:G:158:LEU:HB3	1:G:162:ILE:HD13	1.83	0.59
1:H:175:ARG:HH11	1:H:175:ARG:HG2	1.66	0.59
1:B:295:ARG:HH11	1:B:297:GLU:HG2	1.68	0.59
1:A:67:MET:HE1	1:A:79:ALA:HB2	1.85	0.59
1:G:355:LEU:HD13	1:G:358:LEU:HD12	1.85	0.58
1:C:238:ARG:NH2	1:C:263:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:LYS:O	1:C:385:GLU:HG3	2.03	0.58
1:D:178:SER:HA	1:D:181:GLU:HG3	1.86	0.58
1:A:90:VAL:HG13	1:A:113:GLU:HB3	1.86	0.58
1:F:69:LEU:HD23	1:F:143:ASP:HB2	1.84	0.57
1:E:72:GLU:HB3	1:E:100:GLN:HG3	1.87	0.57
1:F:65:ILE:HD12	1:F:139:ILE:HB	1.85	0.57
1:F:115:TYR:CD1	1:F:131:LYS:HE3	2.39	0.57
1:C:144:GLY:HA3	1:C:313:HIS:CE1	2.39	0.57
1:A:202:ASP:OD2	2:A:501:NOS:O2'	2.23	0.57
1:D:144:GLY:N	1:D:167:GLU:OE2	2.36	0.57
1:H:369:MET:HA	1:H:369:MET:HE2	1.86	0.57
1:C:69:LEU:HD23	1:C:143:ASP:HB2	1.86	0.57
1:H:129:LEU:HD13	1:H:147:LEU:HD23	1.87	0.57
1:E:207:THR:HG22	1:E:364:HIS:CE1	2.39	0.56
1:B:339:GLU:HG3	1:B:348:TYR:CE1	2.40	0.56
1:D:67:MET:HB2	1:D:91:ILE:HG13	1.87	0.56
1:D:123:GLU:O	1:D:127:GLU:HG3	2.04	0.56
1:H:288:THR:HG21	1:H:293:ILE:CG1	2.34	0.56
1:H:67:MET:HE2	1:H:89:ILE:HG23	1.87	0.56
1:F:257:ASN:ND2	4:F:501:PG4:H32	2.20	0.56
1:H:238:ARG:HH21	1:H:263:GLU:CD	2.14	0.56
1:H:296:MET:SD	1:H:326:LEU:HD11	2.45	0.56
1:F:196:TYR:O	1:F:200:LEU:HB2	2.05	0.56
1:A:148:ILE:HG21	1:A:176:LEU:HD21	1.88	0.56
1:E:56:ASN:C	1:E:58:LYS:H	2.14	0.56
1:H:234:GLY:O	1:H:238:ARG:HG3	2.06	0.55
1:H:400:GLU:CD	1:H:400:GLU:H	2.14	0.55
1:B:67:MET:HE2	1:B:89:ILE:HD12	1.87	0.55
1:B:55:LYS:HD2	1:B:84:GLU:HB3	1.89	0.55
1:C:40:ALA:O	1:C:44:MET:HG3	2.07	0.55
2:G:502:NOS:H8	3:G:503:NAD:H72N	1.69	0.55
1:H:190:VAL:HG11	1:H:379:SER:HB3	1.88	0.55
1:G:44:MET:HG2	1:G:370:ASP:HB2	1.88	0.55
1:E:121:THR:HG22	1:E:123:GLU:H	1.72	0.55
1:G:213:ASP:OD2	1:G:217:ARG:NH2	2.33	0.55
2:G:502:NOS:H2'	3:G:503:NAD:H71N	1.72	0.55
1:B:223:ILE:HG22	1:B:249:ALA:HB2	1.89	0.55
1:C:213:ASP:OD2	1:C:217:ARG:NH2	2.35	0.55
1:C:68:ALA:HB3	1:C:142:ASP:OD1	2.07	0.54
1:B:37:MET:HE3	1:B:76:ALA:HB1	1.89	0.54
1:F:368:VAL:HG13	1:G:222:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:MET:HB3	1:C:91:ILE:HD12	1.89	0.54
1:B:302:MET:HE2	1:B:347:ILE:HD12	1.89	0.54
1:A:295:ARG:NH1	1:A:297:GLU:HG2	2.19	0.54
1:D:90:VAL:HG13	1:D:113:GLU:HB3	1.90	0.54
1:H:137:PRO:HD2	1:H:158:LEU:HD22	1.90	0.54
1:H:349:LEU:HD21	1:H:352:GLU:HA	1.89	0.54
1:B:97:LEU:HD12	1:B:354:ARG:HD3	1.89	0.54
1:D:333:ALA:HB2	1:D:339:GLU:HB2	1.90	0.54
1:G:426:LYS:NZ	1:G:430:ASP:HB2	2.23	0.53
1:E:238:ARG:NH2	1:E:263:GLU:OE2	2.41	0.53
1:E:148:ILE:HG21	1:E:176:LEU:HD21	1.90	0.53
1:E:197:THR:OG1	1:E:402:ASP:OD1	2.27	0.53
1:H:390:LEU:HD22	1:H:395:TYR:CE2	2.43	0.53
1:H:199:HIS:O	1:H:203:ASN:HB2	2.08	0.53
1:D:129:LEU:HD22	1:D:147:LEU:HD13	1.90	0.53
1:D:202:ASP:OD2	2:D:501:NOS:O2'	2.27	0.53
1:G:233:TYR:OH	1:G:267:ASP:OD2	2.24	0.52
1:H:142:ASP:OD2	1:H:143:ASP:N	2.42	0.52
1:H:198:LYS:HE2	1:H:202:ASP:OD2	2.09	0.52
1:C:364:HIS:HB2	1:C:369:MET:HE3	1.90	0.52
1:F:67:MET:HE1	1:F:79:ALA:HB2	1.92	0.52
1:H:140:ILE:HD12	1:H:147:LEU:HD13	1.90	0.52
1:B:302:MET:HE1	1:B:308:LEU:HD11	1.91	0.52
1:G:60:PHE:HA	1:G:63:LEU:HD23	1.90	0.52
1:G:425:ARG:HG3	1:G:425:ARG:HH11	1.74	0.52
1:G:55:LYS:NZ	1:G:84:GLU:HB2	2.25	0.52
1:G:211:ALA:O	1:G:215:ILE:HG13	2.09	0.52
1:C:163:MET:HE3	1:C:387:LYS:HG3	1.91	0.52
1:B:90:VAL:HG13	1:B:113:GLU:HB3	1.92	0.52
1:E:56:ASN:O	1:E:58:LYS:N	2.43	0.52
1:B:143:ASP:OD1	1:B:169:THR:OG1	2.28	0.52
1:H:287:THR:HG22	1:H:311:ALA:HB3	1.91	0.52
1:D:312:GLY:HA3	1:D:317:GLU:OE2	2.09	0.51
1:F:25:LYS:HG2	1:F:117:TRP:HB2	1.93	0.51
1:C:90:VAL:HG13	1:C:113:GLU:HB3	1.92	0.51
1:D:195:ALA:HB2	1:D:397:ILE:HD12	1.93	0.51
1:E:389:LYS:O	1:H:387:LYS:NZ	2.40	0.51
1:A:158:LEU:O	1:A:162:ILE:HG13	2.11	0.51
1:E:22:SER:HA	1:E:115:TYR:HE1	1.76	0.51
1:F:188:PRO:HG3	1:F:390:LEU:HB2	1.91	0.51
1:F:409:LYS:O	1:F:413:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:423:GLU:CD	1:H:423:GLU:H	2.19	0.51
1:D:68:ALA:HB2	1:D:147:LEU:HD22	1.93	0.50
1:E:97:LEU:HD22	1:E:118:ARG:HE	1.76	0.50
1:F:33:GLY:O	1:F:37:MET:HG3	2.11	0.50
1:E:386:ASN:O	1:E:388:GLY:N	2.44	0.50
1:H:198:LYS:HG2	1:H:372:SER:OG	2.11	0.50
1:C:70:HIS:CE1	1:C:355:LEU:HD12	2.47	0.50
1:E:207:THR:HG22	1:E:364:HIS:NE2	2.26	0.50
1:F:60:PHE:HB3	1:F:87:ALA:HB2	1.93	0.50
1:F:107:CYS:HB3	1:F:112:MET:SD	2.52	0.50
1:F:129:LEU:HD22	1:F:147:LEU:HD21	1.92	0.50
1:H:41:LYS:HB3	1:H:77:ILE:CD1	2.36	0.50
1:H:133:LEU:HD23	1:H:158:LEU:HD13	1.93	0.50
1:H:238:ARG:NH2	1:H:263:GLU:OE2	2.44	0.50
1:H:129:LEU:O	1:H:132:VAL:HG22	2.10	0.50
1:F:381:LYS:O	1:F:385:GLU:HG3	2.11	0.50
1:G:55:LYS:HZ2	1:G:84:GLU:C	2.20	0.50
1:H:195:ALA:O	1:H:199:HIS:HD2	1.95	0.50
1:E:386:ASN:HB3	1:E:390:LEU:HG	1.94	0.49
1:H:311:ALA:O	3:H:503:NAD:H2N	2.12	0.49
1:C:197:THR:OG1	1:C:402:ASP:OD1	2.29	0.49
1:G:234:GLY:HA3	3:G:503:NAD:O5B	2.12	0.49
1:G:287:THR:HG22	1:G:311:ALA:HB3	1.93	0.49
1:B:257:ASN:HD22	4:B:503:PG4:H12	1.77	0.49
1:A:27:MET:HE1	1:A:108:VAL:HB	1.94	0.49
1:G:121:THR:OG1	1:G:124:GLU:HG3	2.13	0.49
1:H:143:ASP:OD1	1:H:169:THR:OG1	2.29	0.49
1:A:157:GLU:HG2	1:A:158:LEU:HD23	1.94	0.49
1:C:34:HIS:O	1:C:38:GLU:HG2	2.13	0.49
1:F:391:GLU:HB2	1:F:393:GLU:HG3	1.93	0.49
1:H:148:ILE:HD13	1:H:176:LEU:HD11	1.94	0.49
1:E:38:GLU:O	1:E:42:ARG:HD3	2.13	0.49
1:G:63:LEU:HD12	1:G:138:ASP:OD2	2.12	0.49
1:G:425:ARG:HH21	1:G:428:LEU:HD23	1.78	0.49
1:H:164:GLY:HA3	1:H:383:ILE:HD12	1.93	0.49
1:C:265:LYS:NZ	1:H:413:MET:HB3	2.28	0.49
1:A:80:GLU:O	1:A:84:GLU:HG2	2.13	0.48
1:D:163:MET:HE3	1:D:387:LYS:HG3	1.94	0.48
1:A:80:GLU:OE2	1:A:110:LYS:HE2	2.12	0.48
1:E:387:LYS:HB3	1:E:387:LYS:HE3	1.55	0.48
1:F:136:ASN:O	1:F:161:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ARG:HE	4:D:503:PG4:H51	1.79	0.48
1:H:91:ILE:HG23	1:H:114:VAL:HG12	1.93	0.48
1:H:92:THR:OG1	1:H:115:TYR:O	2.28	0.48
1:C:207:THR:CG2	1:C:364:HIS:NE2	2.67	0.48
1:C:386:ASN:HB3	1:C:390:LEU:HG	1.96	0.48
1:E:423:GLU:CD	1:E:423:GLU:H	2.22	0.48
1:F:333:ALA:HB2	1:F:339:GLU:HB2	1.96	0.48
1:A:198:LYS:HD3	1:A:202:ASP:HB3	1.95	0.48
1:C:202:ASP:OD2	2:C:501:NOS:O2'	2.31	0.48
1:E:247:HIS:HD2	5:E:617:HOH:O	1.97	0.48
1:B:207:THR:HG22	1:B:364:HIS:NE2	2.29	0.48
1:C:207:THR:CG2	1:C:364:HIS:CE1	2.94	0.48
1:D:38:GLU:O	1:D:42:ARG:HG3	2.13	0.48
1:D:102:ASP:OD1	1:D:103:VAL:N	2.47	0.48
1:G:425:ARG:HG3	1:G:425:ARG:NH1	2.29	0.48
1:A:129:LEU:HD22	1:A:147:LEU:CD1	2.44	0.47
1:C:60:PHE:HA	1:C:63:LEU:HD12	1.96	0.47
1:D:65:ILE:HG12	1:D:139:ILE:HB	1.96	0.47
1:A:159:ILE:HD12	1:A:186:LYS:HB2	1.96	0.47
1:B:196:TYR:O	1:B:200:LEU:HB2	2.13	0.47
1:C:207:THR:HA	1:C:210:SER:HG	1.79	0.47
1:F:123:GLU:O	1:F:127:GLU:HG3	2.14	0.47
1:F:321:ASN:O	1:F:325:GLU:HG3	2.14	0.47
1:F:352:GLU:OE1	1:F:354:ARG:NH1	2.46	0.47
1:G:196:TYR:O	1:G:200:LEU:HB2	2.13	0.47
1:B:257:ASN:ND2	4:B:503:PG4:H12	2.29	0.47
1:G:265:LYS:HG2	1:G:271:VAL:CG2	2.44	0.47
1:G:357:ASN:HD21	3:G:503:NAD:H72N	1.62	0.47
1:B:74:LYS:HD2	1:B:369:MET:HB2	1.96	0.47
1:B:138:ASP:OD1	1:B:161:LYS:NZ	2.45	0.47
1:C:213:ASP:CG	1:C:217:ARG:HH21	2.22	0.47
1:G:90:VAL:HG13	1:G:113:GLU:HB3	1.96	0.47
1:C:256:VAL:C	1:H:417:ILE:HD11	2.39	0.47
1:C:413:MET:HB2	1:H:265:LYS:HE3	1.96	0.47
1:F:75:THR:OG1	2:F:502:NOS:H2	2.14	0.47
1:G:69:LEU:O	1:G:93:GLY:HA2	2.15	0.47
1:H:138:ASP:HB3	1:H:163:MET:CE	2.45	0.47
1:H:157:GLU:H	1:H:157:GLU:CD	2.22	0.47
1:A:413:MET:HE2	1:E:265:LYS:HD3	1.96	0.47
1:C:74:LYS:HB2	1:C:74:LYS:HE2	1.76	0.47
1:F:74:LYS:HE3	1:F:369:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:GLY:O	1:H:210:SER:HB2	2.14	0.47
1:A:69:LEU:HD23	1:A:143:ASP:HB2	1.96	0.47
1:B:148:ILE:HG21	1:B:176:LEU:HD21	1.96	0.47
2:F:502:NOS:H8	3:F:503:NAD:N7N	2.30	0.47
1:H:75:THR:OG1	2:H:502:NOS:H2	2.15	0.47
1:B:107:CYS:O	1:B:112:MET:HG3	2.15	0.46
1:G:55:LYS:HB2	1:G:55:LYS:HE2	1.65	0.46
1:G:207:THR:HA	1:G:210:SER:OG	2.14	0.46
1:H:40:ALA:HB1	1:H:74:LYS:HG3	1.97	0.46
1:H:98:SER:HB2	1:H:358:LEU:HB3	1.97	0.46
1:C:49:ARG:O	1:C:53:GLU:HG3	2.15	0.46
1:E:78:LEU:HD22	1:E:373:PHE:CD1	2.50	0.46
1:F:198:LYS:HD3	1:F:202:ASP:HB3	1.97	0.46
1:F:221:LEU:HD22	1:G:367:GLU:OE2	2.14	0.46
1:B:260:ARG:HH21	4:B:503:PG4:H61	1.80	0.46
1:H:78:LEU:HD21	1:H:376:GLN:HG2	1.97	0.46
1:H:288:THR:HG22	1:H:317:GLU:OE1	2.16	0.46
1:D:300:LEU:HD21	1:D:326:LEU:HD21	1.98	0.46
1:E:40:ALA:O	1:E:44:MET:HG3	2.16	0.46
1:H:167:GLU:OE2	1:H:172:GLY:HA3	2.16	0.46
1:D:167:GLU:OE1	1:D:168:GLU:N	2.49	0.46
1:H:147:LEU:HD23	1:H:147:LEU:HA	1.79	0.46
1:C:147:LEU:HD12	1:C:147:LEU:HA	1.76	0.46
1:E:74:LYS:HB2	1:E:74:LYS:HE2	1.70	0.46
1:E:102:ASP:OD1	1:E:103:VAL:N	2.49	0.46
1:B:34:HIS:O	1:B:38:GLU:HG2	2.15	0.46
1:C:102:ASP:OD1	1:C:103:VAL:N	2.49	0.46
1:D:381:LYS:O	1:D:385:GLU:HG3	2.15	0.46
1:E:22:SER:HA	1:E:115:TYR:CE1	2.51	0.46
1:H:65:ILE:HB	1:H:89:ILE:HD13	1.98	0.46
1:D:185:LEU:HD21	1:D:189:VAL:HG22	1.97	0.45
1:D:131:LYS:N	1:D:131:LYS:HD3	2.31	0.45
1:E:312:GLY:HA3	1:E:317:GLU:OE2	2.15	0.45
1:F:58:LYS:HE3	1:F:84:GLU:O	2.16	0.45
1:D:296:MET:SD	1:D:326:LEU:HG	2.56	0.45
1:E:391:GLU:HB3	1:E:393:GLU:HG2	1.97	0.45
1:A:55:LYS:HD2	1:A:55:LYS:C	2.42	0.45
1:C:207:THR:CG2	1:C:364:HIS:HE2	2.12	0.45
1:G:425:ARG:NH2	1:G:428:LEU:HB3	2.32	0.45
1:E:188:PRO:HG3	1:E:390:LEU:HB2	1.98	0.45
1:A:169:THR:HG23	2:A:501:NOS:O3'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ARG:NH1	5:C:601:HOH:O	2.47	0.45
1:D:168:GLU:O	1:D:193:ASN:HB2	2.17	0.45
1:F:197:THR:HB	1:F:371:MET:HE2	1.99	0.45
1:F:364:HIS:HD1	1:F:369:MET:HE3	1.82	0.45
1:E:219:THR:HB	1:E:221:LEU:HG	1.99	0.45
1:B:219:THR:HB	1:B:221:LEU:HD12	1.98	0.45
1:C:24:VAL:HG12	1:C:25:LYS:N	2.32	0.45
1:C:219:THR:HB	1:C:221:LEU:HG	1.97	0.45
1:G:238:ARG:HH22	1:G:263:GLU:CD	2.24	0.45
1:G:426:LYS:HZ2	1:G:430:ASP:HB2	1.82	0.45
1:B:25:LYS:HE2	1:B:101:ASP:OD2	2.18	0.44
4:D:503:PG4:H52	4:D:503:PG4:H31	1.72	0.44
1:C:126:TYR:O	1:C:130:ASN:ND2	2.51	0.44
1:C:168:GLU:HG2	2:C:501:NOS:O3'	2.16	0.44
1:F:298:HIS:O	1:F:302:MET:HG3	2.17	0.44
1:G:75:THR:HG22	2:G:502:NOS:H2	1.99	0.44
1:H:70:HIS:CE1	1:H:355:LEU:HD12	2.53	0.44
1:A:296:MET:HE2	1:A:296:MET:HB2	1.89	0.44
1:C:212:MET:HE3	1:C:240:VAL:HG13	1.99	0.44
1:G:123:GLU:N	1:G:123:GLU:OE1	2.46	0.44
1:F:238:ARG:NH2	1:F:263:GLU:OE2	2.51	0.44
1:A:431:TRP:CG	1:E:179:MET:HG3	2.53	0.44
1:H:202:ASP:OD1	1:H:202:ASP:C	2.60	0.44
1:A:230:VAL:HB	1:A:253:ILE:HD13	2.00	0.44
1:E:113:GLU:OE2	1:E:115:TYR:OH	2.21	0.44
1:E:251:VAL:HB	1:E:269:PHE:CD1	2.53	0.44
1:G:118:ARG:HG2	1:G:118:ARG:HH11	1.83	0.44
1:D:234:GLY:HA3	3:D:502:NAD:O5B	2.17	0.44
1:E:65:ILE:HG12	1:E:139:ILE:HB	1.99	0.44
1:A:179:MET:HG2	1:E:431:TRP:CE2	2.51	0.44
1:B:387:LYS:HB3	1:B:388:GLY:H	1.68	0.44
1:E:198:LYS:HD3	1:E:202:ASP:HB3	2.00	0.43
1:E:298:HIS:O	1:E:302:MET:HG3	2.18	0.43
1:G:333:ALA:HB2	1:G:339:GLU:HB2	1.99	0.43
1:A:163:MET:HE3	1:A:387:LYS:HG3	2.00	0.43
1:F:219:THR:OG1	1:G:39:TRP:HZ2	2.02	0.43
1:F:326:LEU:HB3	1:F:342:LEU:HG	1.99	0.43
1:G:198:LYS:HD3	1:G:202:ASP:HB3	2.01	0.43
1:H:69:LEU:O	1:H:93:GLY:HA2	2.18	0.43
1:B:247:HIS:HA	1:D:243:ARG:HD2	2.00	0.43
1:F:203:ASN:O	1:F:207:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:PRO:HB3	1:G:391:GLU:O	2.19	0.43
1:A:70:HIS:CE1	1:A:355:LEU:HD12	2.53	0.43
1:H:252:ILE:HG21	1:H:272:LEU:HD12	2.01	0.43
1:D:67:MET:HE1	1:D:79:ALA:HA	2.00	0.43
1:D:158:LEU:O	1:D:162:ILE:HG13	2.19	0.43
1:F:102:ASP:OD1	1:F:103:VAL:HG23	2.19	0.43
1:F:294:LEU:HD13	1:F:302:MET:HE1	2.01	0.43
1:G:70:HIS:O	1:G:75:THR:HG21	2.18	0.43
1:H:175:ARG:HG2	1:H:175:ARG:NH1	2.33	0.43
1:A:140:ILE:O	1:A:165:GLY:HA2	2.19	0.43
1:G:354:ARG:HE	1:G:354:ARG:HB2	1.26	0.43
1:H:121:THR:HB	1:H:124:GLU:HG3	2.00	0.43
1:D:59:PRO:O	1:D:384:LYS:HD2	2.18	0.43
1:E:157:GLU:H	1:E:157:GLU:HG3	1.51	0.43
1:G:37:MET:HE2	1:G:103:VAL:HG13	2.01	0.43
1:G:75:THR:CG2	2:G:502:NOS:H2	2.48	0.43
1:H:117:TRP:CE2	1:H:120:GLU:HG2	2.54	0.43
1:H:159:ILE:HD13	1:H:186:LYS:HB2	2.00	0.43
1:A:218:THR:CG2	1:A:360:CYS:HB3	2.47	0.43
1:B:147:LEU:O	1:B:151:ILE:HG13	2.19	0.43
1:B:302:MET:CE	1:B:347:ILE:HD12	2.49	0.43
1:F:70:HIS:CE1	1:F:355:LEU:HD12	2.53	0.43
1:F:260:ARG:HE	4:F:501:PG4:H41	1.84	0.43
1:H:24:VAL:HG12	1:H:25:LYS:H	1.83	0.43
1:H:108:VAL:HG23	1:H:114:VAL:CG2	2.49	0.43
1:B:96:PRO:HG2	1:B:354:ARG:NH2	2.34	0.43
1:B:417:ILE:HD12	1:B:417:ILE:HA	1.92	0.43
1:D:134:ASP:OD1	1:D:155:ARG:NH2	2.51	0.43
1:F:40:ALA:O	1:F:44:MET:HG3	2.19	0.43
1:G:363:GLY:HA3	2:G:502:NOS:O6	2.18	0.43
1:B:201:PHE:HA	1:B:205:TYR:HD2	1.84	0.43
1:E:115:TYR:CD2	1:E:131:LYS:HE3	2.54	0.43
1:E:409:LYS:HG3	1:E:413:MET:HE3	1.99	0.43
1:G:68:ALA:HB3	1:G:142:ASP:OD1	2.19	0.43
1:H:169:THR:HG21	2:H:502:NOS:H5'1	2.00	0.43
1:B:142:ASP:OD2	1:B:145:ALA:HA	2.19	0.42
1:A:371:MET:HG2	1:A:405:ILE:CG2	2.50	0.42
1:B:169:THR:HG21	2:B:501:NOS:H5'1	2.00	0.42
1:C:298:HIS:O	1:C:302:MET:HG3	2.19	0.42
1:D:136:ASN:O	1:D:161:LYS:HE3	2.19	0.42
1:F:134:ASP:OD1	1:F:155:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:LEU:HD12	1:C:410:LEU:HA	1.91	0.42
1:C:424:GLN:NE2	1:H:291:LYS:O	2.46	0.42
1:C:426:LYS:HG3	1:C:427:TYR:N	2.34	0.42
1:D:260:ARG:NE	4:D:503:PG4:H51	2.35	0.42
1:F:77:ILE:HD13	1:F:77:ILE:HA	1.95	0.42
1:F:92:THR:HG22	1:F:132:VAL:HG21	2.01	0.42
1:B:42:ARG:O	1:B:42:ARG:HG2	2.19	0.42
1:B:49:ARG:NH1	1:B:49:ARG:HG3	2.34	0.42
1:B:185:LEU:HD21	1:B:189:VAL:HG22	2.01	0.42
1:C:168:GLU:HG2	2:C:501:NOS:HO3'	1.85	0.42
1:F:247:HIS:HA	1:G:243:ARG:HD2	2.01	0.42
1:F:364:HIS:ND1	1:F:369:MET:HE3	2.35	0.42
1:H:371:MET:SD	1:H:409:LYS:HG2	2.59	0.42
1:B:203:ASN:O	1:B:207:THR:HG23	2.20	0.42
1:H:140:ILE:HD13	1:H:140:ILE:HA	1.93	0.42
1:E:176:LEU:HA	1:E:179:MET:HE3	2.01	0.42
1:F:91:ILE:HD12	1:F:91:ILE:N	2.34	0.42
1:F:369:MET:HE1	2:F:502:NOS:O2'	2.19	0.42
1:C:203:ASN:O	1:C:236:CYS:HA	2.20	0.42
1:E:390:LEU:HD22	1:E:395:TYR:CZ	2.55	0.42
1:F:90:VAL:HA	1:F:113:GLU:HB2	2.01	0.42
1:H:72:GLU:C	1:H:103:VAL:HG11	2.45	0.42
1:B:158:LEU:O	1:B:162:ILE:HG12	2.19	0.42
1:E:69:LEU:O	1:E:93:GLY:HA2	2.20	0.42
1:G:159:ILE:HG12	1:G:186:LYS:HB3	2.02	0.42
2:A:501:NOS:H3'	3:A:502:NAD:C4N	2.50	0.42
1:H:292:ASP:HB3	1:H:295:ARG:HD3	2.02	0.42
1:B:212:MET:HA	1:B:212:MET:HE3	2.00	0.41
1:E:37:MET:HE1	1:E:110:LYS:HE3	2.02	0.41
1:F:98:SER:HB2	1:F:358:LEU:HB3	2.01	0.41
1:A:102:ASP:OD1	1:A:103:VAL:N	2.53	0.41
1:A:295:ARG:HH11	1:A:295:ARG:HG3	1.85	0.41
1:B:59:PRO:O	1:B:384:LYS:HD2	2.20	0.41
1:D:143:ASP:OD1	1:D:169:THR:OG1	2.34	0.41
1:E:33:GLY:O	1:E:37:MET:HG3	2.20	0.41
1:G:55:LYS:HD3	1:G:55:LYS:HA	1.95	0.41
1:A:176:LEU:CD1	1:A:189:VAL:HG11	2.49	0.41
1:C:149:PHE:CZ	1:C:153:THR:HG21	2.55	0.41
3:C:502:NAD:H2D	3:C:502:NAD:H6N	1.82	0.41
1:D:55:LYS:NZ	1:D:84:GLU:OE1	2.54	0.41
1:D:389:LYS:HE3	1:D:389:LYS:HB3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:LEU:HD22	1:G:368:VAL:HG23	2.02	0.41
1:H:42:ARG:HD3	1:H:43:HIS:CE1	2.55	0.41
1:B:203:ASN:O	1:B:236:CYS:HA	2.20	0.41
1:B:296:MET:SD	1:B:326:LEU:HD21	2.61	0.41
1:E:364:HIS:ND1	1:E:369:MET:HE3	2.35	0.41
1:F:169:THR:HG23	2:F:502:NOS:O3'	2.19	0.41
1:A:238:ARG:NH2	1:A:263:GLU:OE1	2.53	0.41
1:A:321:ASN:O	1:A:325:GLU:HG3	2.21	0.41
1:E:226:LYS:HD2	1:E:282:ASP:HB3	2.02	0.41
1:G:203:ASN:CG	3:G:503:NAD:H5N	2.46	0.41
1:H:61:GLU:OE2	1:H:62:GLY:N	2.54	0.41
2:H:502:NOS:H3'	3:H:503:NAD:C4N	2.51	0.41
1:B:49:ARG:O	1:B:53:GLU:HG3	2.21	0.41
1:B:74:LYS:HB2	1:B:74:LYS:HE2	1.83	0.41
1:B:123:GLU:O	1:B:127:GLU:HG3	2.20	0.41
1:D:213:ASP:O	1:D:217:ARG:HB3	2.20	0.41
1:D:427:TYR:HD1	1:D:427:TYR:O	2.03	0.41
1:E:185:LEU:HD21	1:E:189:VAL:HG23	2.01	0.41
1:F:65:ILE:HG22	1:F:67:MET:HG3	2.02	0.41
1:F:210:SER:OG	1:F:364:HIS:HD2	2.03	0.41
1:G:64:THR:HG22	1:G:88:LYS:HB2	2.02	0.41
1:A:333:ALA:HB2	1:A:339:GLU:HB2	2.03	0.41
1:D:167:GLU:CD	1:D:172:GLY:HA3	2.45	0.41
1:E:90:VAL:HG13	1:E:113:GLU:HB3	2.02	0.41
1:F:334:ARG:HD2	1:G:39:TRP:CD1	2.55	0.41
1:G:358:LEU:HD21	2:G:502:NOS:C5	2.51	0.41
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.73	0.41
1:D:204:ARG:O	1:D:239:GLY:HA3	2.21	0.41
1:F:138:ASP:HB3	1:F:163:MET:HE2	2.03	0.41
1:G:115:TYR:HB3	1:G:128:ASN:OD1	2.20	0.41
1:H:291:LYS:HB3	1:H:316:ASN:OD1	2.20	0.41
1:A:24:VAL:HG12	1:A:25:LYS:N	2.36	0.41
1:B:140:ILE:O	1:B:165:GLY:HA2	2.21	0.41
1:C:75:THR:OG1	2:C:501:NOS:H2	2.20	0.41
1:C:253:ILE:HG13	1:C:264:ALA:HB1	2.02	0.41
1:F:296:MET:HE2	1:F:296:MET:HB2	1.96	0.41
1:G:158:LEU:HG	1:G:161:LYS:HZ1	1.86	0.41
1:H:44:MET:HG2	1:H:370:ASP:HB2	2.03	0.41
1:H:139:ILE:HG23	1:H:383:ILE:HG21	2.03	0.41
1:H:210:SER:OG	1:H:363:GLY:O	2.39	0.41
1:C:157:GLU:HG2	1:C:158:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASN:O	1:C:198:LYS:HB3	2.21	0.41
1:D:168:GLU:HG3	2:D:501:NOS:O3'	2.20	0.41
1:A:74:LYS:HB2	1:A:74:LYS:HE2	1.80	0.40
1:B:355:LEU:HA	1:B:355:LEU:HD23	1.85	0.40
1:H:69:LEU:HD23	1:H:143:ASP:HB2	2.03	0.40
1:H:333:ALA:HB2	1:H:339:GLU:HB2	2.03	0.40
1:A:169:THR:O	1:A:173:ILE:HG12	2.21	0.40
1:B:213:ASP:CG	1:B:217:ARG:HH21	2.28	0.40
1:B:416:ASP:OD1	1:B:417:ILE:N	2.45	0.40
1:F:124:GLU:H	1:F:124:GLU:HG3	1.73	0.40
1:H:176:LEU:HD13	1:H:189:VAL:HG11	2.02	0.40
1:A:179:MET:HE2	1:A:179:MET:HB3	1.98	0.40
1:A:417:ILE:O	1:E:273:LYS:HE2	2.21	0.40
1:F:27:MET:HE3	1:F:27:MET:O	2.21	0.40
1:F:105:ALA:O	1:F:108:VAL:HG22	2.22	0.40
1:G:75:THR:H	1:G:75:THR:HG23	1.69	0.40
1:H:203:ASN:O	1:H:236:CYS:HA	2.20	0.40
1:A:26:ASP:HB3	1:A:29:LEU:HD12	2.03	0.40
1:A:69:LEU:O	1:A:93:GLY:HA2	2.22	0.40
1:C:364:HIS:CB	1:C:369:MET:HE3	2.51	0.40
1:D:69:LEU:O	1:D:93:GLY:HA2	2.22	0.40
1:D:173:ILE:HD12	1:D:191:ASN:CG	2.46	0.40
1:E:212:MET:O	1:E:216:ILE:HG13	2.21	0.40
1:F:169:THR:O	1:F:173:ILE:HG12	2.21	0.40
1:F:260:ARG:HH21	4:F:501:PG4:H41	1.86	0.40
1:G:158:LEU:HD23	1:G:161:LYS:HD2	2.03	0.40
1:G:265:LYS:HG2	1:G:271:VAL:HG23	2.02	0.40
1:A:133:LEU:HD13	1:A:151:ILE:HG12	2.03	0.40
1:A:202:ASP:OD1	1:A:202:ASP:C	2.64	0.40
1:D:65:ILE:HD13	1:D:82:LEU:HD13	2.03	0.40
1:D:430:ASP:OD1	1:D:432:LYS:NZ	2.55	0.40
1:E:164:GLY:HA3	1:E:383:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/435 (94%)	396 (97%)	12 (3%)	1 (0%)	43	62
1	B	409/435 (94%)	392 (96%)	15 (4%)	2 (0%)	24	41
1	C	409/435 (94%)	399 (98%)	9 (2%)	1 (0%)	43	62
1	D	409/435 (94%)	394 (96%)	14 (3%)	1 (0%)	43	62
1	E	409/435 (94%)	394 (96%)	12 (3%)	3 (1%)	18	32
1	F	409/435 (94%)	389 (95%)	17 (4%)	3 (1%)	18	32
1	G	409/435 (94%)	396 (97%)	12 (3%)	1 (0%)	43	62
1	H	409/435 (94%)	395 (97%)	13 (3%)	1 (0%)	43	62
All	All	3272/3480 (94%)	3155 (96%)	104 (3%)	13 (0%)	30	47

