



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 08:01 AM UTC

PDB ID : 6N7L / pdb_00006n7l
Title : Crystal structure of an alcohol dehydrogenase from Elizabethkingia anophelis NUHP1
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2018-11-27
Resolution : 2.10 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

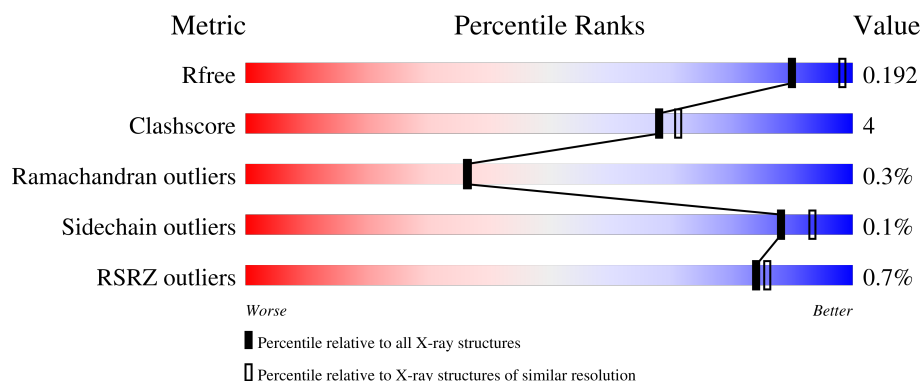
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	353	
1	B	353	
1	C	353	
1	D	353	
1	E	353	

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Mol	Chain	Length	Quality of chain
1	F	353	% 91% 6% .
1	G	353	89% 7% .
1	H	353	% 90% 7% ..
1	I	353	% 86% 10% .
1	J	353	% 90% 7% .
1	K	353	87% 10% ..
1	L	353	% 90% 6% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33393 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 Alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	5	0
			2548	1622	425	483	18			
1	B	342	Total	C	N	O	S	0	4	0
			2524	1608	422	477	17			
1	C	344	Total	C	N	O	S	0	11	0
			2610	1672	437	483	18			
1	D	343	Total	C	N	O	S	0	3	0
			2549	1624	430	478	17			
1	E	340	Total	C	N	O	S	0	3	0
			2506	1595	423	471	17			
1	F	343	Total	C	N	O	S	0	4	0
			2532	1612	427	476	17			
1	G	340	Total	C	N	O	S	0	1	0
			2501	1593	419	472	17			
1	H	342	Total	C	N	O	S	0	3	0
			2525	1610	423	475	17			
1	I	341	Total	C	N	O	S	0	1	0
			2470	1571	420	462	17			
1	J	343	Total	C	N	O	S	0	3	0
			2517	1602	425	472	18			
1	K	342	Total	C	N	O	S	0	3	0
			2518	1602	424	475	17			
1	L	340	Total	C	N	O	S	0	1	0
			2423	1539	412	455	17			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A0A077EGR8
A	-6	ALA	-	expression tag	UNP A0A077EGR8
A	-5	HIS	-	expression tag	UNP A0A077EGR8
A	-4	HIS	-	expression tag	UNP A0A077EGR8
A	-3	HIS	-	expression tag	UNP A0A077EGR8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	expression tag	UNP A0A077EGR8
A	-1	HIS	-	expression tag	UNP A0A077EGR8
A	0	HIS	-	expression tag	UNP A0A077EGR8
B	-7	MET	-	initiating methionine	UNP A0A077EGR8
B	-6	ALA	-	expression tag	UNP A0A077EGR8
B	-5	HIS	-	expression tag	UNP A0A077EGR8
B	-4	HIS	-	expression tag	UNP A0A077EGR8
B	-3	HIS	-	expression tag	UNP A0A077EGR8
B	-2	HIS	-	expression tag	UNP A0A077EGR8
B	-1	HIS	-	expression tag	UNP A0A077EGR8
B	0	HIS	-	expression tag	UNP A0A077EGR8
C	-7	MET	-	initiating methionine	UNP A0A077EGR8
C	-6	ALA	-	expression tag	UNP A0A077EGR8
C	-5	HIS	-	expression tag	UNP A0A077EGR8
C	-4	HIS	-	expression tag	UNP A0A077EGR8
C	-3	HIS	-	expression tag	UNP A0A077EGR8
C	-2	HIS	-	expression tag	UNP A0A077EGR8
C	-1	HIS	-	expression tag	UNP A0A077EGR8
C	0	HIS	-	expression tag	UNP A0A077EGR8
D	-7	MET	-	initiating methionine	UNP A0A077EGR8
D	-6	ALA	-	expression tag	UNP A0A077EGR8
D	-5	HIS	-	expression tag	UNP A0A077EGR8
D	-4	HIS	-	expression tag	UNP A0A077EGR8
D	-3	HIS	-	expression tag	UNP A0A077EGR8
D	-2	HIS	-	expression tag	UNP A0A077EGR8
D	-1	HIS	-	expression tag	UNP A0A077EGR8
D	0	HIS	-	expression tag	UNP A0A077EGR8
E	-7	MET	-	initiating methionine	UNP A0A077EGR8
E	-6	ALA	-	expression tag	UNP A0A077EGR8
E	-5	HIS	-	expression tag	UNP A0A077EGR8
E	-4	HIS	-	expression tag	UNP A0A077EGR8
E	-3	HIS	-	expression tag	UNP A0A077EGR8
E	-2	HIS	-	expression tag	UNP A0A077EGR8
E	-1	HIS	-	expression tag	UNP A0A077EGR8
E	0	HIS	-	expression tag	UNP A0A077EGR8
F	-7	MET	-	initiating methionine	UNP A0A077EGR8
F	-6	ALA	-	expression tag	UNP A0A077EGR8
F	-5	HIS	-	expression tag	UNP A0A077EGR8
F	-4	HIS	-	expression tag	UNP A0A077EGR8
F	-3	HIS	-	expression tag	UNP A0A077EGR8
F	-2	HIS	-	expression tag	UNP A0A077EGR8
F	-1	HIS	-	expression tag	UNP A0A077EGR8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP A0A077EGR8
G	-7	MET	-	initiating methionine	UNP A0A077EGR8
G	-6	ALA	-	expression tag	UNP A0A077EGR8
G	-5	HIS	-	expression tag	UNP A0A077EGR8
G	-4	HIS	-	expression tag	UNP A0A077EGR8
G	-3	HIS	-	expression tag	UNP A0A077EGR8
G	-2	HIS	-	expression tag	UNP A0A077EGR8
G	-1	HIS	-	expression tag	UNP A0A077EGR8
G	0	HIS	-	expression tag	UNP A0A077EGR8
H	-7	MET	-	initiating methionine	UNP A0A077EGR8
H	-6	ALA	-	expression tag	UNP A0A077EGR8
H	-5	HIS	-	expression tag	UNP A0A077EGR8
H	-4	HIS	-	expression tag	UNP A0A077EGR8
H	-3	HIS	-	expression tag	UNP A0A077EGR8
H	-2	HIS	-	expression tag	UNP A0A077EGR8
H	-1	HIS	-	expression tag	UNP A0A077EGR8
H	0	HIS	-	expression tag	UNP A0A077EGR8
I	-7	MET	-	initiating methionine	UNP A0A077EGR8
I	-6	ALA	-	expression tag	UNP A0A077EGR8
I	-5	HIS	-	expression tag	UNP A0A077EGR8
I	-4	HIS	-	expression tag	UNP A0A077EGR8
I	-3	HIS	-	expression tag	UNP A0A077EGR8
I	-2	HIS	-	expression tag	UNP A0A077EGR8
I	-1	HIS	-	expression tag	UNP A0A077EGR8
I	0	HIS	-	expression tag	UNP A0A077EGR8
J	-7	MET	-	initiating methionine	UNP A0A077EGR8
J	-6	ALA	-	expression tag	UNP A0A077EGR8
J	-5	HIS	-	expression tag	UNP A0A077EGR8
J	-4	HIS	-	expression tag	UNP A0A077EGR8
J	-3	HIS	-	expression tag	UNP A0A077EGR8
J	-2	HIS	-	expression tag	UNP A0A077EGR8
J	-1	HIS	-	expression tag	UNP A0A077EGR8
J	0	HIS	-	expression tag	UNP A0A077EGR8
K	-7	MET	-	initiating methionine	UNP A0A077EGR8
K	-6	ALA	-	expression tag	UNP A0A077EGR8
K	-5	HIS	-	expression tag	UNP A0A077EGR8
K	-4	HIS	-	expression tag	UNP A0A077EGR8
K	-3	HIS	-	expression tag	UNP A0A077EGR8
K	-2	HIS	-	expression tag	UNP A0A077EGR8
K	-1	HIS	-	expression tag	UNP A0A077EGR8
K	0	HIS	-	expression tag	UNP A0A077EGR8
L	-7	MET	-	initiating methionine	UNP A0A077EGR8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	ALA	-	expression tag	UNP A0A077EGR8
L	-5	HIS	-	expression tag	UNP A0A077EGR8
L	-4	HIS	-	expression tag	UNP A0A077EGR8
L	-3	HIS	-	expression tag	UNP A0A077EGR8
L	-2	HIS	-	expression tag	UNP A0A077EGR8
L	-1	HIS	-	expression tag	UNP A0A077EGR8
L	0	HIS	-	expression tag	UNP A0A077EGR8

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0

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

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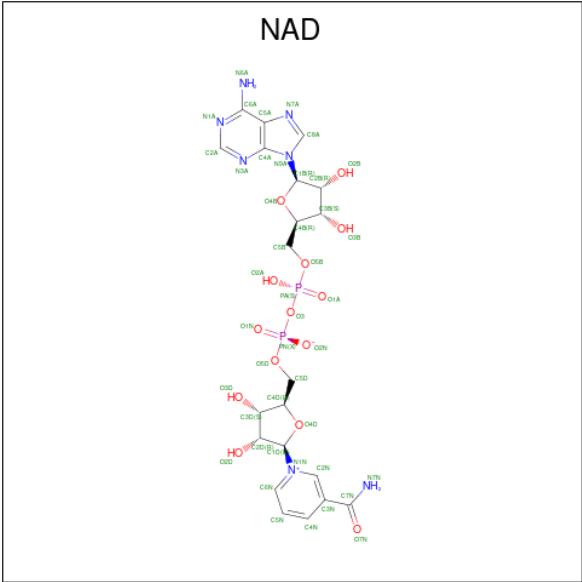
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	B	2	Total Zn 2 2	0	0
4	C	2	Total Zn 2 2	0	0
4	D	2	Total Zn 2 2	0	0
4	E	2	Total Zn 2 2	0	0
4	F	2	Total Zn 2 2	0	0
4	G	2	Total Zn 2 2	0	0
4	H	2	Total Zn 2 2	0	0
4	I	2	Total Zn 2 2	0	0
4	J	2	Total Zn 2 2	0	0
4	K	2	Total Zn 2 2	0	0
4	L	2	Total Zn 2 2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total 1	Cl 1	0	0
5	J	1	Total 1	Cl 1	0	0
5	K	1	Total 1	Cl 1	0	0
5	L	1	Total 1	Cl 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	231	Total 231	O 231	0	0
6	B	237	Total 238	O 238	0	1
6	C	284	Total 284	O 284	0	0
6	D	221	Total 221	O 221	0	0
6	E	196	Total 197	O 197	0	1
6	F	210	Total 210	O 210	0	0
6	G	195	Total 197	O 197	0	2
6	H	198	Total 198	O 198	0	0
6	I	90	Total 90	O 90	0	0
6	J	157	Total 157	O 157	0	0
6	K	149	Total 149	O 149	0	0
6	L	70	Total 70	O 70	0	0

3 Residue-property plots

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.