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	LYS
1	E	387	LYS
1	F	387	LYS
1	B	355	LEU
1	C	355	LEU
1	E	57	ASP
1	F	114	VAL
1	F	355	LEU
1	A	355	LEU
1	D	355	LEU
1	E	355	LEU
1	G	355	LEU
1	H	355	LEU

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	A	339/359 (94%)	336 (99%)	3 (1%)	70	86
1	B	339/359 (94%)	336 (99%)	3 (1%)	70	86
1	C	339/359 (94%)	332 (98%)	7 (2%)	47	72
1	D	339/359 (94%)	333 (98%)	6 (2%)	51	75
1	E	339/359 (94%)	328 (97%)	11 (3%)	34	60
1	F	339/359 (94%)	328 (97%)	11 (3%)	34	60
1	G	339/359 (94%)	326 (96%)	13 (4%)	29	53
1	H	339/359 (94%)	326 (96%)	13 (4%)	29	53
All	All	2712/2872 (94%)	2645 (98%)	67 (2%)	42	67

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	169	THR
1	A	354	ARG
1	B	169	THR
1	B	207	THR
1	B	368	VAL
1	C	22	SER
1	C	108	VAL
1	C	169	THR
1	C	181	GLU
1	C	254	THR
1	C	308	LEU
1	C	430	ASP
1	D	22	SER
1	D	169	THR
1	D	171	THR
1	D	254	THR
1	D	368	VAL
1	D	378	LEU
1	E	57	ASP
1	E	120	GLU
1	E	136	ASN
1	E	153	THR
1	E	156	THR
1	E	169	THR
1	E	197	THR
1	E	207	THR

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Mol	Chain	Res	Type
1	E	265	LYS
1	E	368	VAL
1	E	387	LYS
1	F	25	LYS
1	F	108	VAL
1	F	157	GLU
1	F	169	THR
1	F	171	THR
1	F	207	THR
1	F	217	ARG
1	F	265	LYS
1	F	350	LEU
1	F	368	VAL
1	F	393	GLU
1	G	108	VAL
1	G	133	LEU
1	G	146	ASP
1	G	150	LEU
1	G	151	ILE
1	G	159	ILE
1	G	174	ILE
1	G	207	THR
1	G	254	THR
1	G	349	LEU
1	G	354	ARG
1	G	368	VAL
1	G	428	LEU
1	H	22	SER
1	H	41	LYS
1	H	42	ARG
1	H	52	GLU
1	H	108	VAL
1	H	114	VAL
1	H	129	LEU
1	H	153	THR
1	H	169	THR
1	H	202	ASP
1	H	210	SER
1	H	247	HIS
1	H	254	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	B	357	ASN
1	B	364	HIS
1	C	56	ASN
1	C	130	ASN
1	C	310	ASN
1	C	313	HIS
1	C	357	ASN
1	D	257	ASN
1	D	357	ASN
1	E	375	ASN
1	E	376	GLN
1	E	386	ASN
1	E	401	GLN
1	F	34	HIS
1	F	357	ASN
1	G	392	ASN
1	H	43	HIS
1	H	199	HIS
1	H	220	ASN
1	H	310	ASN
1	H	357	ASN
1	H	376	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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	NOS	E	502	-	21,21,21	1.67	2 (9%)	31,31,31	1.51	2 (6%)
3	NAD	C	502	-	46,48,48	1.51	5 (10%)	64,73,73	1.65	14 (21%)
2	NOS	B	501	-	21,21,21	1.64	2 (9%)	31,31,31	1.54	2 (6%)
2	NOS	A	501	-	21,21,21	1.62	2 (9%)	31,31,31	1.50	2 (6%)
2	NOS	C	501	-	21,21,21	1.63	2 (9%)	31,31,31	1.54	2 (6%)
3	NAD	F	503	-	46,48,48	1.60	8 (17%)	64,73,73	1.74	17 (26%)
4	PG4	C	503	-	12,12,12	0.16	0	11,11,11	0.10	0
3	NAD	B	502	-	46,48,48	1.53	10 (21%)	64,73,73	1.77	17 (26%)
3	NAD	D	502	-	46,48,48	1.52	7 (15%)	64,73,73	1.75	15 (23%)
4	PG4	D	503	-	12,12,12	0.15	0	11,11,11	0.16	0
4	PG4	F	501	-	12,12,12	0.14	0	11,11,11	0.13	0
3	NAD	E	503	-	46,48,48	1.60	7 (15%)	64,73,73	1.73	17 (26%)
4	PG4	H	501	-	12,12,12	0.17	0	11,11,11	0.10	0
2	NOS	G	502	-	21,21,21	1.64	2 (9%)	31,31,31	1.54	3 (9%)
2	NOS	H	502	-	21,21,21	1.66	2 (9%)	31,31,31	1.55	2 (6%)
4	PG4	B	503	-	12,12,12	0.17	0	11,11,11	0.10	0
4	PG4	G	501	-	12,12,12	0.16	0	11,11,11	0.14	0
4	PG4	A	503	-	12,12,12	0.20	0	11,11,11	0.13	0
2	NOS	D	501	-	21,21,21	1.68	2 (9%)	31,31,31	1.51	2 (6%)
2	NOS	F	502	-	21,21,21	1.64	2 (9%)	31,31,31	1.51	2 (6%)
4	PG4	E	501	-	12,12,12	0.19	0	11,11,11	0.14	0
3	NAD	A	502	-	46,48,48	1.51	6 (13%)	64,73,73	1.74	16 (25%)
3	NAD	G	503	-	46,48,48	1.51	6 (13%)	64,73,73	1.76	17 (26%)
3	NAD	H	503	-	46,48,48	1.56	8 (17%)	64,73,73	1.65	16 (25%)

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	NOS	E	502	-	-	1/6/22/22	0/3/3/3
3	NAD	C	502	-	-	8/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NOS	B	501	-	-	1/6/22/22	0/3/3/3
2	NOS	A	501	-	-	0/6/22/22	0/3/3/3
2	NOS	C	501	-	-	0/6/22/22	0/3/3/3
3	NAD	F	503	-	-	9/30/62/62	0/5/5/5
4	PG4	C	503	-	-	4/10/10/10	-
3	NAD	B	502	-	-	11/30/62/62	0/5/5/5
3	NAD	D	502	-	-	8/30/62/62	0/5/5/5
4	PG4	D	503	-	-	3/10/10/10	-
4	PG4	F	501	-	-	3/10/10/10	-
3	NAD	E	503	-	-	12/30/62/62	0/5/5/5
4	PG4	H	501	-	-	4/10/10/10	-
2	NOS	G	502	-	-	0/6/22/22	0/3/3/3
2	NOS	H	502	-	-	0/6/22/22	0/3/3/3
4	PG4	B	503	-	-	4/10/10/10	-
4	PG4	G	501	-	-	2/10/10/10	-
4	PG4	A	503	-	-	4/10/10/10	-
2	NOS	D	501	-	-	0/6/22/22	0/3/3/3
2	NOS	F	502	-	-	0/6/22/22	0/3/3/3
4	PG4	E	501	-	-	4/10/10/10	-
3	NAD	A	502	-	-	8/30/62/62	0/5/5/5
3	NAD	G	503	-	-	7/30/62/62	0/5/5/5
3	NAD	H	503	-	-	9/30/62/62	0/5/5/5

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NOS	O6-C6	6.43	1.35	1.23
2	E	502	NOS	O6-C6	6.42	1.35	1.23
2	H	502	NOS	O6-C6	6.32	1.35	1.23
2	G	502	NOS	O6-C6	6.23	1.35	1.23
2	B	501	NOS	O6-C6	6.22	1.35	1.23
2	F	502	NOS	O6-C6	6.20	1.35	1.23
2	C	501	NOS	O6-C6	6.13	1.35	1.23
2	A	501	NOS	O6-C6	6.08	1.35	1.23
3	E	503	NAD	PN-O5D	5.22	1.79	1.59
3	F	503	NAD	PN-O5D	5.16	1.79	1.59
3	H	503	NAD	PN-O5D	5.10	1.79	1.59
3	G	503	NAD	PN-O5D	5.04	1.79	1.59
3	D	502	NAD	PN-O5D	5.00	1.79	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	NAD	PN-O5D	4.95	1.78	1.59
3	A	502	NAD	PN-O5D	4.84	1.78	1.59
3	B	502	NAD	PN-O5D	4.77	1.78	1.59
3	E	503	NAD	PA-O5B	4.31	1.76	1.59
3	C	502	NAD	PA-O5B	4.11	1.75	1.59
3	A	502	NAD	PA-O5B	4.09	1.75	1.59
3	D	502	NAD	PA-O5B	4.01	1.75	1.59
3	H	503	NAD	PA-O5B	3.98	1.75	1.59
3	F	503	NAD	PA-O5B	3.94	1.74	1.59
3	B	502	NAD	PA-O5B	3.84	1.74	1.59
3	G	503	NAD	PA-O5B	3.70	1.73	1.59
2	A	501	NOS	C6-N1	-3.17	1.32	1.39
2	G	502	NOS	C6-N1	-3.17	1.32	1.39
2	C	501	NOS	C6-N1	-3.15	1.32	1.39
2	D	501	NOS	C6-N1	-3.15	1.32	1.39
2	F	502	NOS	C6-N1	-3.14	1.32	1.39
2	B	501	NOS	C6-N1	-3.13	1.32	1.39
2	E	502	NOS	C6-N1	-3.12	1.32	1.39
2	H	502	NOS	C6-N1	-3.12	1.32	1.39
3	E	503	NAD	C5A-C4A	2.72	1.43	1.39
3	A	502	NAD	C7N-N7N	2.69	1.37	1.33
3	D	502	NAD	C2N-N1N	2.64	1.37	1.35
3	D	502	NAD	C7N-N7N	2.63	1.37	1.33
3	F	503	NAD	C7N-N7N	2.57	1.37	1.33
3	F	503	NAD	PA-O3	2.57	1.62	1.59
3	E	503	NAD	C7N-N7N	2.55	1.37	1.33
3	C	502	NAD	C7N-N7N	2.50	1.37	1.33
3	H	503	NAD	C5A-C4A	2.48	1.43	1.39
3	H	503	NAD	C7N-N7N	2.48	1.37	1.33
3	B	502	NAD	C7N-N7N	2.43	1.37	1.33
3	H	503	NAD	C8A-N9A	2.37	1.41	1.37
3	F	503	NAD	C4A-N3A	2.35	1.38	1.34
3	F	503	NAD	C2N-N1N	2.33	1.37	1.35
3	E	503	NAD	PA-O3	2.33	1.62	1.59
3	C	502	NAD	C5A-C4A	2.33	1.43	1.39
3	F	503	NAD	C5A-C4A	2.32	1.43	1.39
3	A	502	NAD	O5D-C5D	-2.32	1.35	1.44
3	G	503	NAD	C8A-N9A	2.31	1.41	1.37
3	B	502	NAD	C5A-C4A	2.23	1.43	1.39
3	E	503	NAD	C8A-N9A	2.23	1.41	1.37
3	G	503	NAD	C7N-N7N	2.21	1.37	1.33
3	G	503	NAD	C5A-C4A	2.19	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAD	PA-O3	2.17	1.61	1.59
3	B	502	NAD	C8A-N9A	2.16	1.41	1.37
3	B	502	NAD	C4A-N3A	2.15	1.38	1.34
3	F	503	NAD	C2A-N1A	2.15	1.37	1.33
3	H	503	NAD	PA-O3	2.13	1.61	1.59
3	E	503	NAD	C2A-N1A	2.11	1.37	1.33
3	D	502	NAD	C5A-C4A	2.10	1.42	1.39
3	D	502	NAD	C4A-N3A	2.10	1.38	1.34
3	B	502	NAD	C2N-N1N	2.09	1.37	1.35
3	B	502	NAD	O3D-C3D	-2.09	1.37	1.43
3	B	502	NAD	O5D-C5D	-2.05	1.36	1.44
3	A	502	NAD	C5A-C4A	2.03	1.42	1.39
3	H	503	NAD	C2A-N1A	2.02	1.37	1.33
3	G	503	NAD	C2A-N1A	2.02	1.37	1.33
3	D	502	NAD	C8A-N9A	2.02	1.41	1.37
3	H	503	NAD	C2N-N1N	2.01	1.37	1.35
3	C	502	NAD	C8A-N9A	2.00	1.41	1.37
3	B	502	NAD	O2D-C2D	-2.00	1.38	1.43

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NOS	C5-C6-N1	5.74	119.04	110.78
2	H	502	NOS	C5-C6-N1	5.74	119.03	110.78
2	C	501	NOS	C5-C6-N1	5.72	119.00	110.78
2	G	502	NOS	C5-C6-N1	5.69	118.96	110.78
2	F	502	NOS	C5-C6-N1	5.65	118.90	110.78
2	D	501	NOS	C5-C6-N1	5.64	118.89	110.78
2	E	502	NOS	C5-C6-N1	5.61	118.84	110.78
2	A	501	NOS	C5-C6-N1	5.61	118.84	110.78
2	G	502	NOS	C2-N1-C6	-4.97	118.28	125.09
2	H	502	NOS	C2-N1-C6	-4.97	118.28	125.09
2	C	501	NOS	C2-N1-C6	-4.92	118.35	125.09
3	A	502	NAD	O3-PA-O1A	-4.84	96.15	110.70
2	B	501	NOS	C2-N1-C6	-4.83	118.47	125.09
2	E	502	NOS	C2-N1-C6	-4.81	118.50	125.09
2	D	501	NOS	C2-N1-C6	-4.80	118.51	125.09
2	F	502	NOS	C2-N1-C6	-4.77	118.56	125.09
2	A	501	NOS	C2-N1-C6	-4.73	118.60	125.09
3	D	502	NAD	O3-PA-O1A	-4.72	96.51	110.70
3	E	503	NAD	O3-PA-O1A	-4.61	96.84	110.70
3	B	502	NAD	O3-PA-O1A	-4.38	97.54	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	NAD	O3-PA-O1A	-4.36	97.59	110.70
3	G	503	NAD	O3-PA-O1A	-4.35	97.63	110.70
3	F	503	NAD	O3-PA-O1A	-4.34	97.65	110.70
3	D	502	NAD	O2A-PA-O3	4.31	118.91	107.27
3	G	503	NAD	O2A-PA-O3	4.30	118.89	107.27
3	H	503	NAD	O3-PA-O1A	-4.13	98.27	110.70
3	E	503	NAD	O2A-PA-O3	4.10	118.34	107.27
3	E	503	NAD	O2A-PA-O1A	4.05	131.28	112.44
3	B	502	NAD	O2A-PA-O3	4.05	118.21	107.27
3	A	502	NAD	O2A-PA-O3	4.03	118.16	107.27
3	B	502	NAD	O2A-PA-O1A	4.01	131.10	112.44
3	A	502	NAD	O2A-PA-O1A	3.99	131.02	112.44
3	C	502	NAD	O2A-PA-O1A	3.97	130.91	112.44
3	A	502	NAD	O2N-PN-O1N	3.95	130.80	112.44
3	G	503	NAD	O2A-PA-O1A	3.94	130.76	112.44
3	D	502	NAD	O2A-PA-O1A	3.92	130.67	112.44
3	F	503	NAD	O2A-PA-O1A	3.92	130.66	112.44
3	F	503	NAD	O2A-PA-O3	3.89	117.79	107.27
3	H	503	NAD	O2A-PA-O1A	3.89	130.53	112.44
3	D	502	NAD	O2N-PN-O1N	3.89	130.52	112.44
3	B	502	NAD	O2N-PN-O1N	3.85	130.37	112.44
3	G	503	NAD	O2N-PN-O1N	3.84	130.32	112.44
3	F	503	NAD	O2N-PN-O1N	3.84	130.31	112.44
3	H	503	NAD	O2A-PA-O3	3.78	117.48	107.27
3	C	502	NAD	O2N-PN-O1N	3.75	129.90	112.44
3	H	503	NAD	O2N-PN-O1N	3.72	129.76	112.44
3	E	503	NAD	O2N-PN-O1N	3.63	129.31	112.44
3	C	502	NAD	O2A-PA-O3	3.62	117.05	107.27
3	B	502	NAD	C4D-O4D-C1D	-3.56	106.66	109.92
3	F	503	NAD	C4D-O4D-C1D	-3.54	106.69	109.92
3	D	502	NAD	O3-PN-O1N	3.30	120.64	110.70
3	G	503	NAD	O3-PN-O1N	3.13	120.11	110.70
3	C	502	NAD	O3-PN-O1N	3.08	119.97	110.70
3	D	502	NAD	O5B-PA-O1A	-3.08	96.74	108.94
3	G	503	NAD	C4D-O4D-C1D	-3.04	107.14	109.92
3	E	503	NAD	O3-PN-O1N	2.97	119.64	110.70
3	D	502	NAD	PN-O5D-C5D	-2.94	104.51	121.35
3	H	503	NAD	O3-PN-O1N	2.91	119.47	110.70
3	F	503	NAD	O5D-PN-O1N	-2.91	97.40	108.94
3	B	502	NAD	O3-PN-O1N	2.90	119.44	110.70
3	G	503	NAD	O5B-PA-O1A	-2.88	97.53	108.94
3	H	503	NAD	C4D-O4D-C1D	-2.81	107.35	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	503	NAD	PN-O5D-C5D	-2.78	105.41	121.35
3	F	503	NAD	O3-PN-O1N	2.78	119.06	110.70
3	E	503	NAD	PN-O5D-C5D	-2.78	105.44	121.35
3	B	502	NAD	O5B-PA-O1A	-2.77	97.94	108.94
3	E	503	NAD	C4D-O4D-C1D	-2.76	107.40	109.92
3	H	503	NAD	O5D-PN-O1N	-2.71	98.18	108.94
3	D	502	NAD	O2N-PN-O3	-2.68	100.02	107.27
3	C	502	NAD	O5B-PA-O1A	-2.68	98.30	108.94
3	A	502	NAD	C5B-C4B-C3B	-2.68	105.56	115.21
3	C	502	NAD	C5B-C4B-C3B	-2.67	105.61	115.21
3	C	502	NAD	O5D-PN-O1N	-2.67	98.37	108.94
3	G	503	NAD	C5B-C4B-C3B	-2.66	105.64	115.21
3	B	502	NAD	O7N-C7N-C3N	2.65	122.84	119.60
3	A	502	NAD	O3-PN-O1N	2.64	118.64	110.70
3	B	502	NAD	PN-O5D-C5D	-2.63	106.29	121.35
3	D	502	NAD	C5B-C4B-C3B	-2.61	105.82	115.21
3	A	502	NAD	O5D-PN-O1N	-2.61	98.61	108.94
3	D	502	NAD	O5D-PN-O1N	-2.57	98.76	108.94
3	F	503	NAD	O5B-PA-O1A	-2.56	98.77	108.94
3	B	502	NAD	C5D-C4D-C3D	-2.56	105.98	115.21
3	B	502	NAD	O5D-PN-O1N	-2.56	98.78	108.94
3	H	503	NAD	O5B-PA-O1A	-2.55	98.82	108.94
3	F	503	NAD	O2N-PN-O5D	-2.53	96.08	107.57
3	A	502	NAD	PA-O5B-C5B	-2.53	106.86	121.35
3	A	502	NAD	PN-O5D-C5D	-2.52	106.92	121.35
3	B	502	NAD	C5B-C4B-C3B	-2.48	106.27	115.21
3	H	503	NAD	O2N-PN-O5D	-2.47	96.39	107.57
3	G	503	NAD	PA-O5B-C5B	-2.46	107.28	121.35
3	E	503	NAD	O5D-PN-O1N	-2.45	99.24	108.94
3	C	502	NAD	PA-O5B-C5B	-2.44	107.34	121.35
3	D	502	NAD	O3B-C3B-C4B	-2.44	104.07	111.08
3	E	503	NAD	C5B-C4B-C3B	-2.44	106.42	115.21
3	A	502	NAD	C4D-O4D-C1D	-2.44	107.69	109.92
3	D	502	NAD	C4D-O4D-C1D	-2.44	107.69	109.92
3	G	503	NAD	O5D-PN-O1N	-2.43	99.32	108.94
3	F	503	NAD	C5B-C4B-C3B	-2.43	106.48	115.21
3	G	503	NAD	O2N-PN-O5D	-2.41	96.65	107.57
3	E	503	NAD	O2N-PN-O3	-2.40	100.78	107.27
3	A	502	NAD	O5B-PA-O1A	-2.40	99.43	108.94
3	C	502	NAD	PN-O5D-C5D	-2.40	107.62	121.35
3	B	502	NAD	PA-O5B-C5B	-2.39	107.68	121.35
3	B	502	NAD	O3B-C3B-C4B	-2.38	104.25	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	NAD	O2N-PN-O5D	-2.37	96.82	107.57
3	E	503	NAD	O5B-PA-O1A	-2.37	99.55	108.94
3	F	503	NAD	O7N-C7N-C3N	2.34	122.46	119.60
3	H	503	NAD	C5B-C4B-C3B	-2.33	106.81	115.21
3	H	503	NAD	PA-O5B-C5B	-2.33	108.01	121.35
3	G	503	NAD	O2N-PN-O3	-2.32	101.02	107.27
3	G	503	NAD	O3B-C3B-C4B	-2.31	104.44	111.08
3	D	502	NAD	O2N-PN-O5D	-2.31	97.10	107.57
3	C	502	NAD	O2N-PN-O5D	-2.30	97.13	107.57
3	B	502	NAD	O2N-PN-O3	-2.27	101.13	107.27
3	E	503	NAD	C5D-C4D-C3D	-2.27	107.04	115.21
3	E	503	NAD	PA-O5B-C5B	-2.27	108.35	121.35
3	D	502	NAD	PA-O5B-C5B	-2.27	108.36	121.35
3	A	502	NAD	O2N-PN-O5D	-2.26	97.30	107.57
3	H	503	NAD	O2N-PN-O3	-2.26	101.16	107.27
3	H	503	NAD	PN-O5D-C5D	-2.26	108.39	121.35
3	F	503	NAD	PA-O5B-C5B	-2.26	108.39	121.35
3	E	503	NAD	O2N-PN-O5D	-2.26	97.34	107.57
3	A	502	NAD	O7N-C7N-C3N	2.24	122.34	119.60
3	F	503	NAD	O3B-C3B-C4B	-2.23	104.69	111.08
3	F	503	NAD	O4B-C1B-C2B	-2.22	101.86	106.62
3	F	503	NAD	PN-O5D-C5D	-2.21	108.70	121.35
3	G	503	NAD	C4B-O4B-C1B	-2.20	104.61	109.47
3	E	503	NAD	O3B-C3B-C4B	-2.16	104.89	111.08
3	H	503	NAD	O7N-C7N-C3N	2.15	122.23	119.60
3	H	503	NAD	C5D-C4D-C3D	-2.14	107.49	115.21
3	D	502	NAD	O7N-C7N-C3N	2.14	122.22	119.60
3	C	502	NAD	C5D-C4D-C3D	-2.13	107.54	115.21
3	A	502	NAD	O2N-PN-O3	-2.13	101.51	107.27
3	C	502	NAD	O2N-PN-O3	-2.13	101.51	107.27
2	G	502	NOS	N1-C2-N3	2.13	127.94	125.50
3	G	503	NAD	C4A-N9A-C1B	-2.13	121.66	126.63
3	A	502	NAD	O3D-C3D-C4D	-2.12	105.00	111.08
3	F	503	NAD	N3A-C4A-N9A	2.10	130.75	127.17
3	C	502	NAD	O7N-C7N-C3N	2.10	122.16	119.60
3	H	503	NAD	O3B-C3B-C4B	-2.09	105.08	111.08
3	F	503	NAD	O3D-C3D-C4D	-2.09	105.09	111.08
3	B	502	NAD	O3D-C3D-C4D	-2.08	105.10	111.08
3	A	502	NAD	O3B-C3B-C4B	-2.08	105.11	111.08
3	G	503	NAD	C5D-C4D-C3D	-2.04	107.86	115.21
3	E	503	NAD	N3A-C4A-N9A	2.04	130.63	127.17
3	E	503	NAD	O7N-C7N-C3N	2.02	122.07	119.60