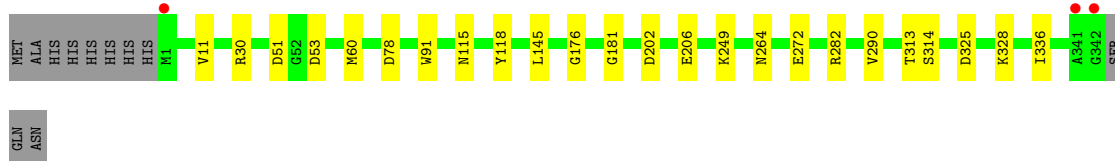
- Molecule 1: Alcohol dehydrogenase

Chain A: 



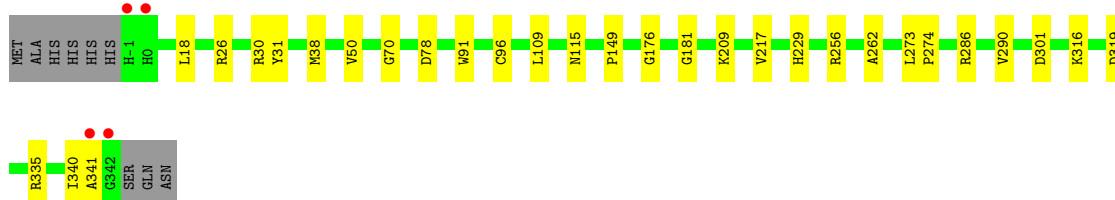
- Molecule 1: Alcohol dehydrogenase

Chain B: 



- Molecule 1: Alcohol dehydrogenase

Chain C: 



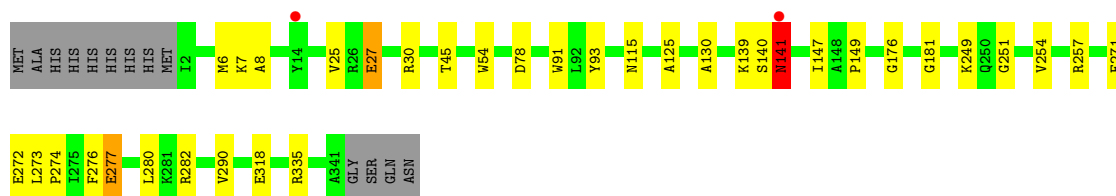
- Molecule 1: Alcohol dehydrogenase

Chain D: 

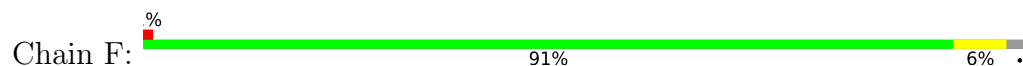


- Molecule 1: Alcohol dehydrogenase

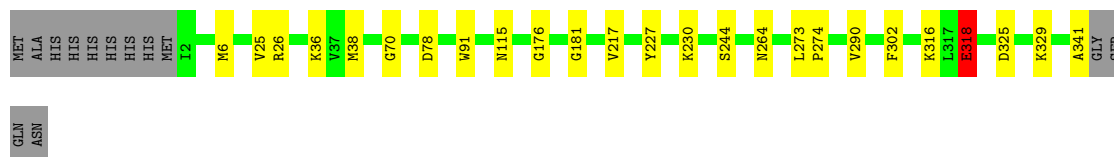
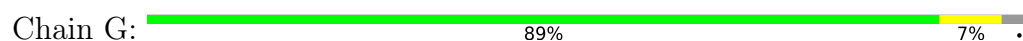
Chain E: 



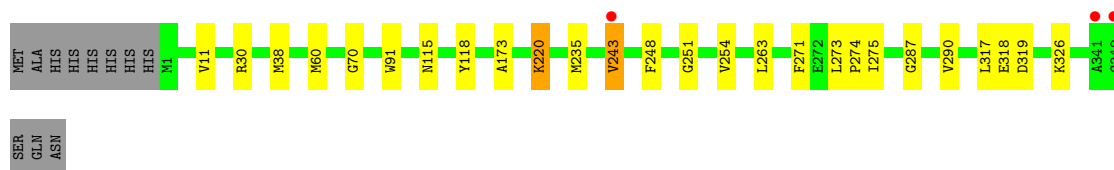
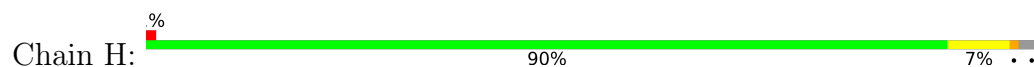
- Molecule 1: Alcohol dehydrogenase



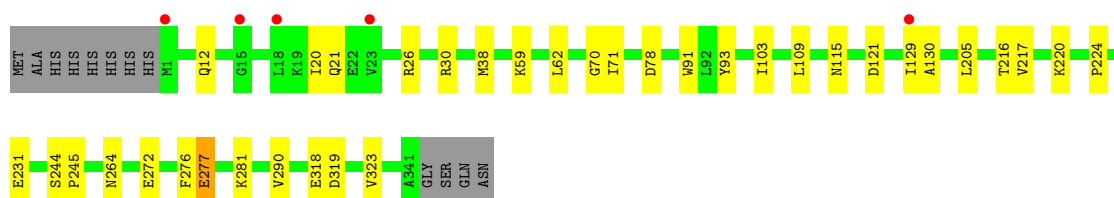
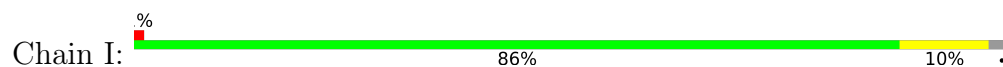
- Molecule 1: Alcohol dehydrogenase



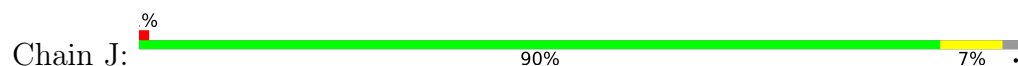
- Molecule 1: Alcohol dehydrogenase



- Molecule 1: Alcohol dehydrogenase

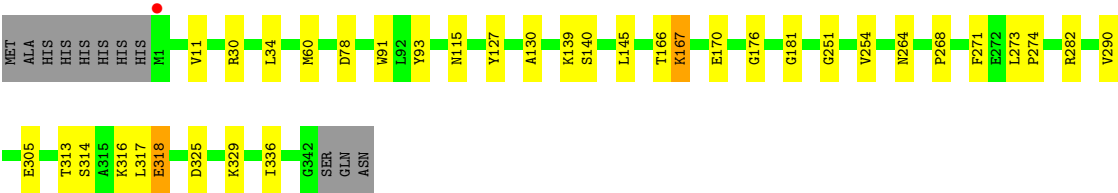
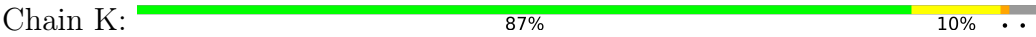


- Molecule 1: Alcohol dehydrogenase

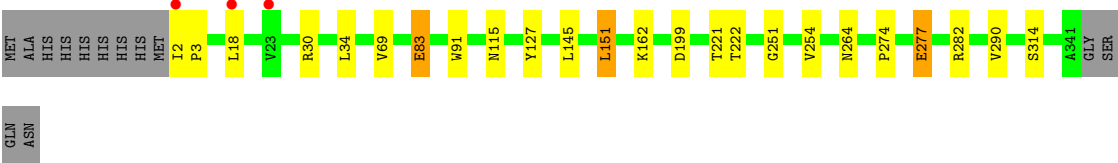
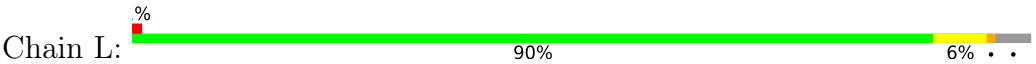




● Molecule 1: Alcohol dehydrogenase



● Molecule 1: Alcohol dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.15Å 168.29Å 199.73Å 90.00° 97.97° 90.00°	Depositor
Resolution (Å)	48.79 – 2.10 48.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (48.79-2.10) 95.2 (48.79-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.149 , 0.191 0.151 , 0.192	Depositor DCC
R_{free} test set	15384 reflections (5.77%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33393	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: CL, ZN, EDO, 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	0.36	1/2612 (0.0%)	0.53	2/3549 (0.1%)
1	B	0.32	0/2585	0.49	0/3518
1	C	0.32	0/2692	0.50	0/3649
1	D	0.30	0/2607	0.50	0/3541
1	E	0.36	0/2564	0.70	9/3489 (0.3%)
1	F	0.36	1/2593 (0.0%)	0.57	6/3527 (0.2%)
1	G	0.35	1/2553 (0.0%)	0.60	6/3474 (0.2%)
1	H	0.36	1/2583 (0.0%)	0.72	9/3515 (0.3%)
1	I	0.31	1/2522 (0.0%)	0.58	5/3438 (0.1%)
1	J	0.28	0/2575	0.53	2/3505 (0.1%)
1	K	0.31	0/2576	0.67	9/3506 (0.3%)
1	L	0.31	2/2475 (0.1%)	0.55	3/3382 (0.1%)
All	All	0.33	7/30937 (0.0%)	0.58	51/42093 (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	E	0	2
1	G	0	1
1	I	0	1
1	K	0	1
1	L	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	318	GLU	CD-OE2	6.43	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	7	LYS	CE-NZ	-6.38	1.30	1.49
1	I	244	SER	N-CA	5.91	1.55	1.45
1	A	329	LYS	CB-CG	5.91	1.70	1.52
1	L	83	GLU	CD-OE2	5.50	1.35	1.25

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	318	GLU	CA-CB-CG	19.73	153.56	114.10
1	J	36	LYS	CG-CD-CE	-15.29	76.14	111.30
1	K	167	LYS	CB-CG-CD	14.12	143.79	111.30
1	E	140	SER	CA-C-N	11.22	141.05	122.54
1	E	140	SER	C-N-CA	11.22	141.05	122.54

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	141	ASN	Sidechain
1	E	27	GLU	Sidechain
1	G	318	GLU	Sidechain
1	I	231	GLU	Sidechain
1	K	139	LYS	Peptide

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	2548	0	2552	18	0
1	B	2524	0	2511	18	0
1	C	2610	0	2684	25	0
1	D	2549	0	2566	17	0
1	E	2506	0	2488	33	0
1	F	2532	0	2522	21	0
1	G	2501	0	2485	20	0
1	H	2525	0	2525	16	0
1	I	2470	0	2417	26	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2517	0	2498	20	0
1	K	2518	0	2498	23	0
1	L	2423	0	2316	16	0
2	A	48	0	72	3	0
2	B	28	0	42	2	0
2	C	48	0	72	8	0
2	D	32	0	48	2	0
2	E	36	0	54	4	0
2	F	40	0	60	4	0
2	G	28	0	42	3	0
2	H	24	0	36	3	1
2	I	24	0	36	3	0
2	J	28	0	42	2	0
2	K	16	0	24	0	0
2	L	12	0	18	0	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	0	0
3	D	44	0	26	2	0
3	E	44	0	26	0	0
3	F	44	0	26	0	0
3	G	44	0	26	1	0
3	H	44	0	26	1	0
3	I	44	0	26	1	0
3	J	44	0	26	1	0
3	K	44	0	26	1	0
3	L	44	0	26	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	231	0	0	5	0
6	B	238	0	0	3	0
6	C	284	0	0	2	0
6	D	221	0	0	1	0
6	E	197	0	0	1	0
6	F	210	0	0	4	0
6	G	197	0	0	1	0
6	H	198	0	0	1	0
6	I	90	0	0	1	0
6	J	157	0	0	0	0
6	K	149	0	0	1	0
6	L	70	0	0	1	0
All	All	33393	0	30920	221	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 4.

The worst 5 of 221 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:E:6:MET:CE	1:E:8:ALA:HB2	1.77	1.15
1:G:316:LYS:NZ	1:G:318:GLU:OE2	1.93	1.01
1:E:6:MET:HE1	1:E:125:ALA:HB1	1.44	0.99
1:A:36:LYS:NZ	6:A:501:HOH:O	1.98	0.97
1:E:6:MET:HE1	1:E:8:ALA:HB2	1.49	0.92

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)
1:I:220:LYS:NZ	2:H:706:EDO:O2[1_656]	1.30	0.90

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/353 (98%)	335 (97%)	9 (3%)	1 (0%)	36	36
1	B	344/353 (98%)	333 (97%)	10 (3%)	1 (0%)	36	36
1	C	353/353 (100%)	342 (97%)	10 (3%)	1 (0%)	36	36
1	D	344/353 (98%)	333 (97%)	10 (3%)	1 (0%)	36	36
1	E	341/353 (97%)	331 (97%)	9 (3%)	1 (0%)	36	36
1	F	345/353 (98%)	335 (97%)	9 (3%)	1 (0%)	36	36
1	G	339/353 (96%)	328 (97%)	10 (3%)	1 (0%)	36	36
1	H	343/353 (97%)	333 (97%)	9 (3%)	1 (0%)	36	36
1	I	340/353 (96%)	329 (97%)	10 (3%)	1 (0%)	36	36
1	J	344/353 (98%)	332 (96%)	11 (3%)	1 (0%)	36	36
1	K	343/353 (97%)	332 (97%)	9 (3%)	2 (1%)	21	18
1	L	339/353 (96%)	327 (96%)	11 (3%)	1 (0%)	36	36
All	All	4120/4236 (97%)	3990 (97%)	117 (3%)	13 (0%)	36	36

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	140	SER
1	A	290	VAL
1	B	290	VAL
1	C	290	VAL
1	D	290	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/278 (96%)	267 (100%)	0	100	100
1	B	261/278 (94%)	261 (100%)	0	100	100
1	C	278/278 (100%)	274 (99%)	4 (1%)	59	67
1	D	266/278 (96%)	266 (100%)	0	100	100
1	E	258/278 (93%)	258 (100%)	0	100	100
1	F	261/278 (94%)	261 (100%)	0	100	100
1	G	258/278 (93%)	258 (100%)	0	100	100
1	H	262/278 (94%)	262 (100%)	0	100	100
1	I	247/278 (89%)	247 (100%)	0	100	100
1	J	258/278 (93%)	258 (100%)	0	100	100
1	K	259/278 (93%)	259 (100%)	0	100	100
1	L	235/278 (84%)	235 (100%)	0	100	100
All	All	3110/3336 (93%)	3106 (100%)	4 (0%)	88	93