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NAD	C5B-O5B-PA-O1A
3	A	502	NAD	O4D-C1D-N1N-C2N
3	A	502	NAD	O4D-C1D-N1N-C6N
3	A	502	NAD	C2D-C1D-N1N-C2N
3	A	502	NAD	C2D-C1D-N1N-C6N
3	B	502	NAD	C5B-O5B-PA-O1A
3	B	502	NAD	O4D-C1D-N1N-C2N
3	B	502	NAD	O4D-C1D-N1N-C6N
3	B	502	NAD	C2D-C1D-N1N-C2N
3	B	502	NAD	C2D-C1D-N1N-C6N
3	C	502	NAD	C5B-O5B-PA-O1A
3	C	502	NAD	O4D-C1D-N1N-C2N
3	C	502	NAD	O4D-C1D-N1N-C6N
3	C	502	NAD	C2D-C1D-N1N-C2N
3	C	502	NAD	C2D-C1D-N1N-C6N
3	D	502	NAD	C5D-O5D-PN-O3
3	D	502	NAD	O4D-C1D-N1N-C2N
3	D	502	NAD	O4D-C1D-N1N-C6N
3	D	502	NAD	C2D-C1D-N1N-C2N
3	D	502	NAD	C2D-C1D-N1N-C6N
3	E	503	NAD	C5B-O5B-PA-O1A
3	E	503	NAD	C5D-O5D-PN-O3
3	E	503	NAD	O4D-C1D-N1N-C2N
3	E	503	NAD	O4D-C1D-N1N-C6N
3	E	503	NAD	C2D-C1D-N1N-C2N
3	E	503	NAD	C2D-C1D-N1N-C6N
3	F	503	NAD	C5B-O5B-PA-O1A
3	F	503	NAD	O4D-C1D-N1N-C2N
3	F	503	NAD	O4D-C1D-N1N-C6N
3	F	503	NAD	C2D-C1D-N1N-C2N
3	F	503	NAD	C2D-C1D-N1N-C6N
3	G	503	NAD	O4D-C1D-N1N-C2N
3	G	503	NAD	O4D-C1D-N1N-C6N
3	G	503	NAD	C2D-C1D-N1N-C2N
3	G	503	NAD	C2D-C1D-N1N-C6N
3	H	503	NAD	C5B-O5B-PA-O1A
3	H	503	NAD	O4D-C1D-N1N-C2N
3	H	503	NAD	O4D-C1D-N1N-C6N
3	H	503	NAD	C2D-C1D-N1N-C2N
3	H	503	NAD	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	C	502	NAD	O4B-C4B-C5B-O5B
3	E	503	NAD	O4B-C4B-C5B-O5B
3	H	503	NAD	O4B-C4B-C5B-O5B
4	B	503	PG4	C6-C5-O3-C4
3	A	502	NAD	C3B-C4B-C5B-O5B
3	B	502	NAD	C3B-C4B-C5B-O5B
3	C	502	NAD	C3B-C4B-C5B-O5B
3	E	503	NAD	C3B-C4B-C5B-O5B
3	E	503	NAD	O4D-C4D-C5D-O5D
3	H	503	NAD	C3B-C4B-C5B-O5B
3	A	502	NAD	O4B-C4B-C5B-O5B
3	B	502	NAD	O4B-C4B-C5B-O5B
3	B	502	NAD	O4D-C4D-C5D-O5D
3	F	503	NAD	C3B-C4B-C5B-O5B
4	A	503	PG4	O4-C7-C8-O5
4	C	503	PG4	O4-C7-C8-O5
4	E	501	PG4	O4-C7-C8-O5
4	H	501	PG4	O4-C7-C8-O5
3	F	503	NAD	O4B-C4B-C5B-O5B
4	E	501	PG4	O1-C1-C2-O2
4	D	503	PG4	O2-C3-C4-O3
4	A	503	PG4	O1-C1-C2-O2
4	C	503	PG4	O1-C1-C2-O2
4	H	501	PG4	O1-C1-C2-O2
4	B	503	PG4	C4-C3-O2-C2
4	C	503	PG4	O3-C5-C6-O4
4	A	503	PG4	O3-C5-C6-O4
4	E	501	PG4	O3-C5-C6-O4
4	H	501	PG4	O3-C5-C6-O4
4	F	501	PG4	O1-C1-C2-O2
4	D	503	PG4	C3-C4-O3-C5
3	D	502	NAD	O4D-C4D-C5D-O5D
3	A	502	NAD	C5B-O5B-PA-O2A
3	B	502	NAD	C5B-O5B-PA-O2A
3	B	502	NAD	C5D-O5D-PN-O3
3	C	502	NAD	C5B-O5B-PA-O2A
3	E	503	NAD	C5B-O5B-PA-O2A
3	F	503	NAD	C5B-O5B-PA-O2A
3	G	503	NAD	C5D-O5D-PN-O3
3	H	503	NAD	C5B-O5B-PA-O2A
4	B	503	PG4	O2-C3-C4-O3
4	F	501	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
4	C	503	PG4	C8-C7-O4-C6
3	D	502	NAD	O4B-C4B-C5B-O5B
4	H	501	PG4	C8-C7-O4-C6
3	G	503	NAD	O4D-C4D-C5D-O5D
4	A	503	PG4	C8-C7-O4-C6
4	E	501	PG4	C8-C7-O4-C6
3	D	502	NAD	C3B-C4B-C5B-O5B
3	B	502	NAD	PA-O3-PN-O1N
4	B	503	PG4	O3-C5-C6-O4
4	D	503	PG4	C4-C3-O2-C2
2	B	501	NOS	C3'-C4'-C5'-O5'
3	G	503	NAD	O4B-C4B-C5B-O5B
4	G	501	PG4	O2-C3-C4-O3
3	E	503	NAD	C3D-C4D-C5D-O5D
4	F	501	PG4	O2-C3-C4-O3
4	G	501	PG4	O3-C5-C6-O4
2	E	502	NOS	C3'-C4'-C5'-O5'
3	E	503	NAD	PA-O3-PN-O1N
3	F	503	NAD	PA-O3-PN-O1N
3	H	503	NAD	O4D-C4D-C5D-O5D

There are no ring outliers.

19 monomers are involved in 56 short contacts:

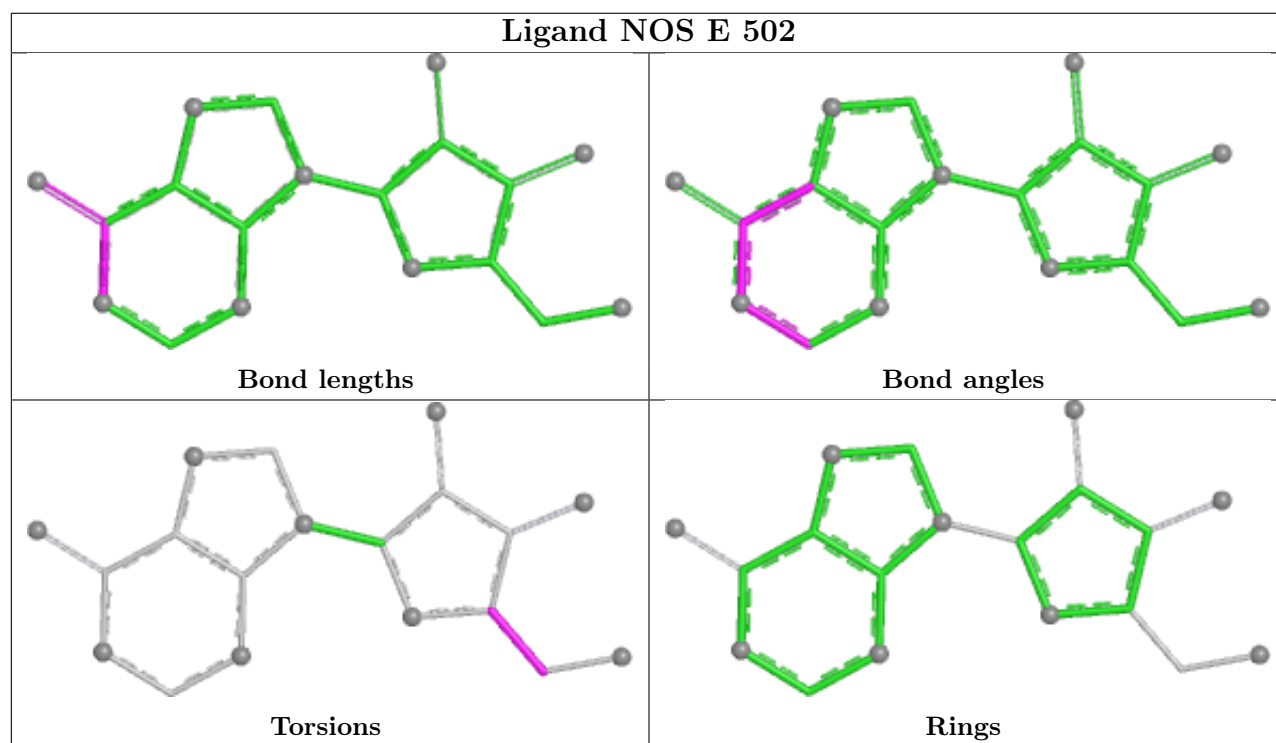
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	NAD	3	0
2	B	501	NOS	1	0
2	A	501	NOS	3	0
2	C	501	NOS	4	0
3	F	503	NAD	2	0
3	B	502	NAD	2	0
3	D	502	NAD	3	0
4	D	503	PG4	4	0
4	F	501	PG4	4	0
3	E	503	NAD	2	0
2	G	502	NOS	7	0
2	H	502	NOS	3	0
4	B	503	PG4	3	0
4	A	503	PG4	1	0
2	D	501	NOS	2	0
2	F	502	NOS	4	0
3	A	502	NAD	3	0

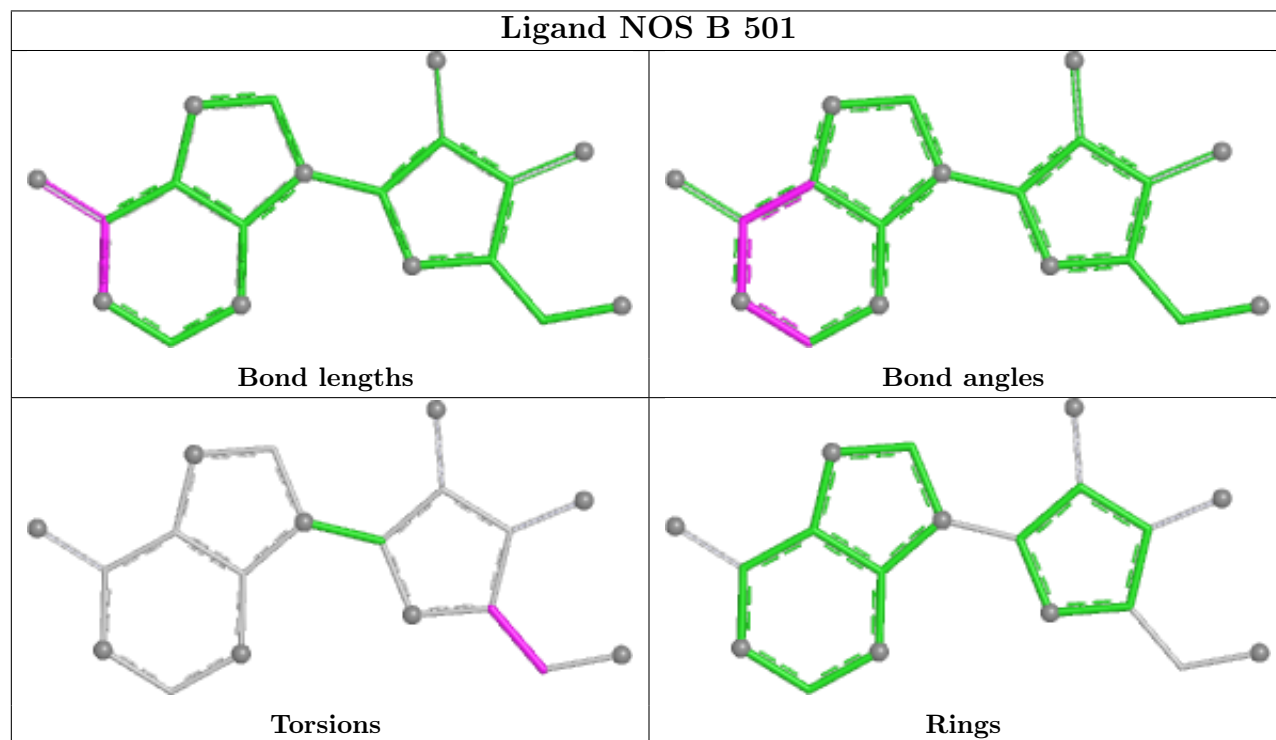
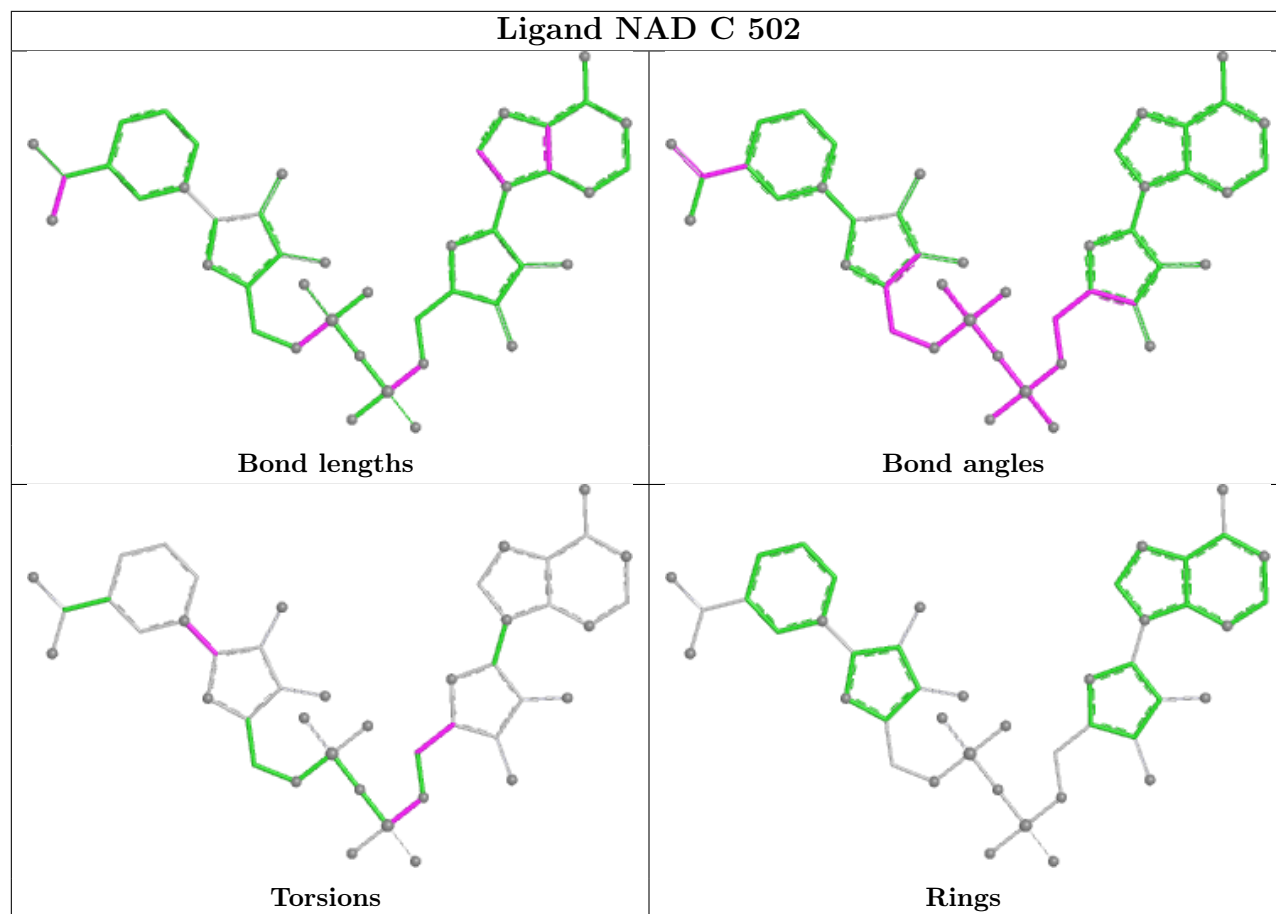
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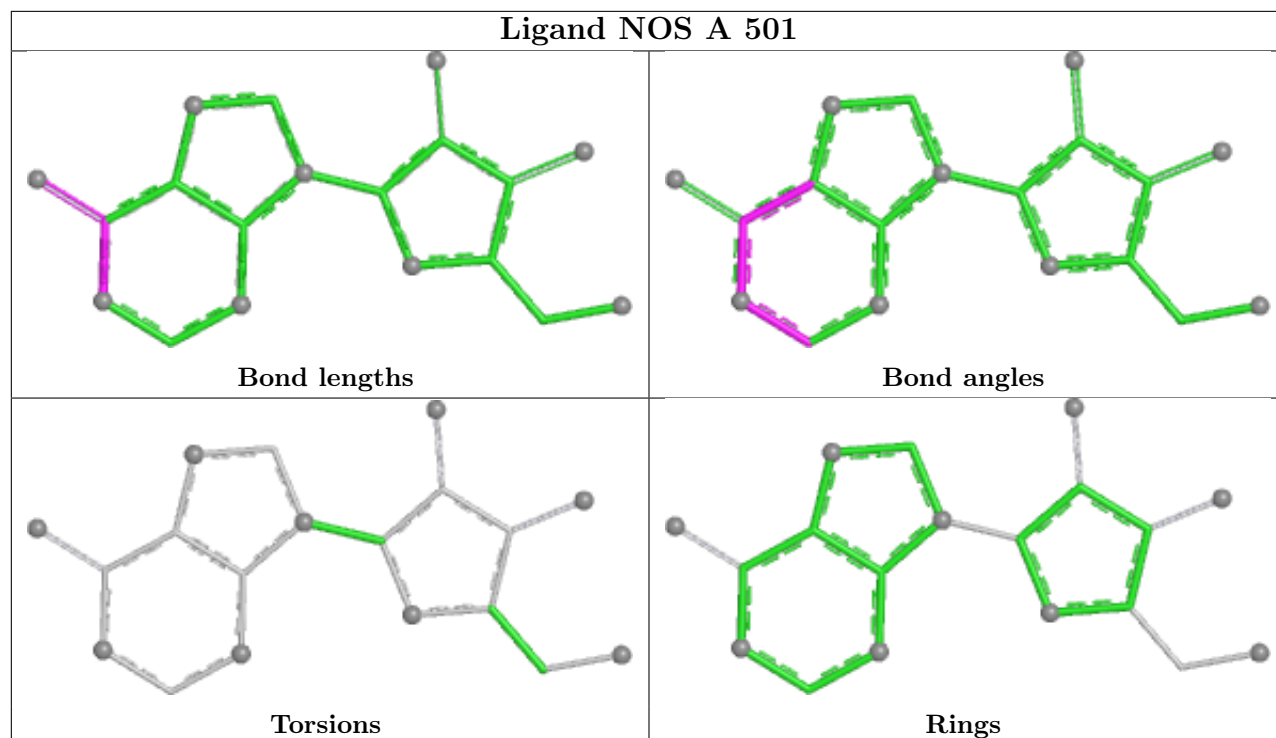
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	503	NAD	7	0
3	H	503	NAD	4	0

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.