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

Mol	Chain	Res	Type
1	C	217[A]	VAL
1	C	217[B]	VAL
1	C	340[A]	ILE
1	C	340[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	264	ASN
1	L	304	ASN
1	G	331	GLN
1	K	264	ASN
1	G	264	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 139 ligands modelled in this entry, 36 are monoatomic - leaving 103 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	EDO	I	404	-	3,3,3	0.35	0	2,2,2	0.42	0
2	EDO	H	707	-	3,3,3	0.43	0	2,2,2	0.30	0
2	EDO	C	409	-	3,3,3	0.43	0	2,2,2	0.43	0
2	EDO	E	408	-	3,3,3	0.46	0	2,2,2	0.59	0
2	EDO	K	404	-	3,3,3	0.49	0	2,2,2	0.22	0
2	EDO	C	413	-	3,3,3	0.60	0	2,2,2	0.07	0
3	NAD	I	402	-	46,48,48	0.37	0	64,73,73	0.56	1 (1%)
2	EDO	C	406	-	3,3,3	0.54	0	2,2,2	0.08	0
2	EDO	J	403	-	3,3,3	0.41	0	2,2,2	0.52	0
2	EDO	C	407	-	3,3,3	0.45	0	2,2,2	0.47	0
2	EDO	A	406	-	3,3,3	0.35	0	2,2,2	0.87	0
2	EDO	D	505	-	3,3,3	0.39	0	2,2,2	0.54	0
2	EDO	I	403	-	3,3,3	0.43	0	2,2,2	0.43	0
3	NAD	E	402	-	46,48,48	0.36	0	64,73,73	0.61	2 (3%)
2	EDO	A	409[A]	-	3,3,3	0.49	0	2,2,2	0.24	0
2	EDO	D	507	-	3,3,3	0.46	0	2,2,2	0.38	0
2	EDO	E	410	-	3,3,3	0.38	0	2,2,2	0.28	0
2	EDO	E	405	-	3,3,3	0.46	0	2,2,2	0.28	0
2	EDO	I	405	-	3,3,3	0.46	0	2,2,2	0.31	0
3	NAD	L	402	-	46,48,48	0.32	0	64,73,73	0.59	2 (3%)
2	EDO	H	705	-	3,3,3	0.45	0	2,2,2	0.19	0
2	EDO	F	409	-	3,3,3	0.46	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	F	406	-	3,3,3	0.45	0	2,2,2	0.39	0
2	EDO	D	509	-	3,3,3	0.40	0	2,2,2	0.31	0
2	EDO	C	412	-	3,3,3	0.41	0	2,2,2	0.41	0
2	EDO	H	706	-	3,3,3	0.46	0	2,2,2	0.44	0
2	EDO	B	407	-	3,3,3	0.49	0	2,2,2	0.12	0
3	NAD	D	501	-	46,48,48	0.41	0	64,73,73	0.60	1 (1%)
2	EDO	J	406	-	3,3,3	0.38	0	2,2,2	0.63	0
2	EDO	J	405	-	3,3,3	0.51	0	2,2,2	0.15	0
3	NAD	G	501	-	46,48,48	0.37	0	64,73,73	0.58	1 (1%)
2	EDO	A	401	-	3,3,3	0.66	0	2,2,2	0.53	0
2	EDO	E	401	-	3,3,3	0.66	0	2,2,2	0.10	0
3	NAD	F	402	-	46,48,48	0.35	0	64,73,73	0.58	0
2	EDO	A	408	-	3,3,3	0.40	0	2,2,2	0.52	0
2	EDO	C	408	-	3,3,3	0.43	0	2,2,2	0.34	0
3	NAD	K	402	-	46,48,48	0.37	0	64,73,73	0.56	0
2	EDO	J	401	-	3,3,3	0.57	0	2,2,2	0.11	0
2	EDO	F	411	-	3,3,3	0.47	0	2,2,2	0.22	0
2	EDO	D	508	-	3,3,3	0.44	0	2,2,2	0.14	0
2	EDO	K	403	-	3,3,3	0.38	0	2,2,2	0.53	0
2	EDO	H	701	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EDO	G	503	-	3,3,3	0.39	0	2,2,2	0.39	0
3	NAD	J	402	-	46,48,48	0.36	0	64,73,73	0.60	1 (1%)
2	EDO	I	406	-	3,3,3	0.40	0	2,2,2	0.64	0
2	EDO	G	507	-	3,3,3	0.45	0	2,2,2	0.32	0
3	NAD	C	402	-	46,48,48	0.41	0	64,73,73	0.61	0
2	EDO	G	506	-	3,3,3	0.42	0	2,2,2	0.42	0
3	NAD	A	402	-	46,48,48	0.40	0	64,73,73	0.64	1 (1%)
2	EDO	A	403	-	3,3,3	0.45	0	2,2,2	0.34	0
2	EDO	D	504	-	3,3,3	0.73	0	2,2,2	0.26	0
2	EDO	C	410	-	3,3,3	0.43	0	2,2,2	0.40	0
2	EDO	E	403	-	3,3,3	0.39	0	2,2,2	0.49	0
2	EDO	D	502	-	3,3,3	0.45	0	2,2,2	0.26	0
2	EDO	F	407	-	3,3,3	0.44	0	2,2,2	0.19	0
2	EDO	D	506	-	3,3,3	0.44	0	2,2,2	0.32	0
2	EDO	F	401	-	3,3,3	0.58	0	2,2,2	0.19	0
2	EDO	G	504	-	3,3,3	0.47	0	2,2,2	0.33	0
2	EDO	I	401	-	3,3,3	0.62	0	2,2,2	0.14	0
2	EDO	F	404	-	3,3,3	0.36	0	2,2,2	0.72	0
2	EDO	C	401	-	3,3,3	0.68	0	2,2,2	0.50	0
2	EDO	F	403	-	3,3,3	0.44	0	2,2,2	0.49	0
2	EDO	J	407	-	3,3,3	0.43	0	2,2,2	0.58	0
2	EDO	L	404	-	3,3,3	0.42	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	E	406	-	3,3,3	0.39	0	2,2,2	0.51	0
2	EDO	L	401	-	3,3,3	0.54	0	2,2,2	0.11	0
2	EDO	A	405	-	3,3,3	0.50	0	2,2,2	0.34	0
3	NAD	B	402	-	46,48,48	0.34	0	64,73,73	0.57	0
2	EDO	E	404	-	3,3,3	0.38	0	2,2,2	0.51	0
2	EDO	A	412	-	3,3,3	0.35	0	2,2,2	0.80	0
2	EDO	H	704	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	E	409	-	3,3,3	0.34	0	2,2,2	0.72	0
2	EDO	C	404	-	3,3,3	0.34	0	2,2,2	0.66	0
2	EDO	C	403	-	3,3,3	0.47	0	2,2,2	0.41	0
2	EDO	D	503	-	3,3,3	0.45	0	2,2,2	0.42	0
2	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	A	409[B]	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	F	410	-	3,3,3	0.50	0	2,2,2	0.18	0
2	EDO	B	405	-	3,3,3	0.41	0	2,2,2	0.52	0
2	EDO	F	405	-	3,3,3	0.48	0	2,2,2	0.18	0
2	EDO	K	401	-	3,3,3	0.53	0	2,2,2	0.25	0
2	EDO	G	502	-	3,3,3	0.41	0	2,2,2	0.42	0
2	EDO	J	408	-	3,3,3	0.41	0	2,2,2	0.52	0
2	EDO	K	405	-	3,3,3	0.42	0	2,2,2	0.52	0
3	NAD	H	703	-	46,48,48	0.34	0	64,73,73	0.56	1 (1%)
2	EDO	L	403	-	3,3,3	0.41	0	2,2,2	0.38	0
2	EDO	C	411	-	3,3,3	0.43	0	2,2,2	0.28	0
2	EDO	B	403	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	C	405	-	3,3,3	0.47	0	2,2,2	0.33	0
2	EDO	A	411	-	3,3,3	0.45	0	2,2,2	0.45	0
2	EDO	H	702	-	3,3,3	0.66	0	2,2,2	0.16	0
2	EDO	B	401	-	3,3,3	0.55	0	2,2,2	0.17	0
2	EDO	J	404	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	B	406	-	3,3,3	0.37	0	2,2,2	0.66	0
2	EDO	A	407	-	3,3,3	0.49	0	2,2,2	0.26	0
2	EDO	F	408	-	3,3,3	0.39	0	2,2,2	0.56	0
2	EDO	E	407	-	3,3,3	0.46	0	2,2,2	0.21	0
2	EDO	I	407	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	A	410	-	3,3,3	0.46	0	2,2,2	0.35	0
2	EDO	G	508	-	3,3,3	0.40	0	2,2,2	0.61	0
2	EDO	B	404	-	3,3,3	0.38	0	2,2,2	0.55	0
2	EDO	G	505	-	3,3,3	0.44	0	2,2,2	0.39	0
2	EDO	B	408	-	3,3,3	0.46	0	2,2,2	0.46	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	EDO	I	404	-	-	1/1/1/1	-
2	EDO	H	707	-	-	0/1/1/1	-
2	EDO	C	409	-	-	0/1/1/1	-
2	EDO	E	408	-	-	1/1/1/1	-
2	EDO	K	404	-	-	0/1/1/1	-
2	EDO	C	413	-	-	1/1/1/1	-
3	NAD	I	402	-	-	4/30/62/62	0/5/5/5
2	EDO	C	406	-	-	1/1/1/1	-
2	EDO	J	403	-	-	1/1/1/1	-
2	EDO	C	407	-	-	0/1/1/1	-
2	EDO	A	406	-	-	1/1/1/1	-
2	EDO	D	505	-	-	0/1/1/1	-
2	EDO	I	403	-	-	0/1/1/1	-
3	NAD	E	402	-	-	6/30/62/62	0/5/5/5
2	EDO	A	409[A]	-	-	0/1/1/1	-
2	EDO	D	507	-	-	0/1/1/1	-
2	EDO	E	410	-	-	0/1/1/1	-
2	EDO	E	405	-	-	0/1/1/1	-
2	EDO	I	405	-	-	0/1/1/1	-
3	NAD	L	402	-	-	4/30/62/62	0/5/5/5
2	EDO	H	705	-	-	0/1/1/1	-
2	EDO	F	409	-	-	0/1/1/1	-
2	EDO	F	406	-	-	0/1/1/1	-
2	EDO	D	509	-	-	0/1/1/1	-
2	EDO	C	412	-	-	1/1/1/1	-
2	EDO	H	706	-	-	0/1/1/1	-
2	EDO	B	407	-	-	0/1/1/1	-
3	NAD	D	501	-	-	4/30/62/62	0/5/5/5
2	EDO	J	406	-	-	1/1/1/1	-
2	EDO	J	405	-	-	1/1/1/1	-
3	NAD	G	501	-	-	5/30/62/62	0/5/5/5
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	E	401	-	-	0/1/1/1	-
3	NAD	F	402	-	-	5/30/62/62	0/5/5/5
2	EDO	A	408	-	-	0/1/1/1	-
2	EDO	C	408	-	-	0/1/1/1	-
3	NAD	K	402	-	-	5/30/62/62	0/5/5/5
2	EDO	J	401	-	-	0/1/1/1	-
2	EDO	F	411	-	-	0/1/1/1	-
2	EDO	D	508	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	K	403	-	-	1/1/1/1	-
2	EDO	H	701	-	-	0/1/1/1	-
2	EDO	G	503	-	-	0/1/1/1	-
3	NAD	J	402	-	-	5/30/62/62	0/5/5/5
2	EDO	I	406	-	-	1/1/1/1	-
2	EDO	G	507	-	-	0/1/1/1	-
3	NAD	C	402	-	-	5/30/62/62	0/5/5/5
2	EDO	G	506	-	-	0/1/1/1	-
3	NAD	A	402	-	-	4/30/62/62	0/5/5/5
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	D	504	-	-	0/1/1/1	-
2	EDO	C	410	-	-	0/1/1/1	-
2	EDO	E	403	-	-	0/1/1/1	-
2	EDO	D	502	-	-	0/1/1/1	-
2	EDO	F	407	-	-	0/1/1/1	-
2	EDO	D	506	-	-	0/1/1/1	-
2	EDO	F	401	-	-	0/1/1/1	-
2	EDO	G	504	-	-	1/1/1/1	-
2	EDO	I	401	-	-	0/1/1/1	-
2	EDO	F	404	-	-	0/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	F	403	-	-	0/1/1/1	-
2	EDO	J	407	-	-	1/1/1/1	-
2	EDO	L	404	-	-	1/1/1/1	-
2	EDO	E	406	-	-	1/1/1/1	-
2	EDO	L	401	-	-	0/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-
3	NAD	B	402	-	-	5/30/62/62	0/5/5/5
2	EDO	E	404	-	-	0/1/1/1	-
2	EDO	A	412	-	-	1/1/1/1	-
2	EDO	H	704	-	-	0/1/1/1	-
2	EDO	E	409	-	-	0/1/1/1	-
2	EDO	C	404	-	-	0/1/1/1	-
2	EDO	C	403	-	-	1/1/1/1	-
2	EDO	D	503	-	-	0/1/1/1	-
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	A	409[B]	-	-	0/1/1/1	-
2	EDO	F	410	-	-	0/1/1/1	-
2	EDO	B	405	-	-	0/1/1/1	-
2	EDO	F	405	-	-	0/1/1/1	-
2	EDO	K	401	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	G	502	-	-	0/1/1/1	-
2	EDO	J	408	-	-	1/1/1/1	-
2	EDO	K	405	-	-	0/1/1/1	-
3	NAD	H	703	-	-	5/30/62/62	0/5/5/5
2	EDO	L	403	-	-	1/1/1/1	-
2	EDO	C	411	-	-	0/1/1/1	-
2	EDO	B	403	-	-	0/1/1/1	-
2	EDO	C	405	-	-	0/1/1/1	-
2	EDO	A	411	-	-	1/1/1/1	-
2	EDO	H	702	-	-	0/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	J	404	-	-	1/1/1/1	-
2	EDO	B	406	-	-	1/1/1/1	-
2	EDO	A	407	-	-	0/1/1/1	-
2	EDO	F	408	-	-	0/1/1/1	-
2	EDO	E	407	-	-	0/1/1/1	-
2	EDO	I	407	-	-	1/1/1/1	-
2	EDO	A	410	-	-	0/1/1/1	-
2	EDO	G	508	-	-	0/1/1/1	-
2	EDO	B	404	-	-	0/1/1/1	-
2	EDO	G	505	-	-	0/1/1/1	-
2	EDO	B	408	-	-	1/1/1/1	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	402	NAD	C2N-N1N-C1D	-2.32	114.02	119.13
3	E	402	NAD	C2N-N1N-C1D	-2.19	114.30	119.13
3	L	402	NAD	C6N-N1N-C1D	2.19	124.02	119.73
3	J	402	NAD	C2N-N1N-C1D	-2.19	114.31	119.13
3	D	501	NAD	C2N-N1N-C1D	-2.17	114.33	119.13

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAD	O4D-C1D-N1N-C2N
3	A	402	NAD	O4D-C1D-N1N-C6N
3	A	402	NAD	C2D-C1D-N1N-C2N
3	A	402	NAD	C2D-C1D-N1N-C6N

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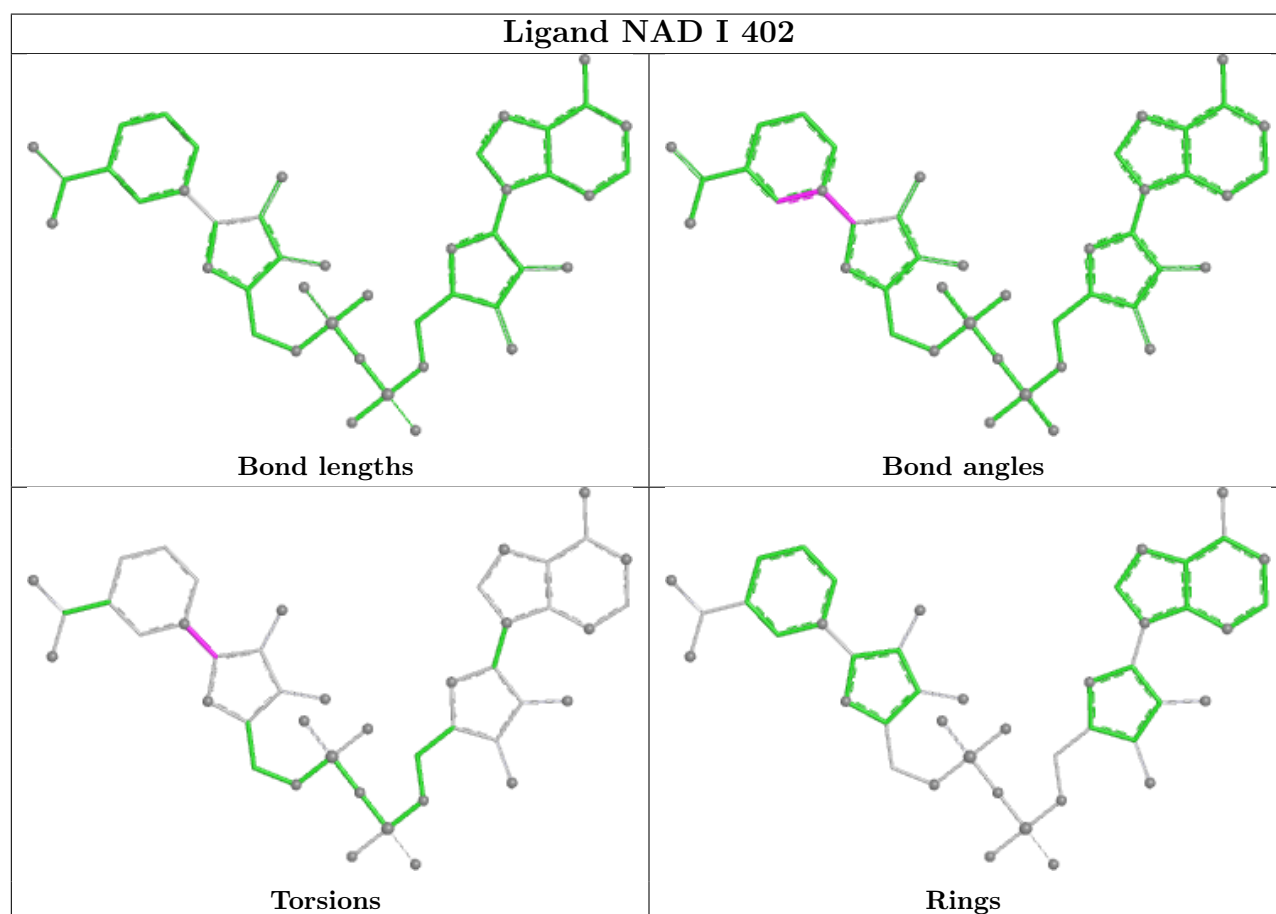
Mol	Chain	Res	Type	Atoms
3	B	402	NAD	O4D-C1D-N1N-C2N

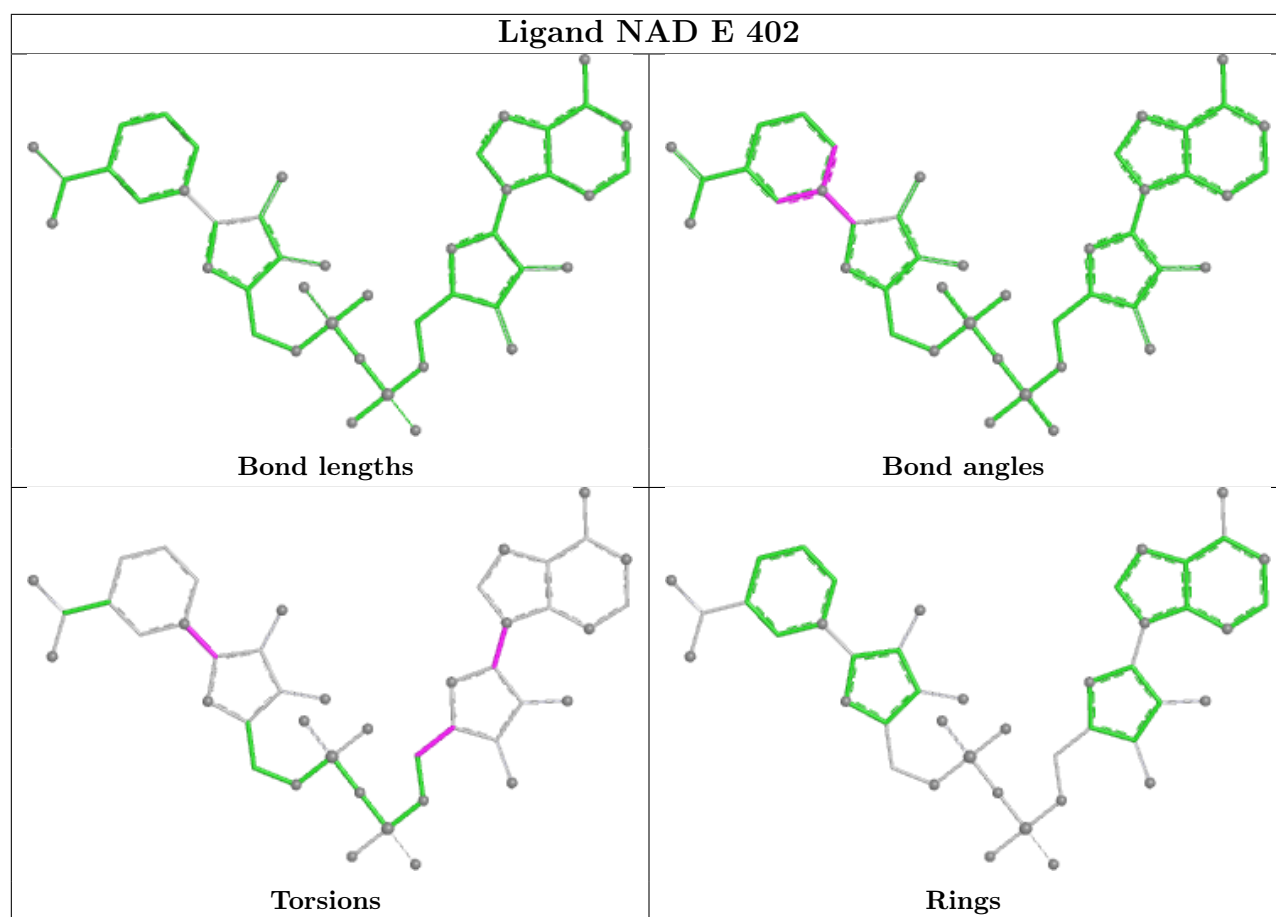
There are no ring outliers.

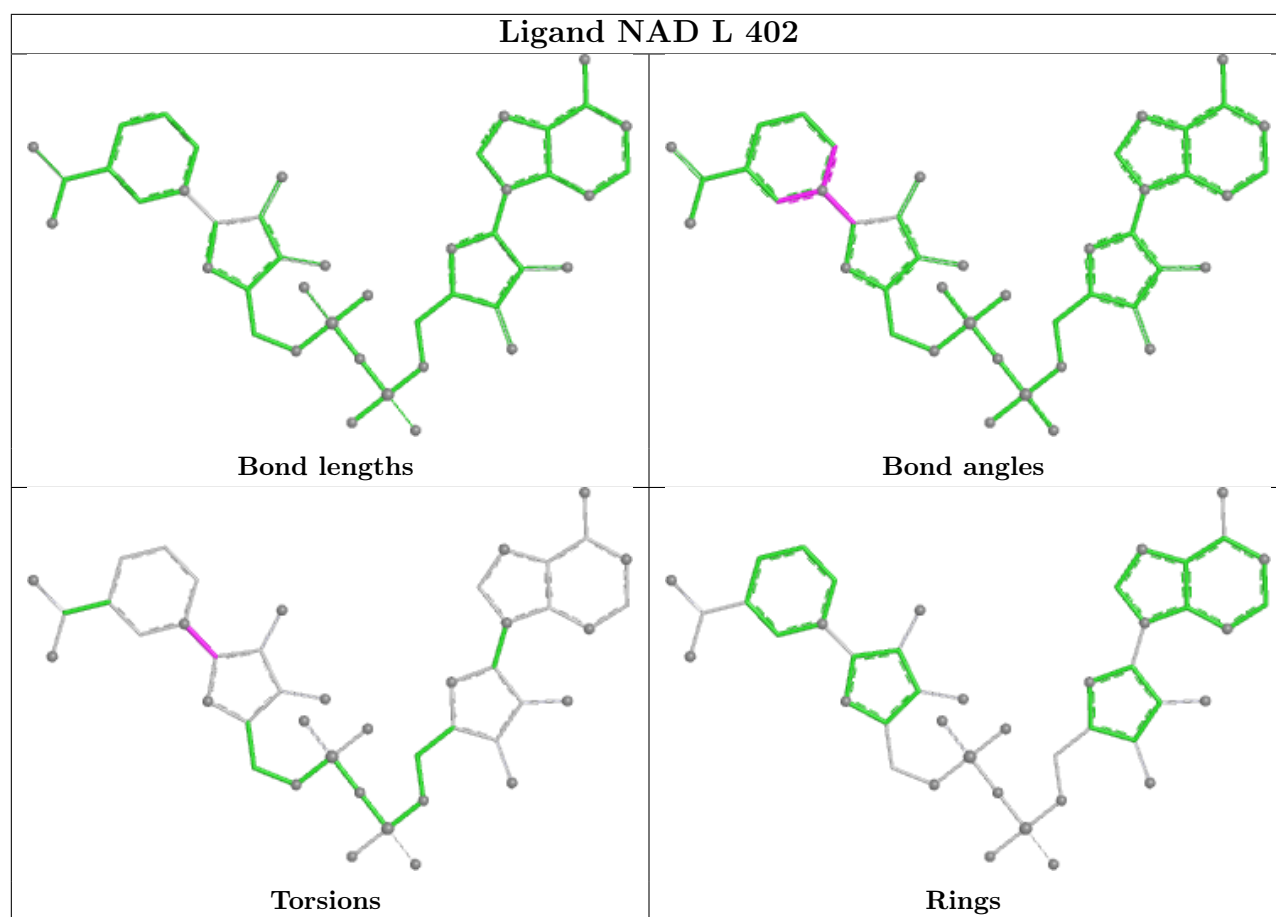
35 monomers are involved in 45 short contacts:

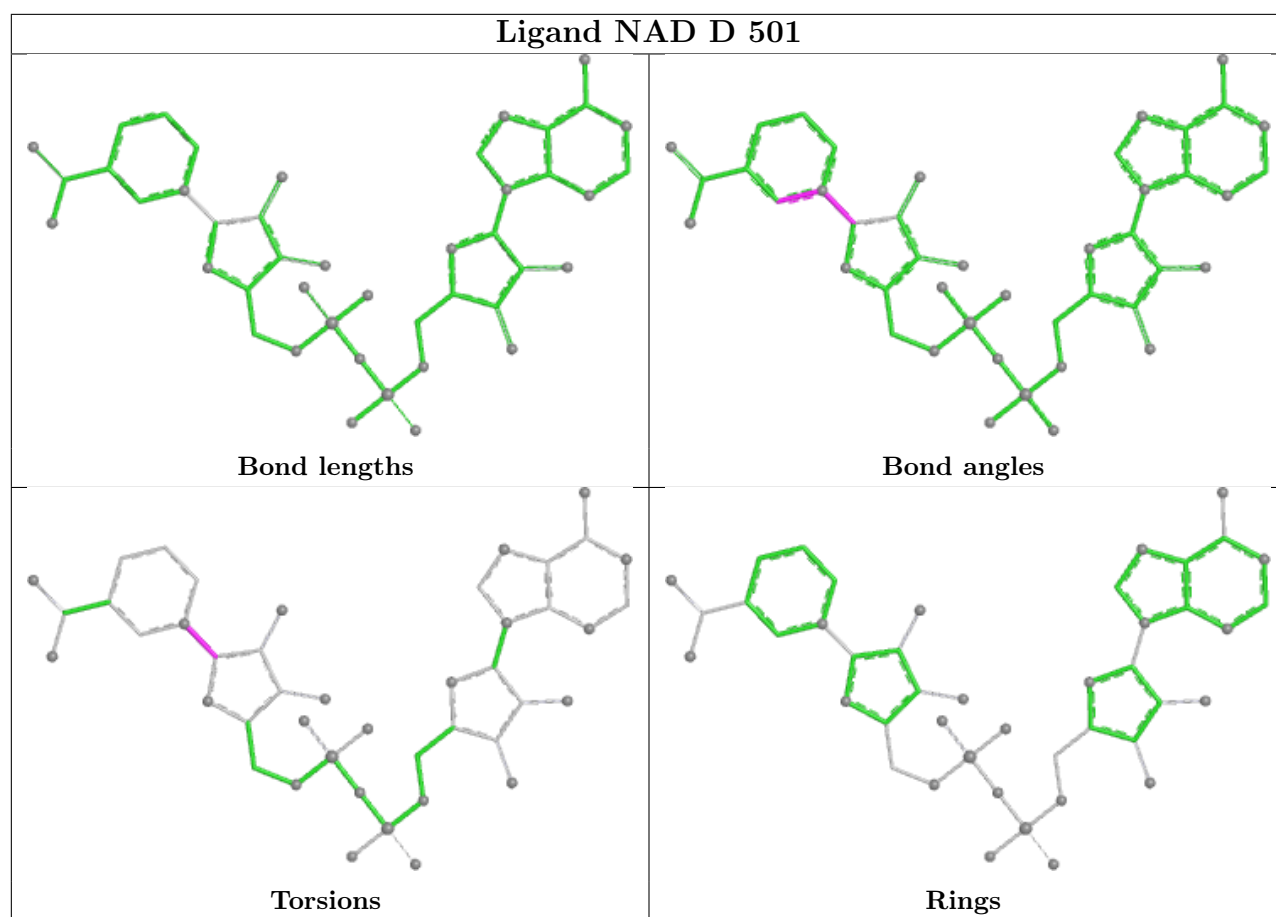
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	404	EDO	2	0
3	I	402	NAD	1	0
2	C	406	EDO	2	0
2	C	407	EDO	2	0
2	A	406	EDO	1	0
2	D	505	EDO	1	0
2	E	410	EDO	1	0
2	I	405	EDO	1	0
3	L	402	NAD	2	0
2	F	409	EDO	1	0
2	C	412	EDO	1	0
2	H	706	EDO	0	1
3	D	501	NAD	2	0
3	G	501	NAD	1	0
2	A	401	EDO	1	0
3	K	402	NAD	1	0
2	F	411	EDO	1	0
2	D	508	EDO	1	0
2	H	701	EDO	2	0
2	G	503	EDO	2	0
3	J	402	NAD	1	0
2	F	407	EDO	1	0
2	F	404	EDO	1	0
2	C	401	EDO	2	0
2	J	407	EDO	2	0
2	E	406	EDO	2	0
3	B	402	NAD	1	0
2	H	704	EDO	1	0
2	C	404	EDO	1	0
2	A	409[B]	EDO	1	0
3	H	703	NAD	1	0
2	B	403	EDO	1	0
2	E	407	EDO	1	0
2	G	508	EDO	1	0
2	B	404	EDO	1	0

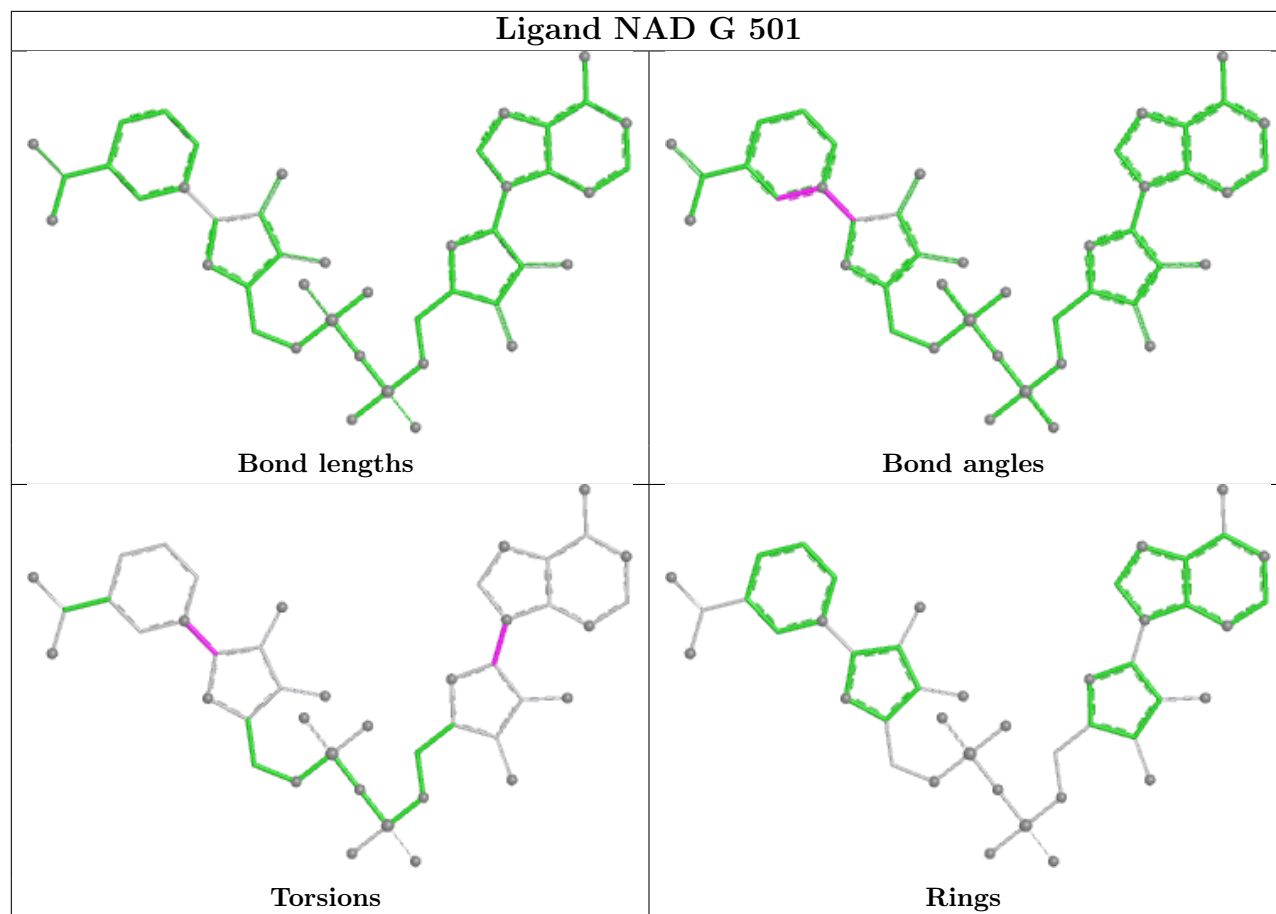
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