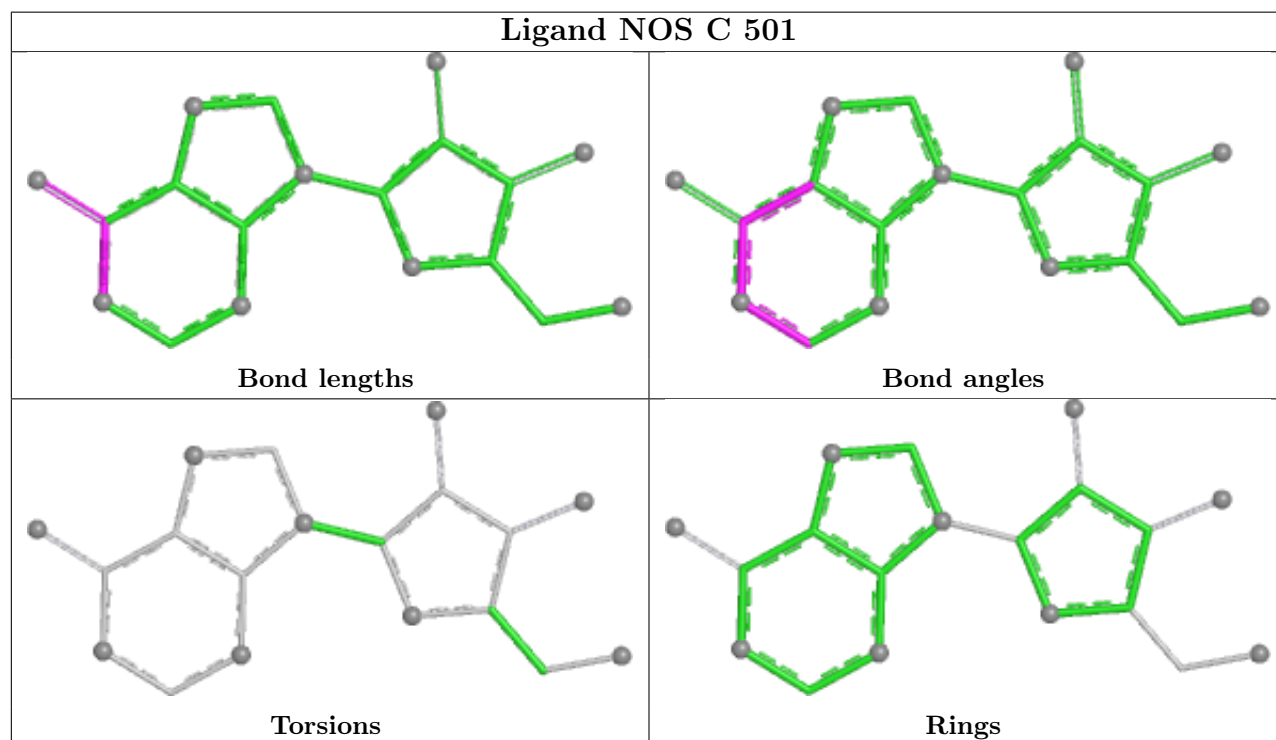


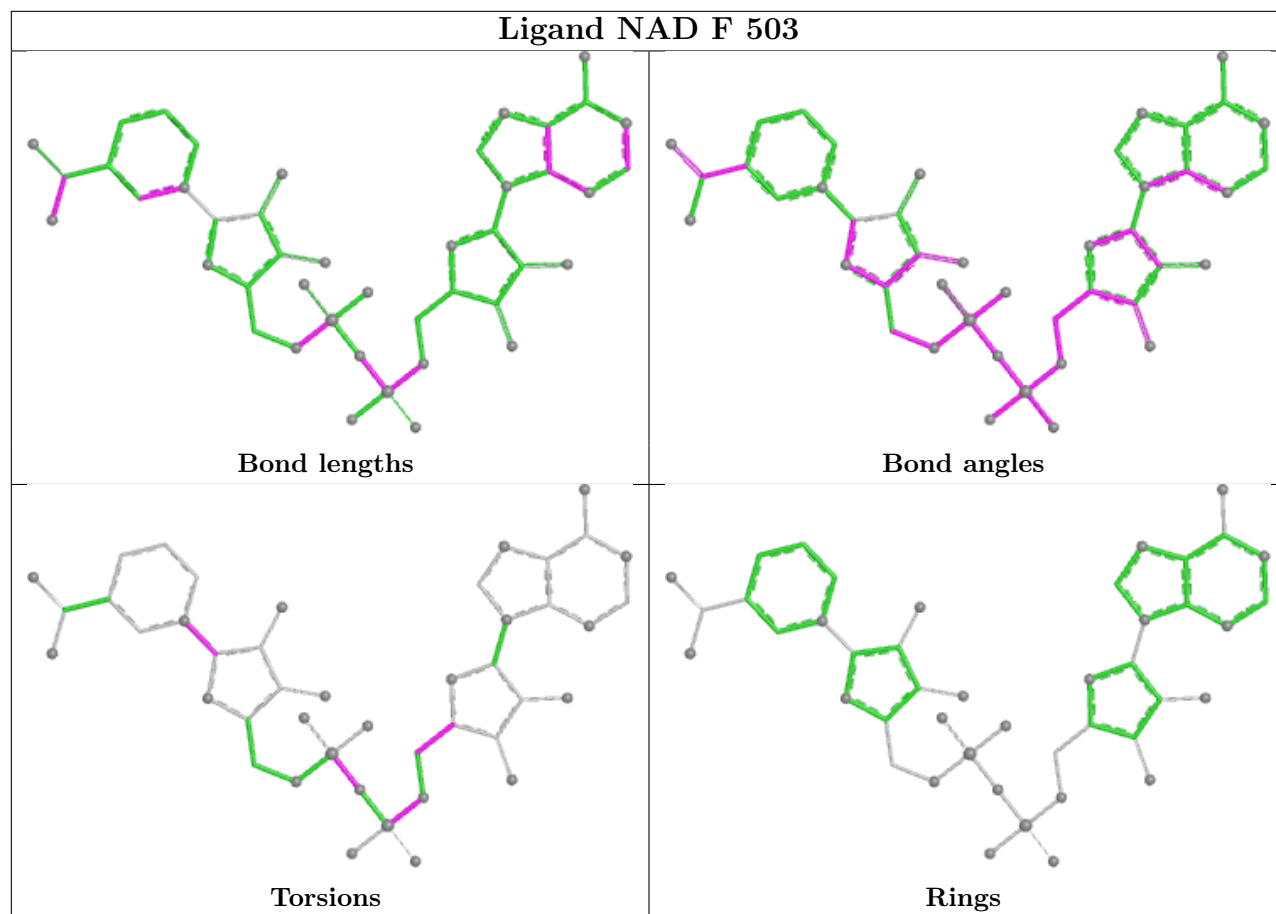


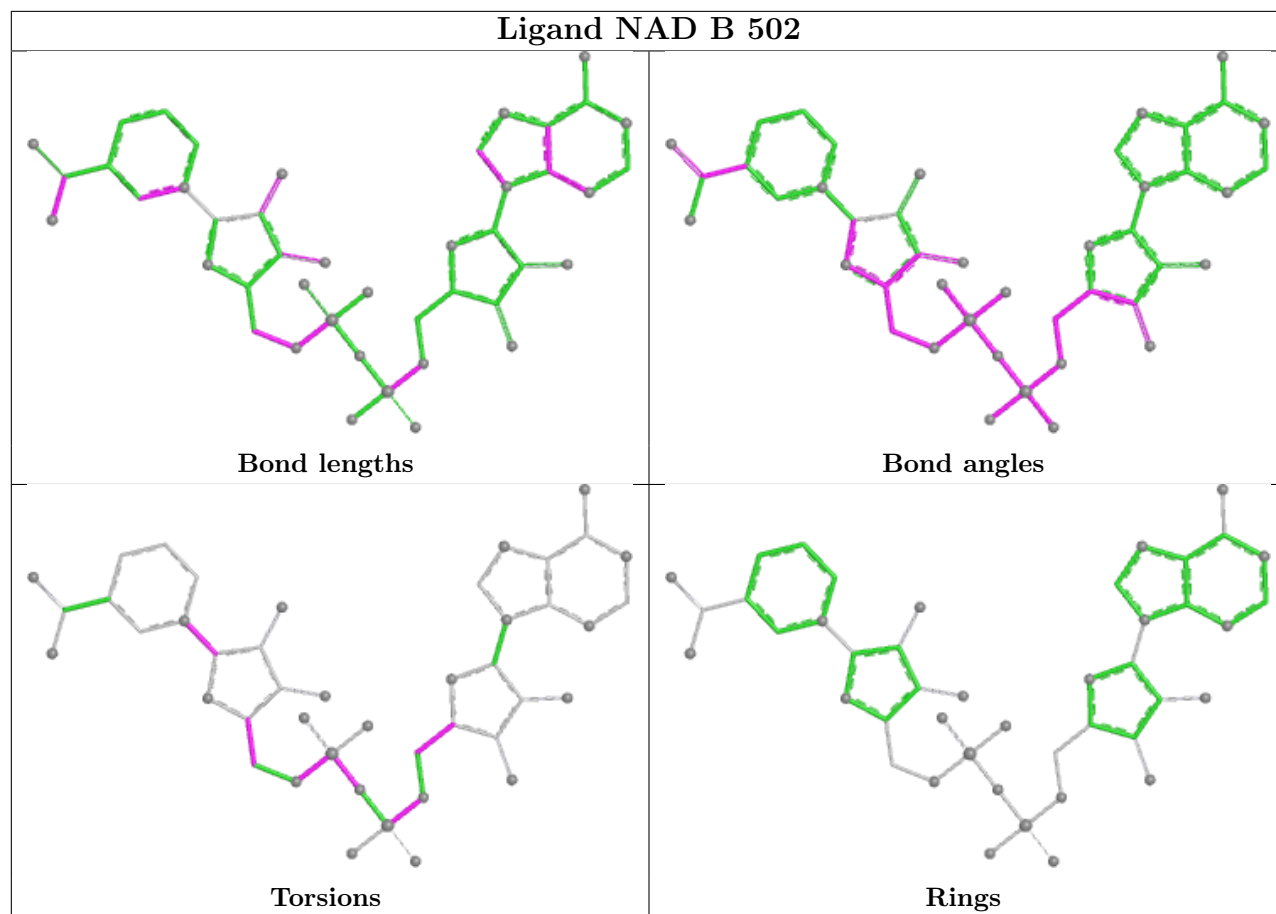
Ligand NOS A 501

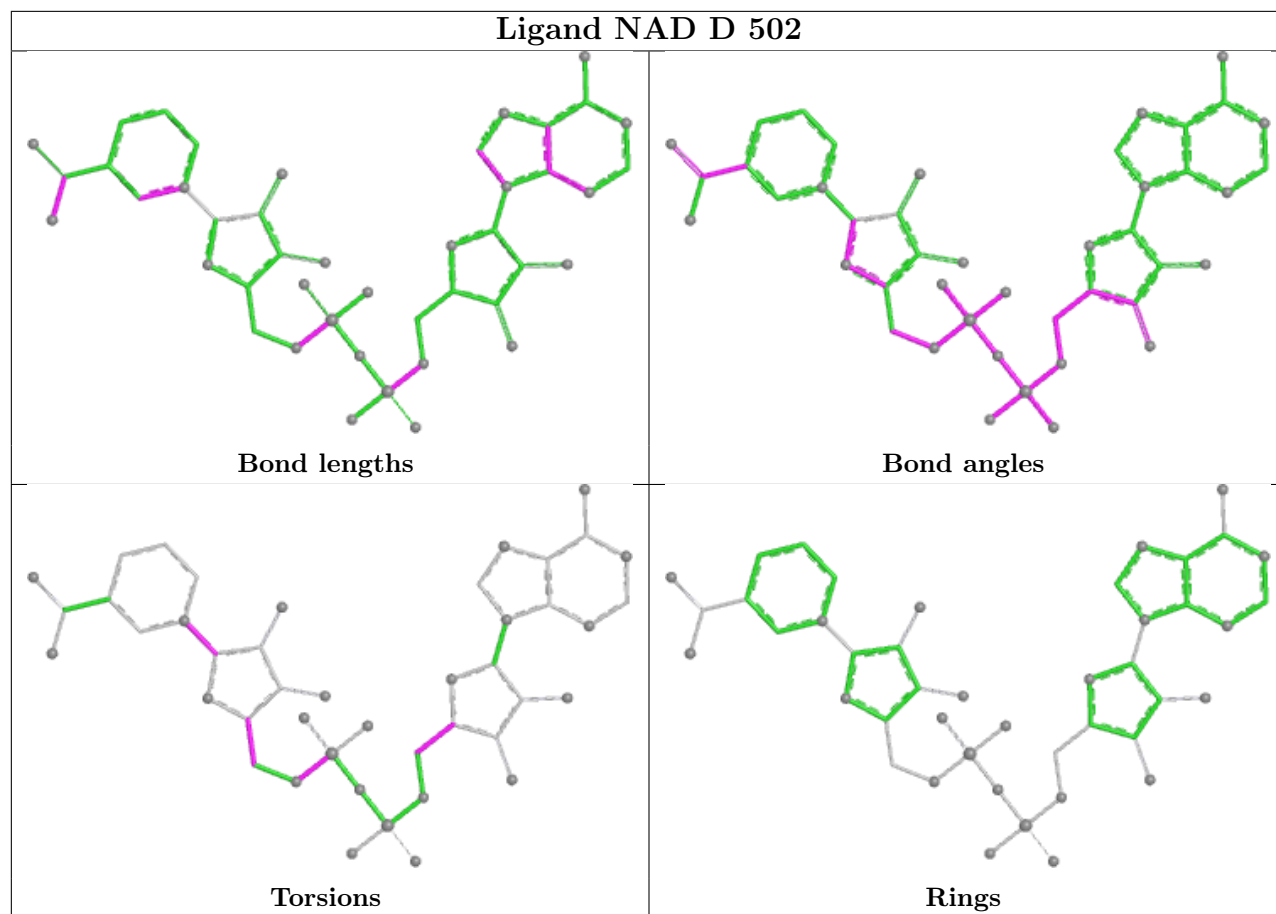


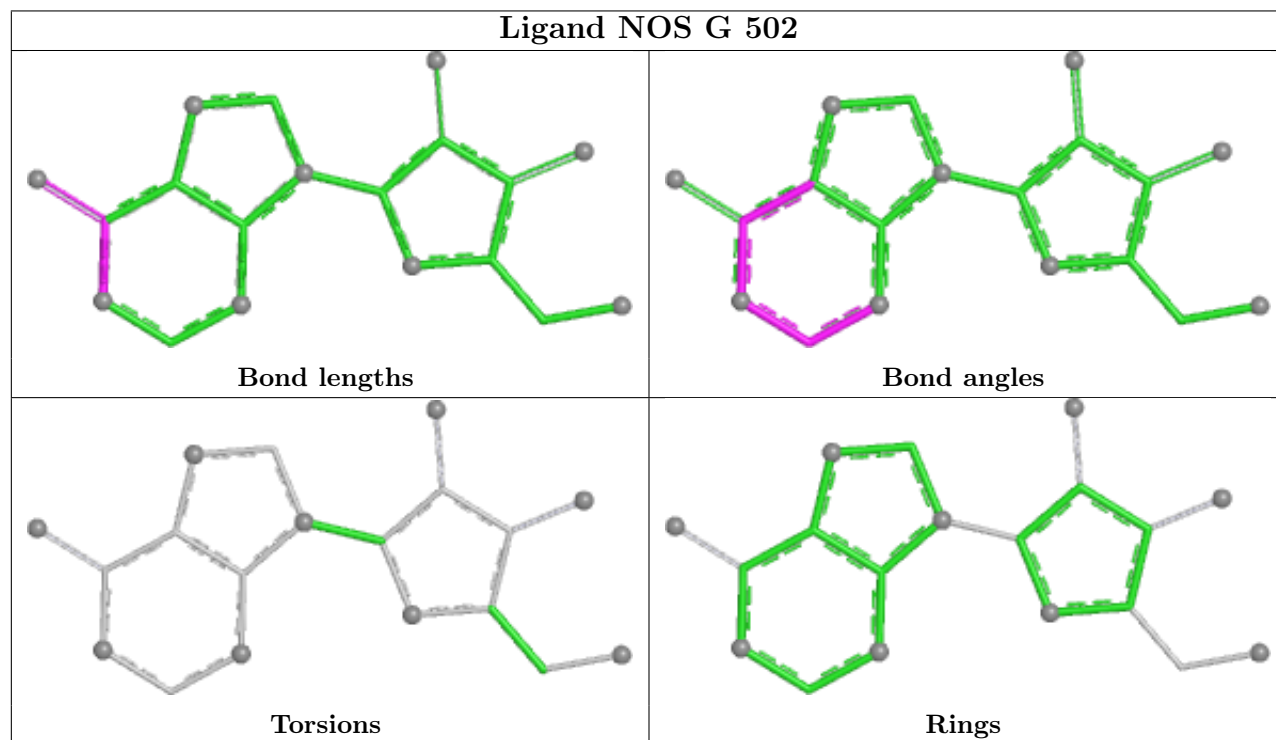
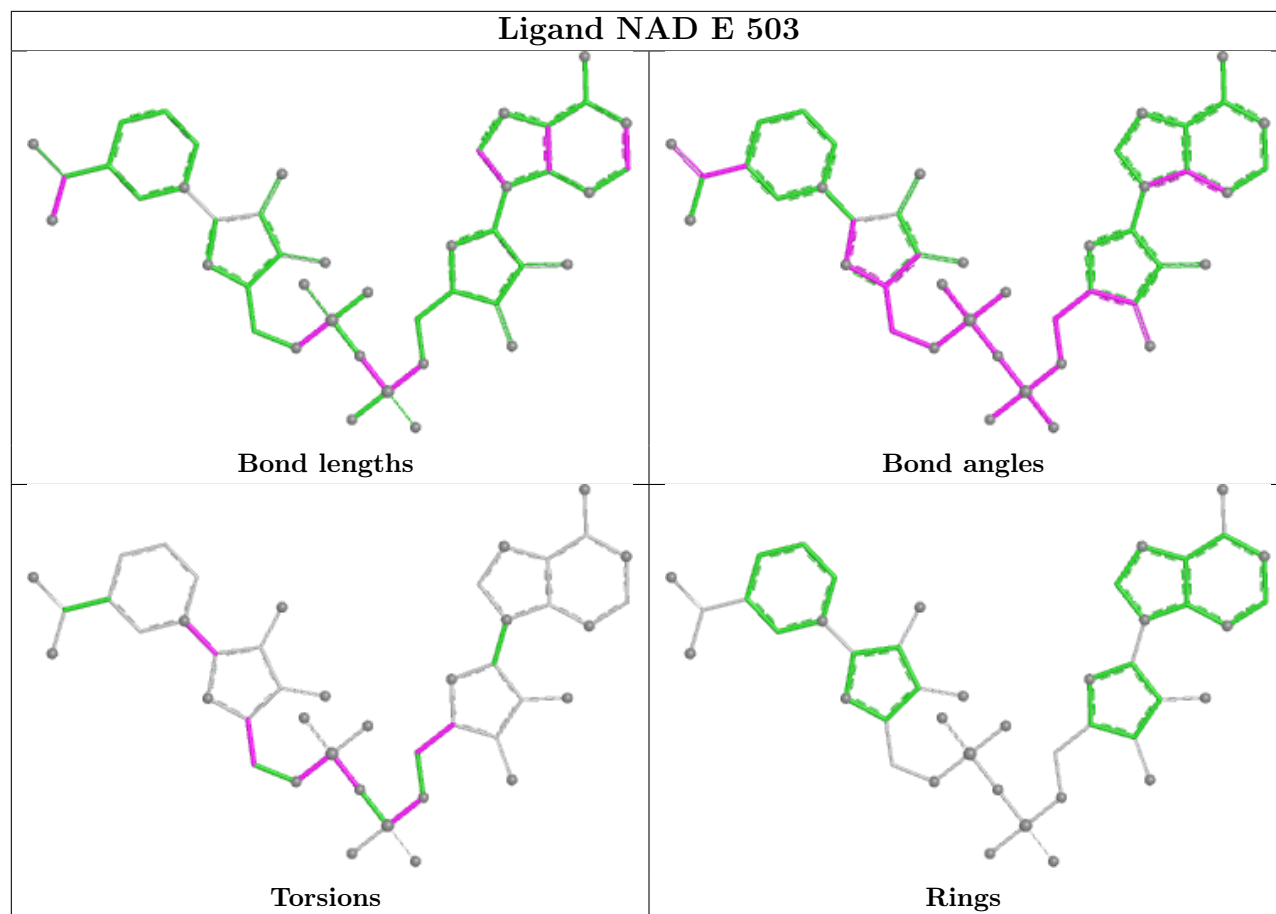
Ligand NOS C 501