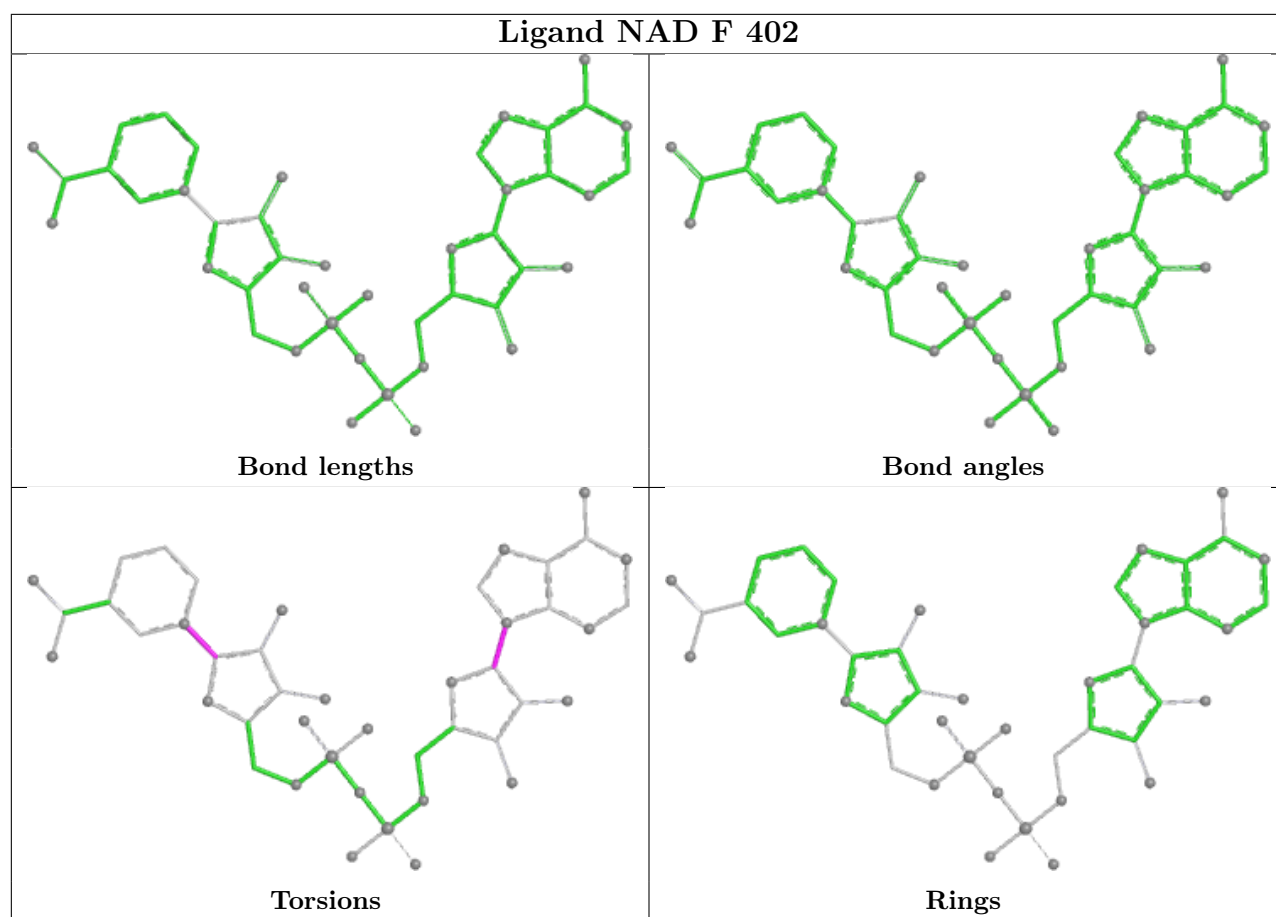


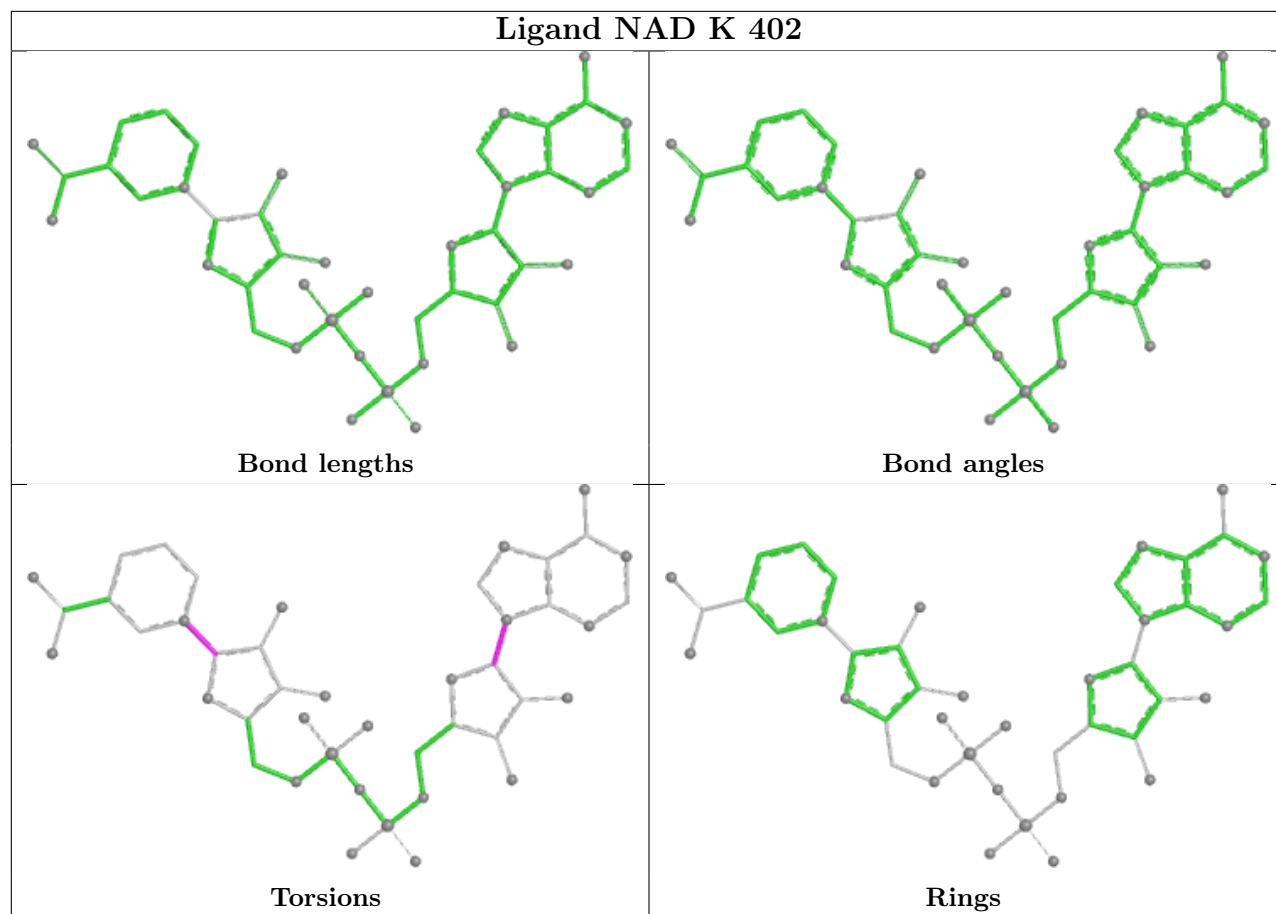


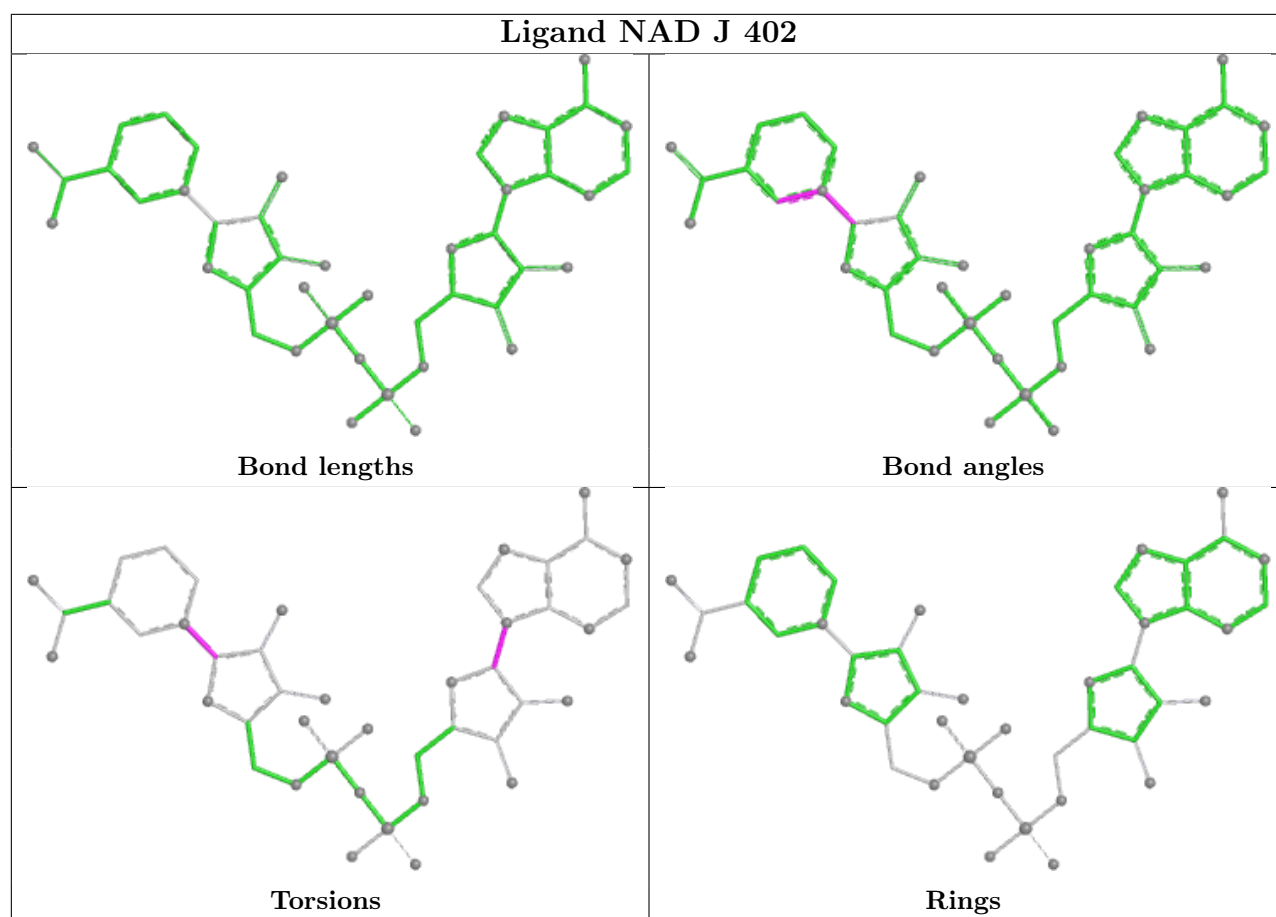