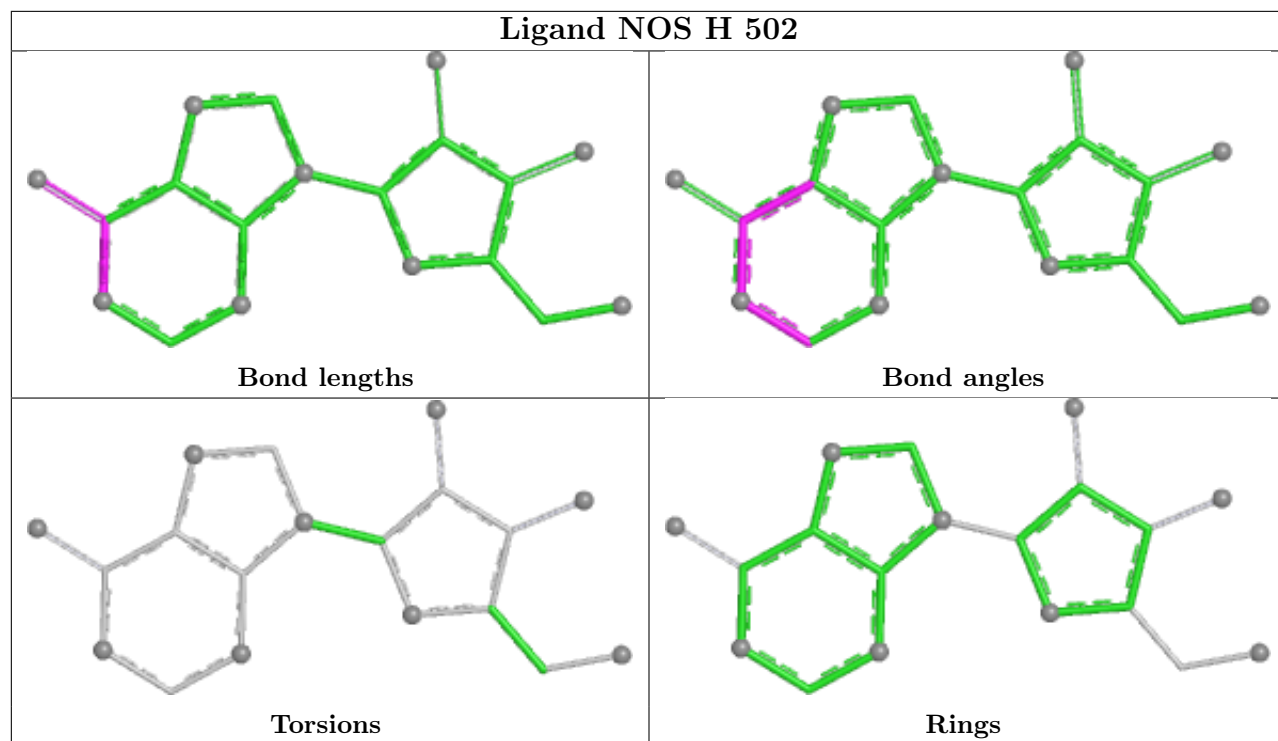




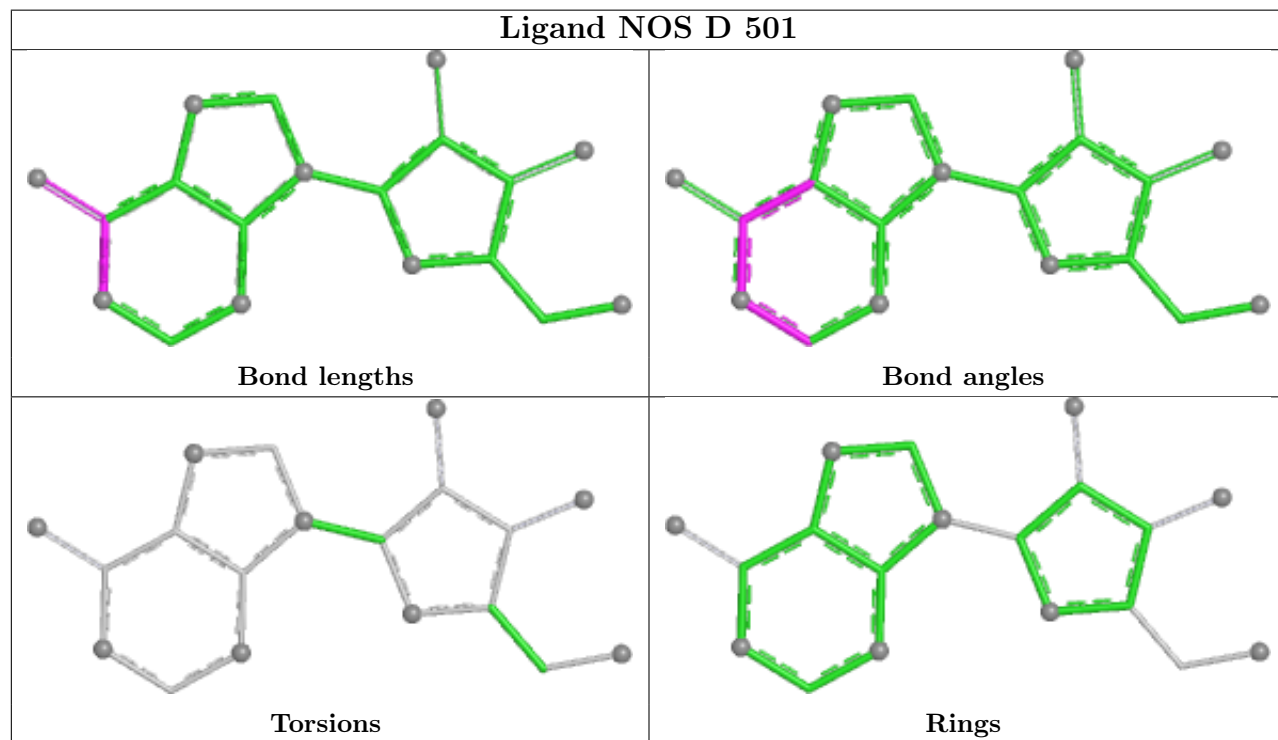




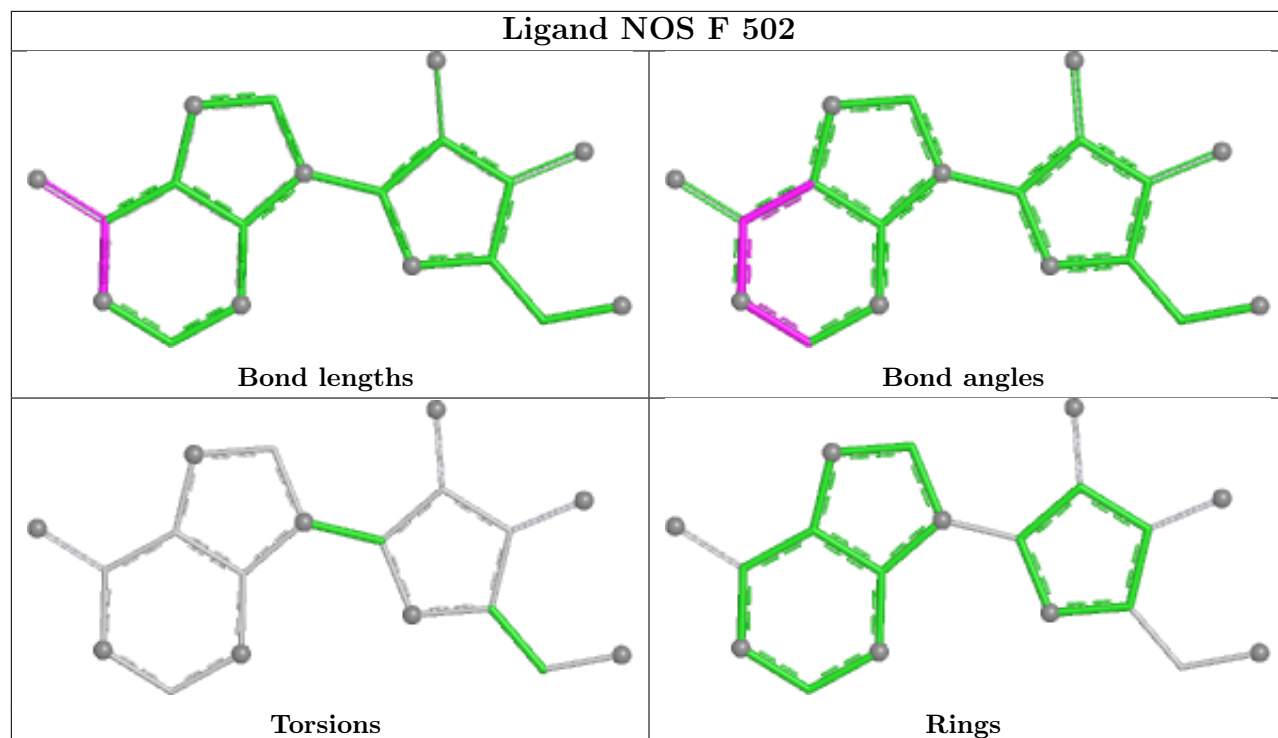
Ligand NOS H 502



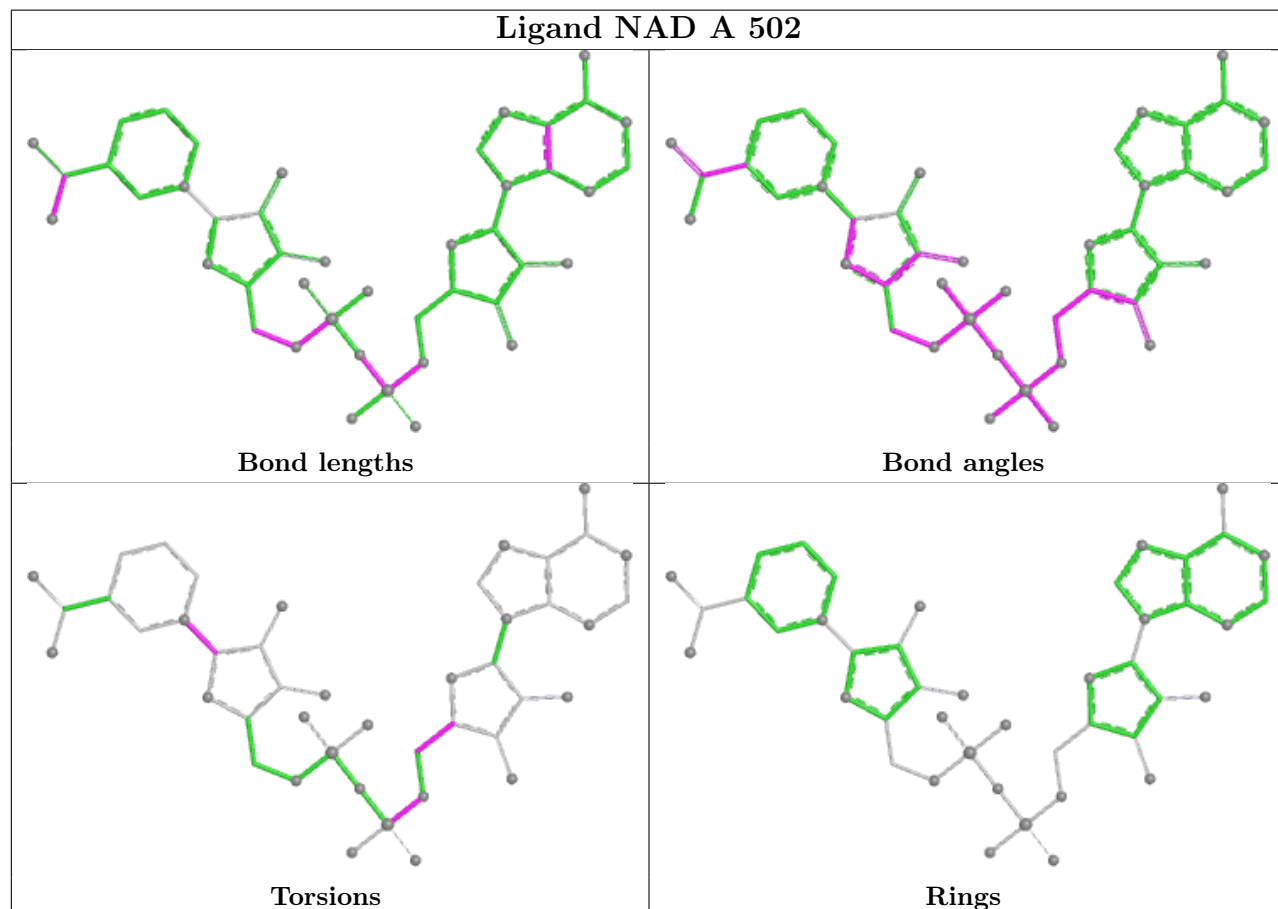
Ligand NOS D 501

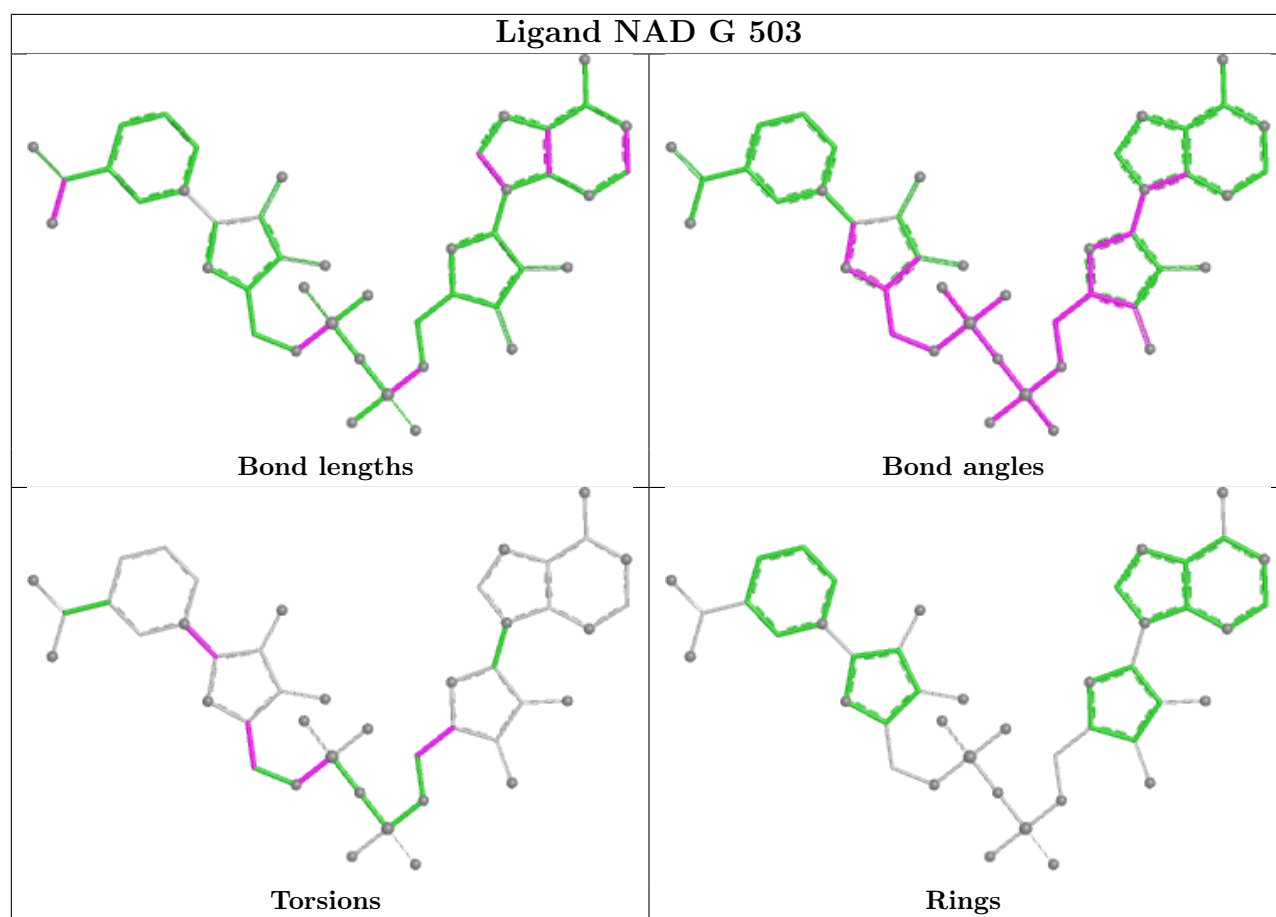


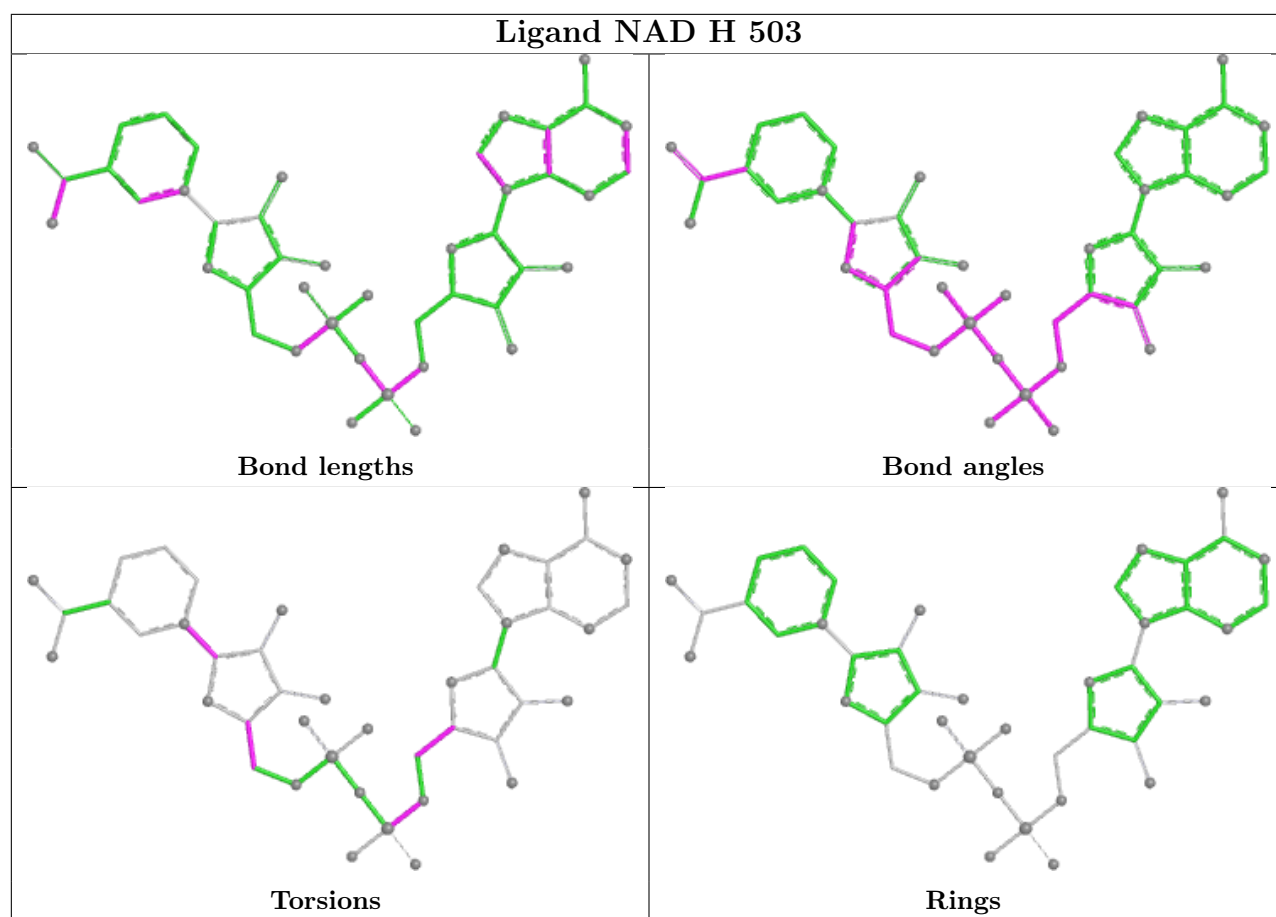
Ligand NOS F 502



Ligand NAD A 502







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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	411/435 (94%)	-0.13	0 100 100	31, 54, 80, 98	0
1	B	411/435 (94%)	-0.11	1 (0%) 91 90	33, 57, 84, 94	0
1	C	411/435 (94%)	0.04	3 (0%) 84 82	31, 66, 98, 111	0
1	D	411/435 (94%)	-0.11	1 (0%) 91 90	32, 61, 98, 130	0
1	E	411/435 (94%)	0.02	3 (0%) 84 82	33, 62, 89, 102	0
1	F	411/435 (94%)	0.07	0 100 100	36, 73, 100, 114	0
1	G	411/435 (94%)	0.40	9 (2%) 62 59	40, 92, 135, 146	0
1	H	411/435 (94%)	0.22	4 (0%) 79 77	42, 82, 118, 125	0
All	All	3288/3480 (94%)	0.05	21 (0%) 85 84	31, 67, 113, 146	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	90	VAL	3.4
1	G	115	TYR	3.0
1	H	141	ILE	2.8
1	G	133	LEU	2.7
1	E	164	GLY	2.6
1	G	172	GLY	2.6
1	C	145	ALA	2.5
1	G	111	GLY	2.5
1	H	432	LYS	2.4
1	G	68	ALA	2.4
1	H	60	PHE	2.3
1	D	432	LYS	2.3
1	B	168	GLU	2.3
1	G	107	CYS	2.3
1	G	130	ASN	2.2
1	G	104	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	66	GLY	2.1
1	C	417	ILE	2.1
1	H	140	ILE	2.1
1	C	142	ASP	2.1
1	E	432	LYS	2.1

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.

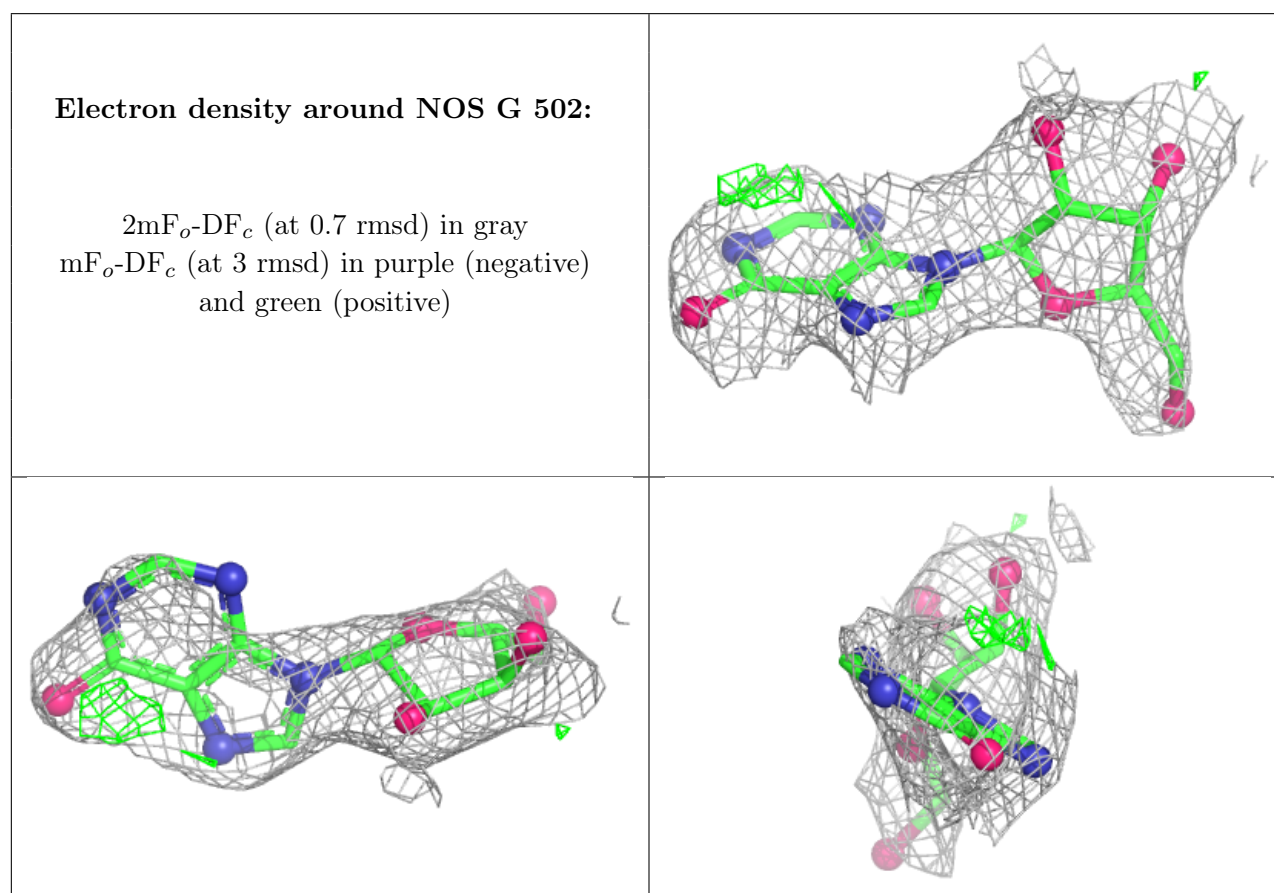
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PG4	B	503	13/13	0.85	0.17	75,88,115,116	0
4	PG4	F	501	13/13	0.85	0.17	73,83,89,94	0
4	PG4	G	501	13/13	0.85	0.18	87,95,121,123	0
4	PG4	H	501	13/13	0.85	0.14	70,82,94,97	0
4	PG4	C	503	13/13	0.87	0.13	77,81,98,99	0
2	NOS	G	502	19/19	0.87	0.13	89,113,130,134	0
4	PG4	A	503	13/13	0.89	0.13	60,66,81,82	0
4	PG4	E	501	13/13	0.90	0.12	53,59,68,69	0
4	PG4	D	503	13/13	0.90	0.15	80,84,113,115	0
2	NOS	H	502	19/19	0.91	0.11	61,71,87,90	0
2	NOS	F	502	19/19	0.91	0.12	65,70,88,89	0
2	NOS	D	501	19/19	0.91	0.10	54,60,67,68	0
3	NAD	H	503	44/44	0.93	0.11	56,75,93,106	0
2	NOS	B	501	19/19	0.93	0.11	37,45,68,70	0
3	NAD	G	503	44/44	0.93	0.10	46,65,84,86	0
2	NOS	E	502	19/19	0.94	0.09	41,54,71,73	0
3	NAD	D	502	44/44	0.94	0.08	36,50,57,61	0
2	NOS	C	501	19/19	0.94	0.10	50,57,85,87	0

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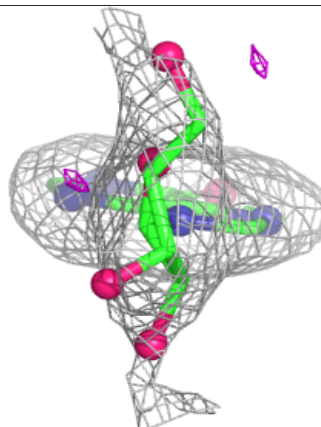
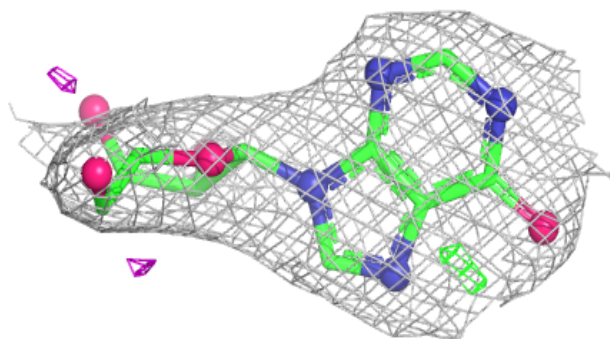
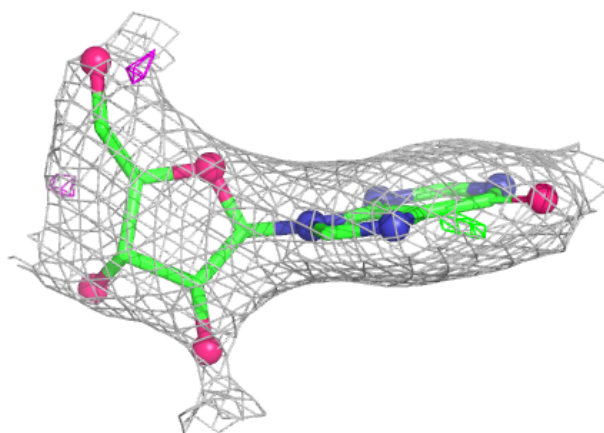
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NOS	A	501	19/19	0.94	0.09	37,46,67,74	0
3	NAD	B	502	44/44	0.96	0.09	43,54,62,66	0
3	NAD	C	502	44/44	0.96	0.07	48,55,61,67	0
3	NAD	A	502	44/44	0.96	0.07	28,45,51,58	0
3	NAD	E	503	44/44	0.96	0.07	38,46,51,57	0
3	NAD	F	503	44/44	0.96	0.08	42,56,64,68	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.

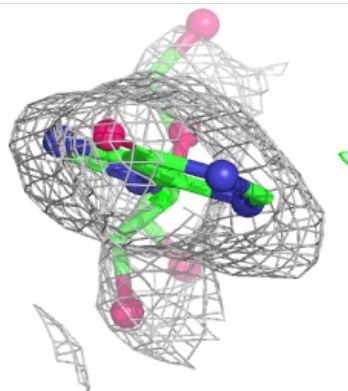
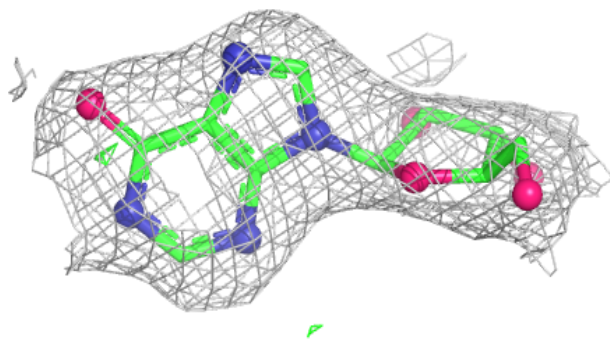
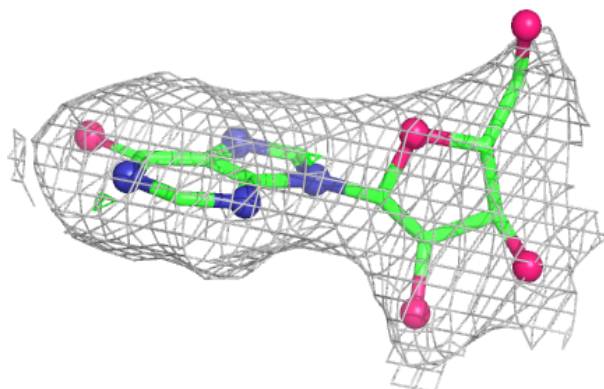


Electron density around NOS H 502:

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

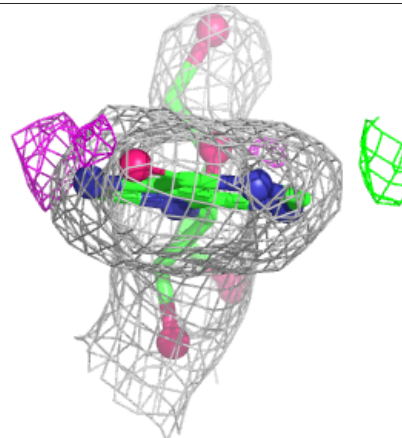
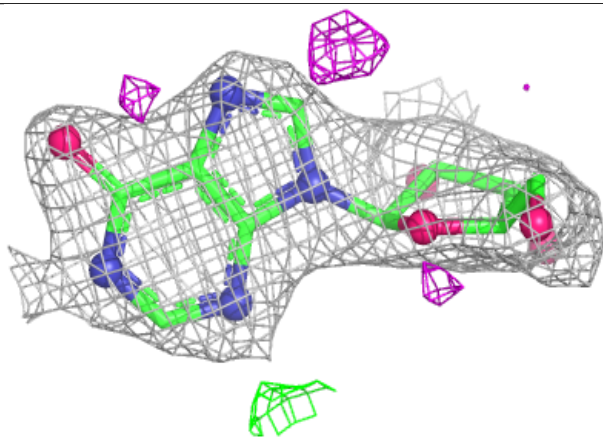
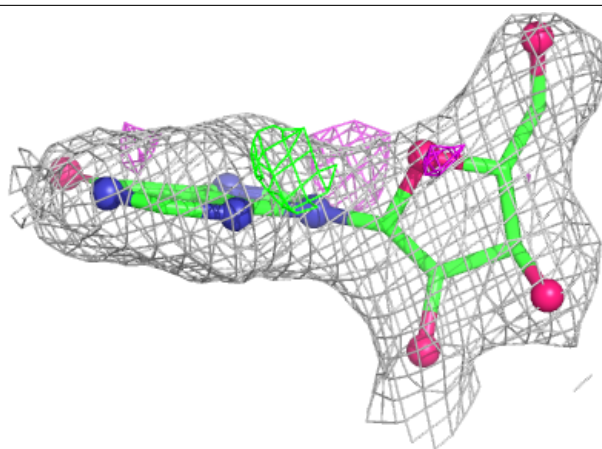
**Electron density around NOS F 502:**

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and green (positive)

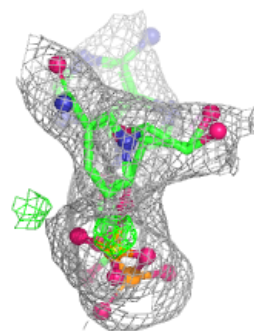
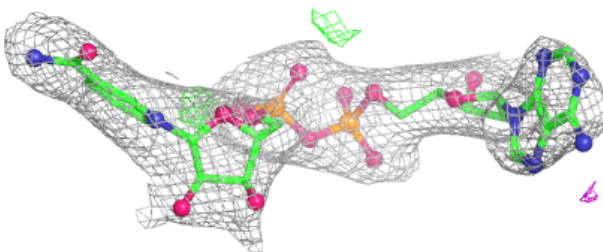
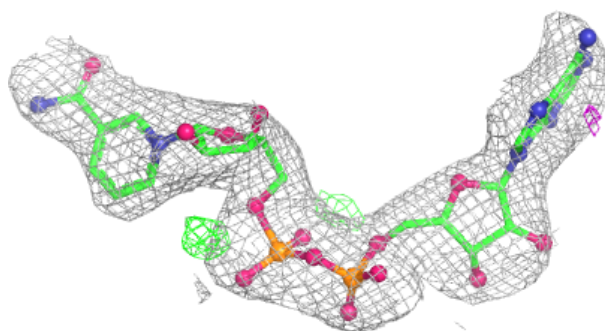


Electron density around NOS D 501:

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and green (positive)

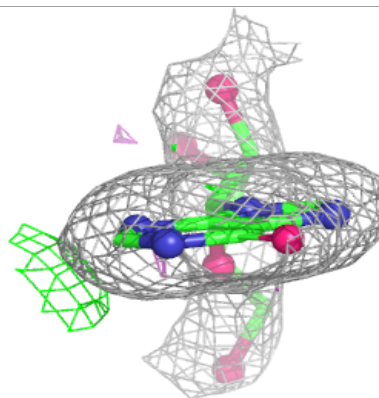
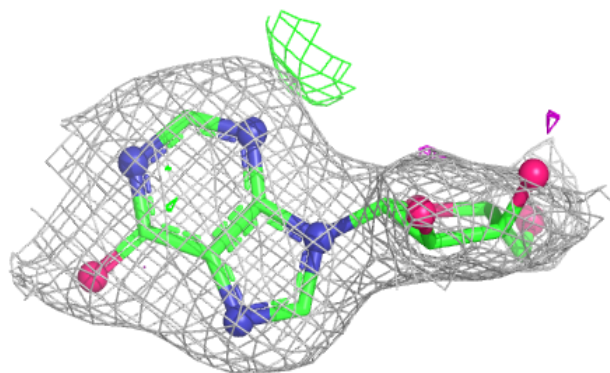
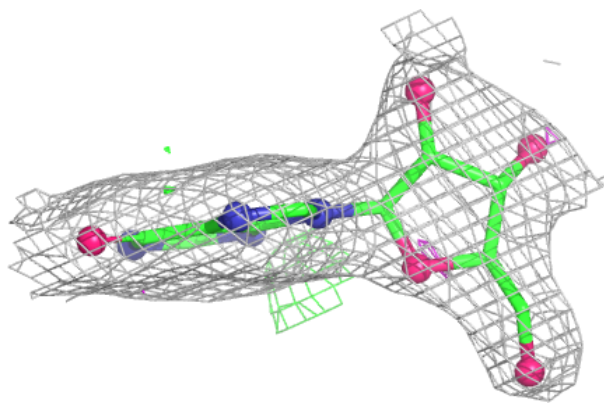
**Electron density around NAD H 503:**

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and green (positive)

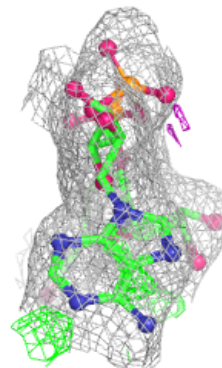
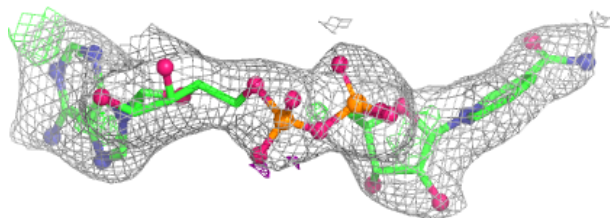
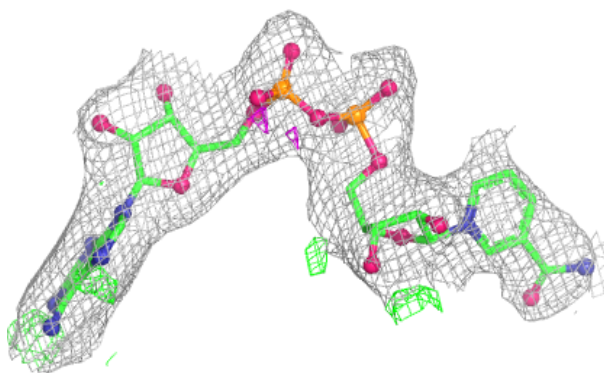


Electron density around NOS B 501:

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and green (positive)

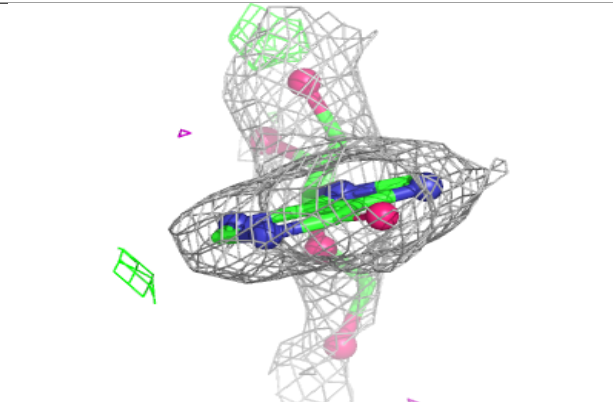
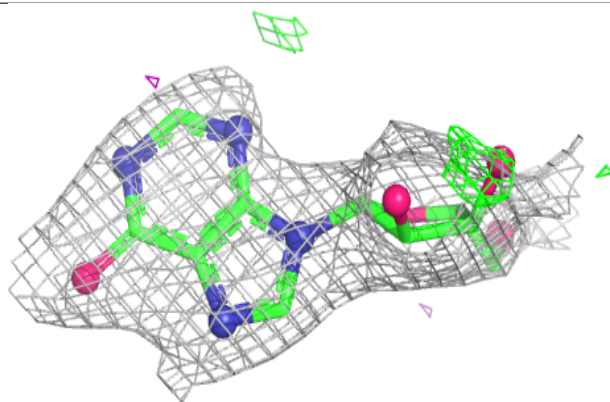
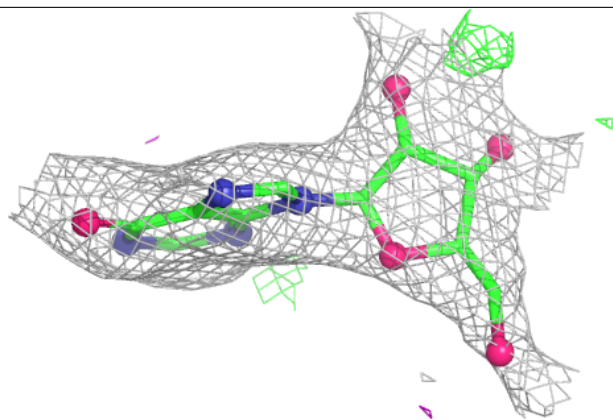
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and green (positive)

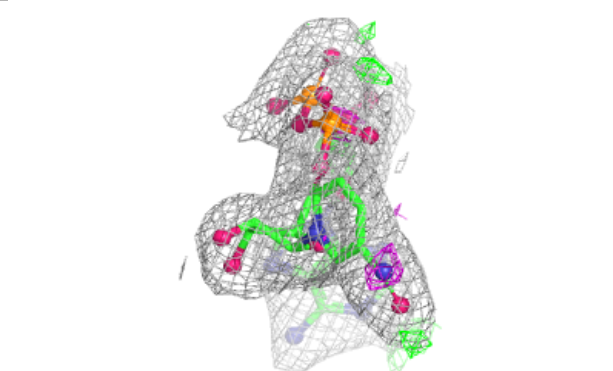
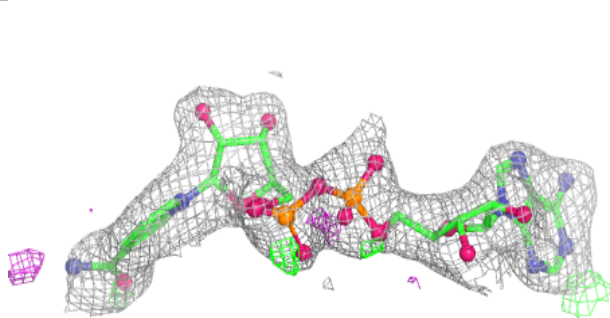
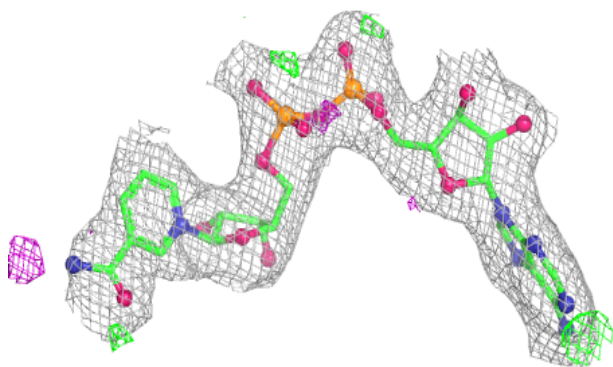


Electron density around NOS E 502:

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and green (positive)

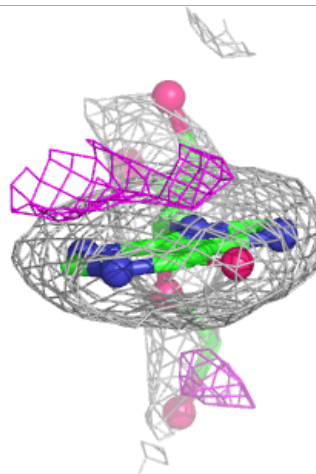
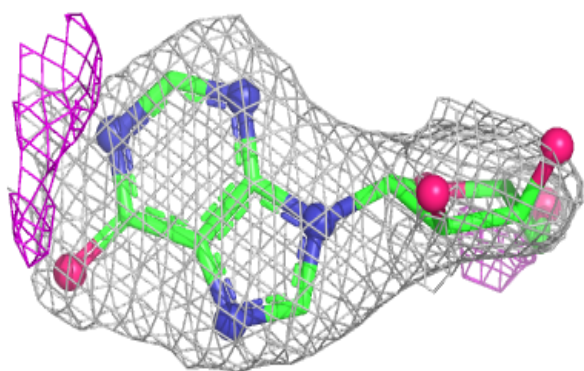
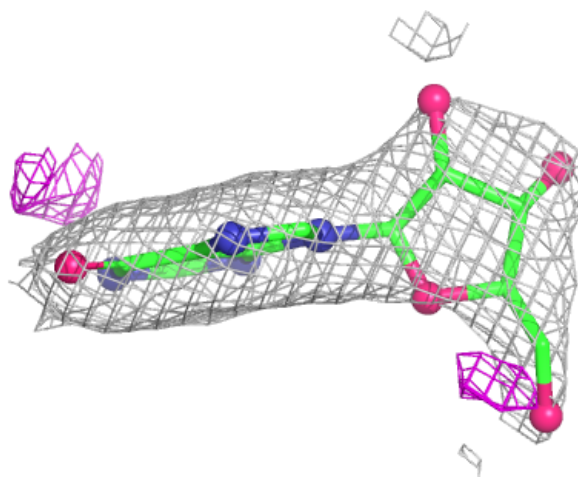
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and green (positive)



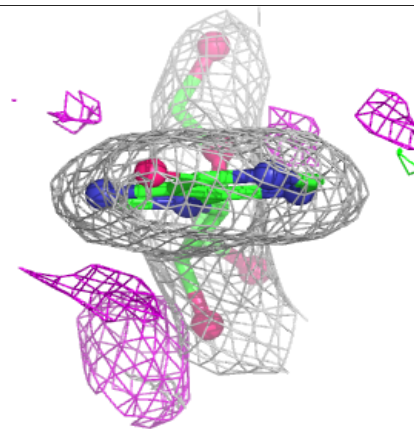
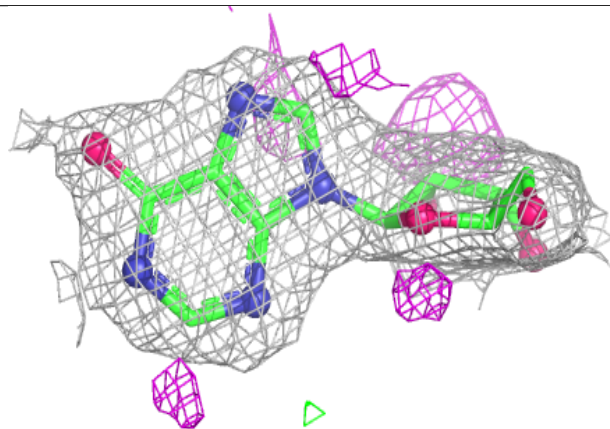
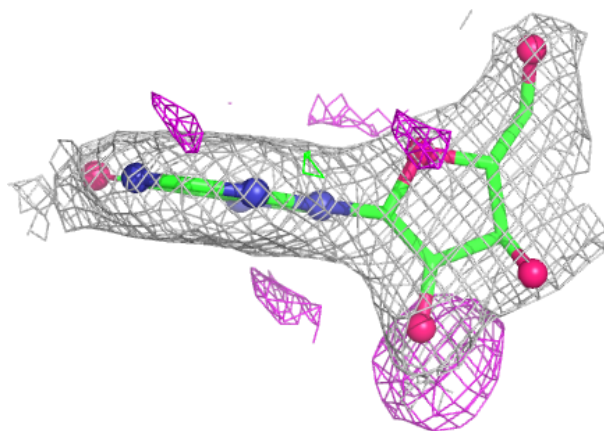
Electron density around NOS C 501:

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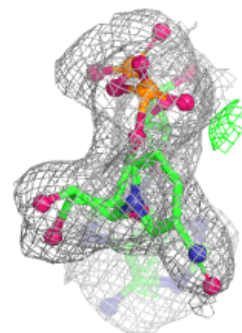
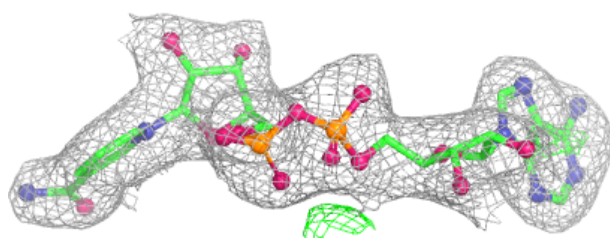
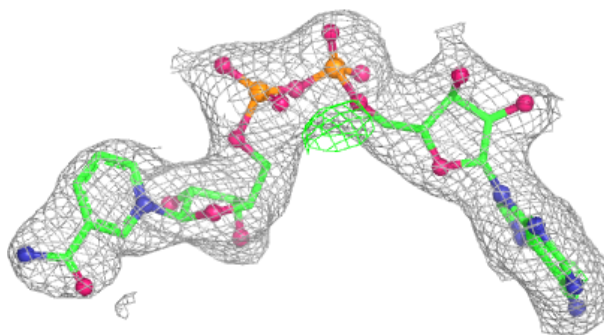


Electron density around NOS A 501:

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and green (positive)

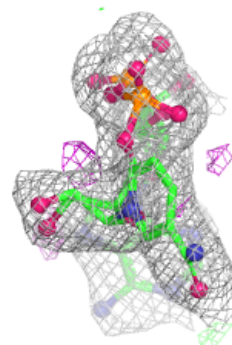
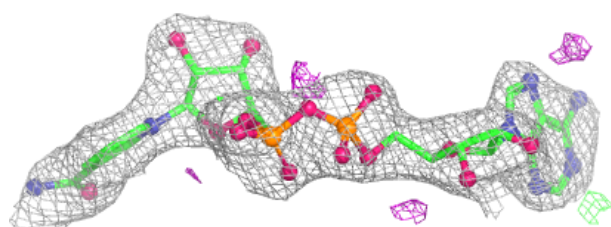
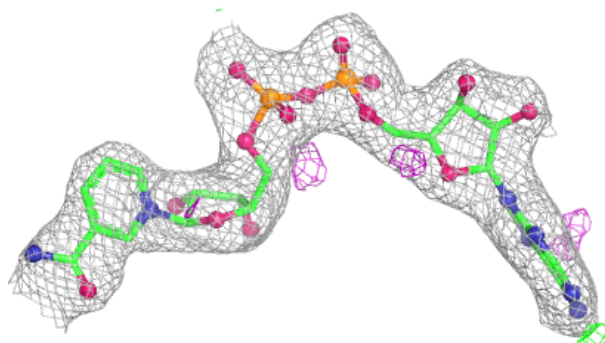
**Electron density around NAD B 502:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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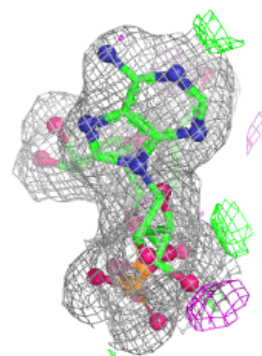
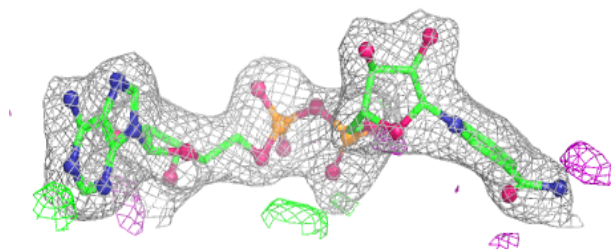
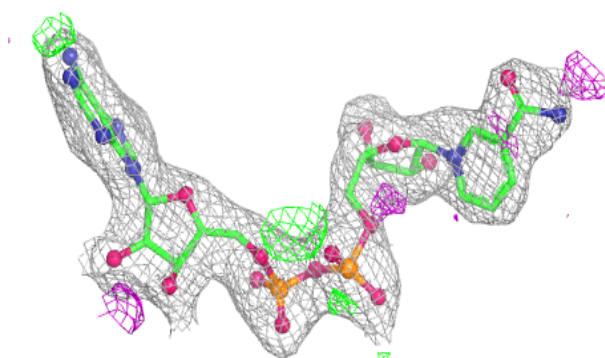


Electron density around NAD C 502:

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

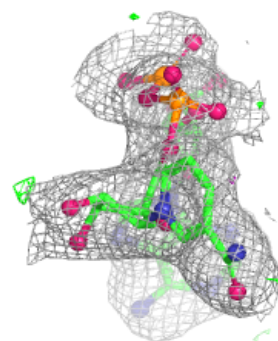
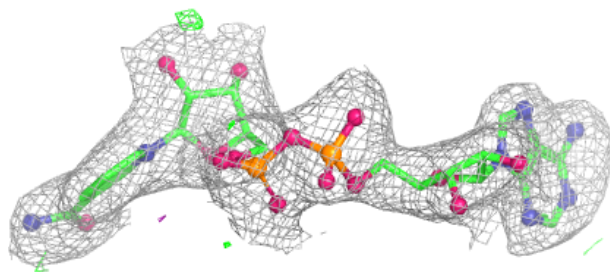
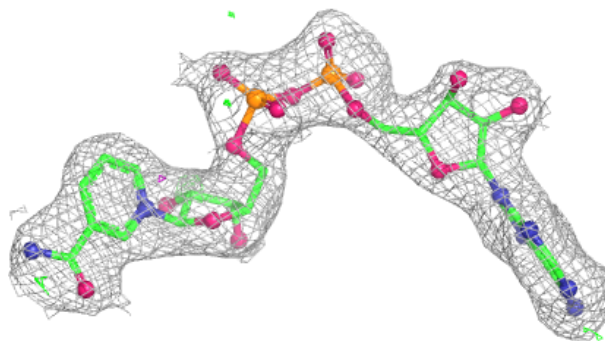
**Electron density around NAD A 502:**

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

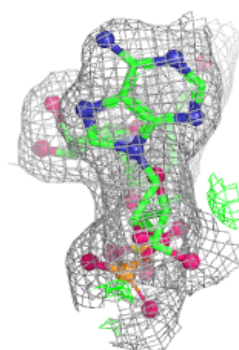
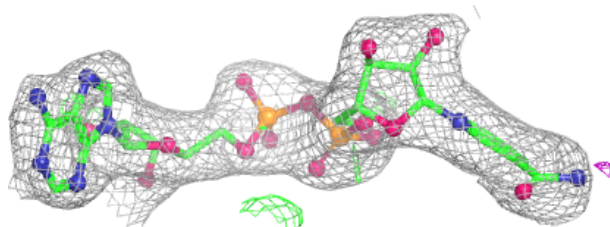
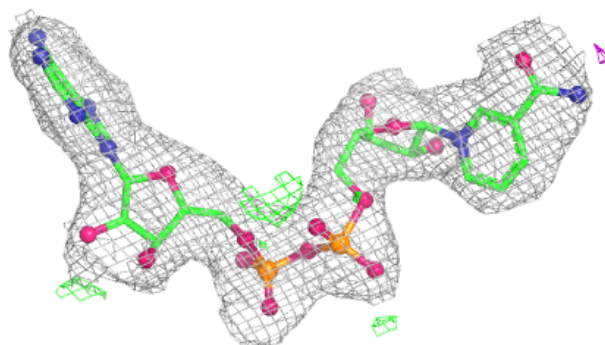


Electron density around NAD E 503:

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

**Electron density around NAD F 503:**

$2mF_o-DF_c$ (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.