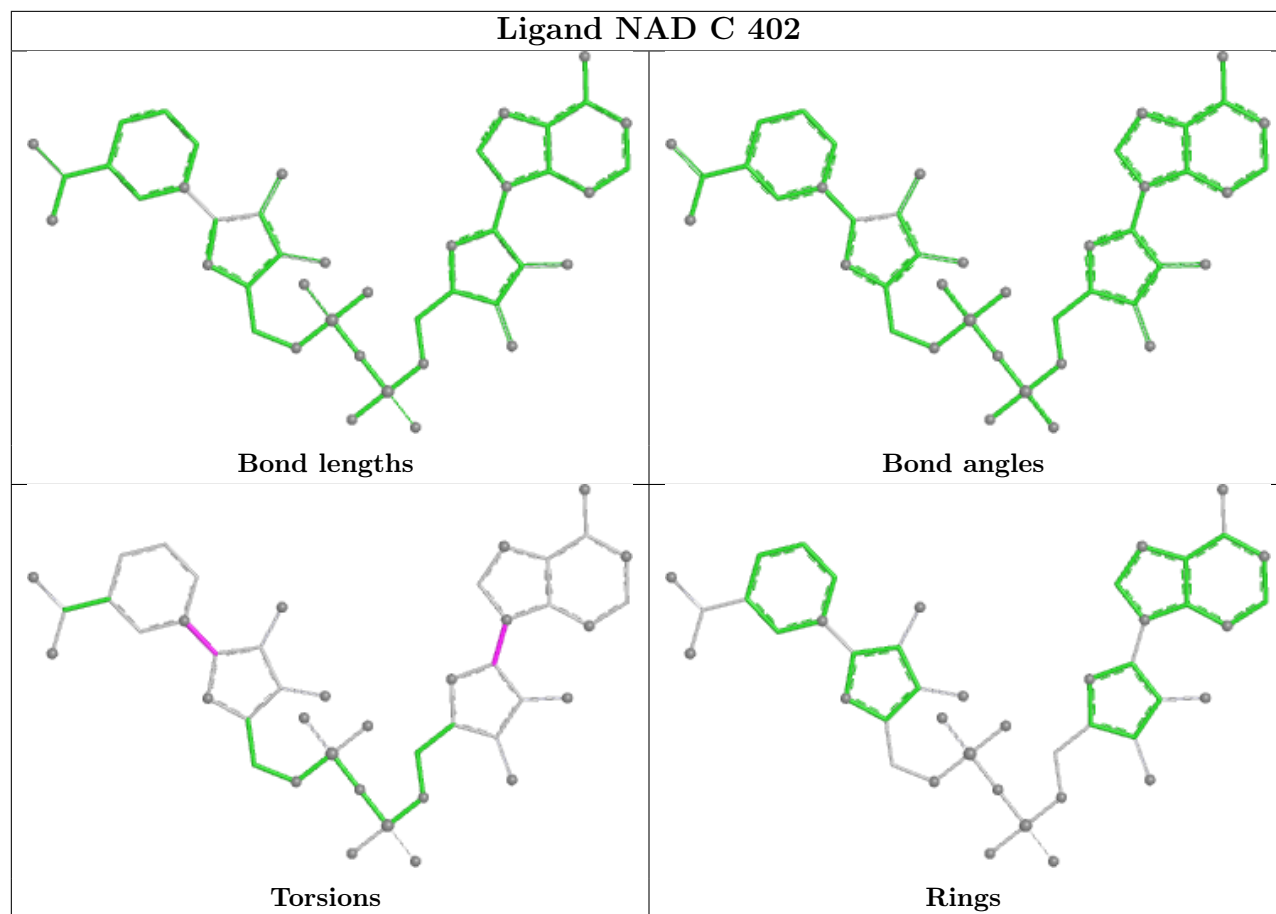


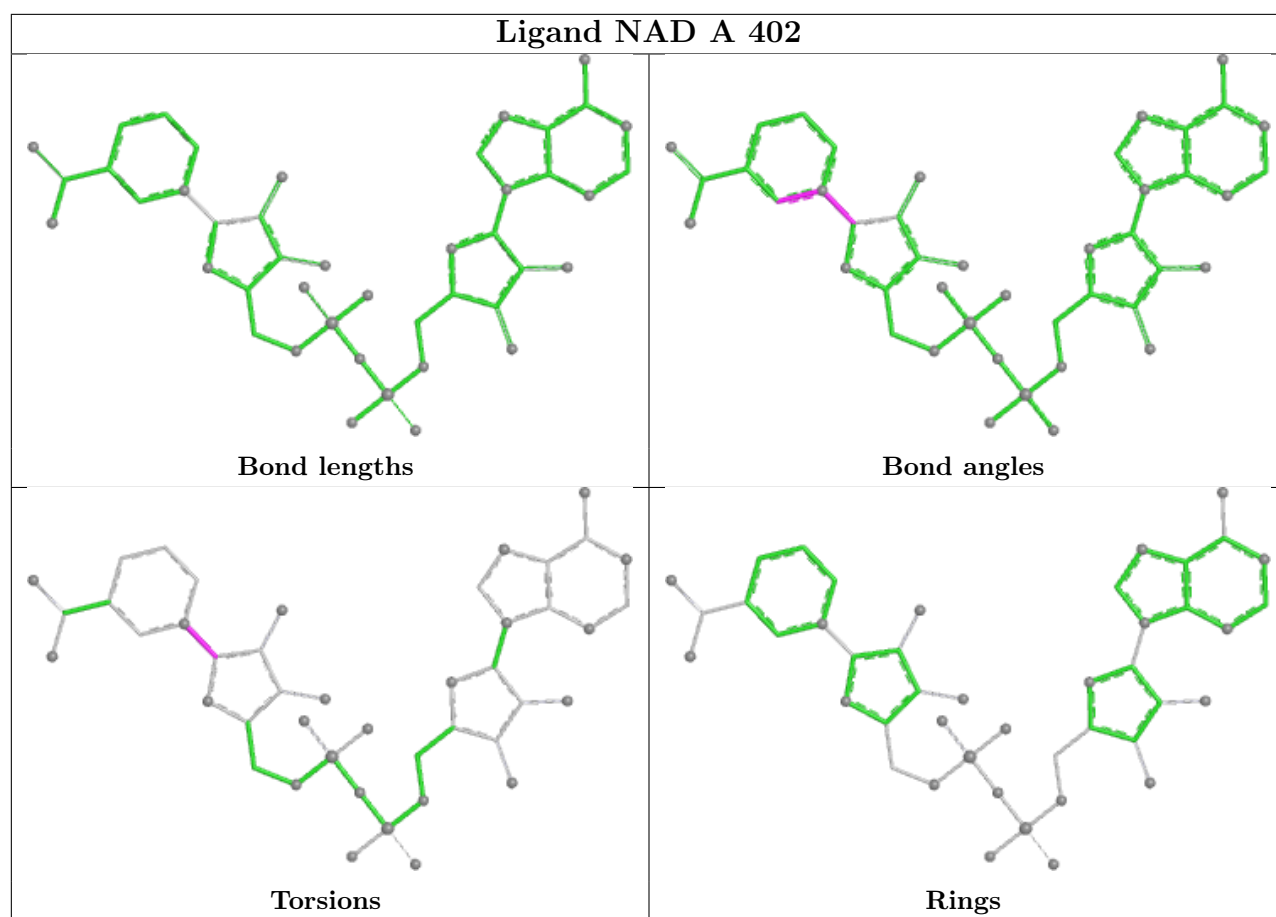


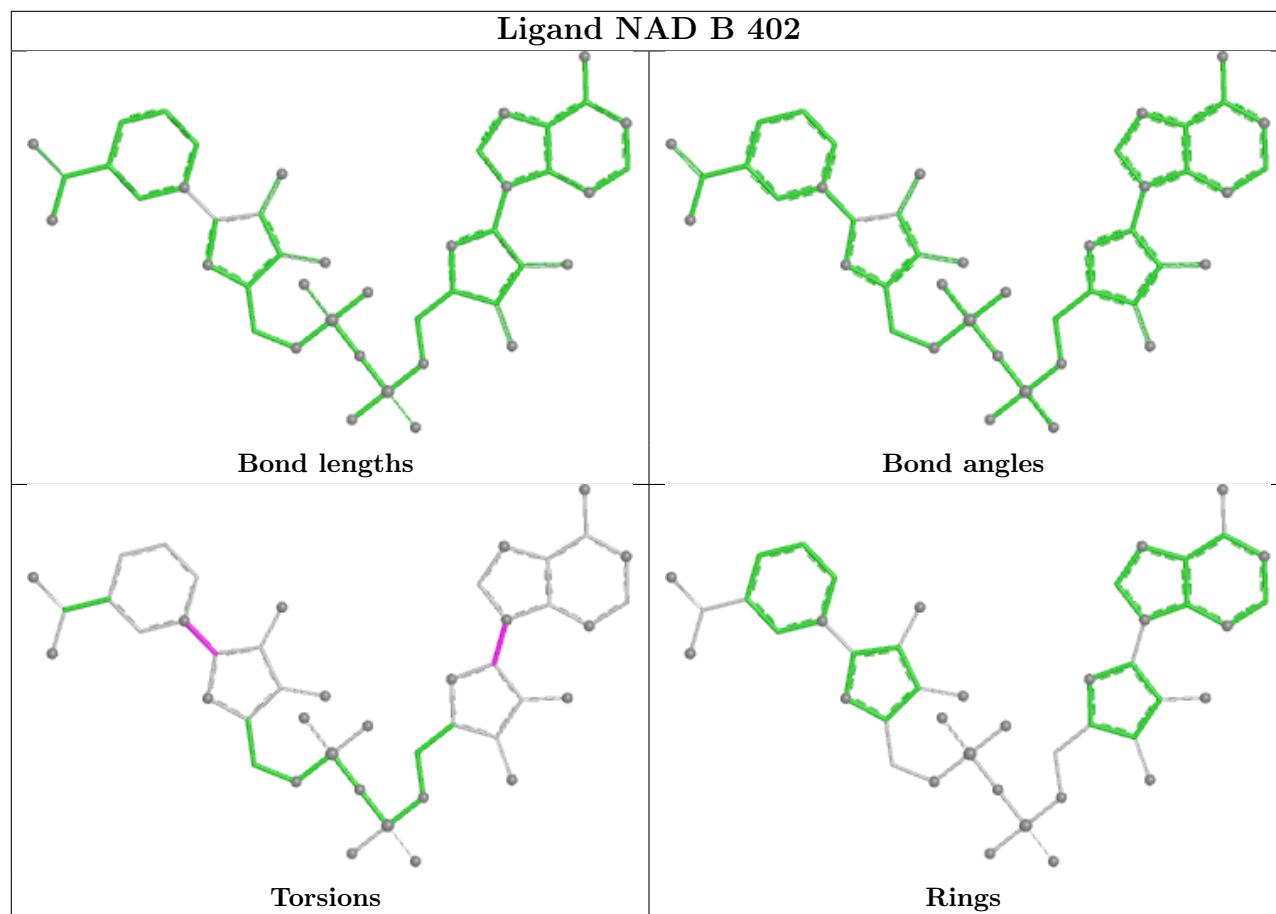


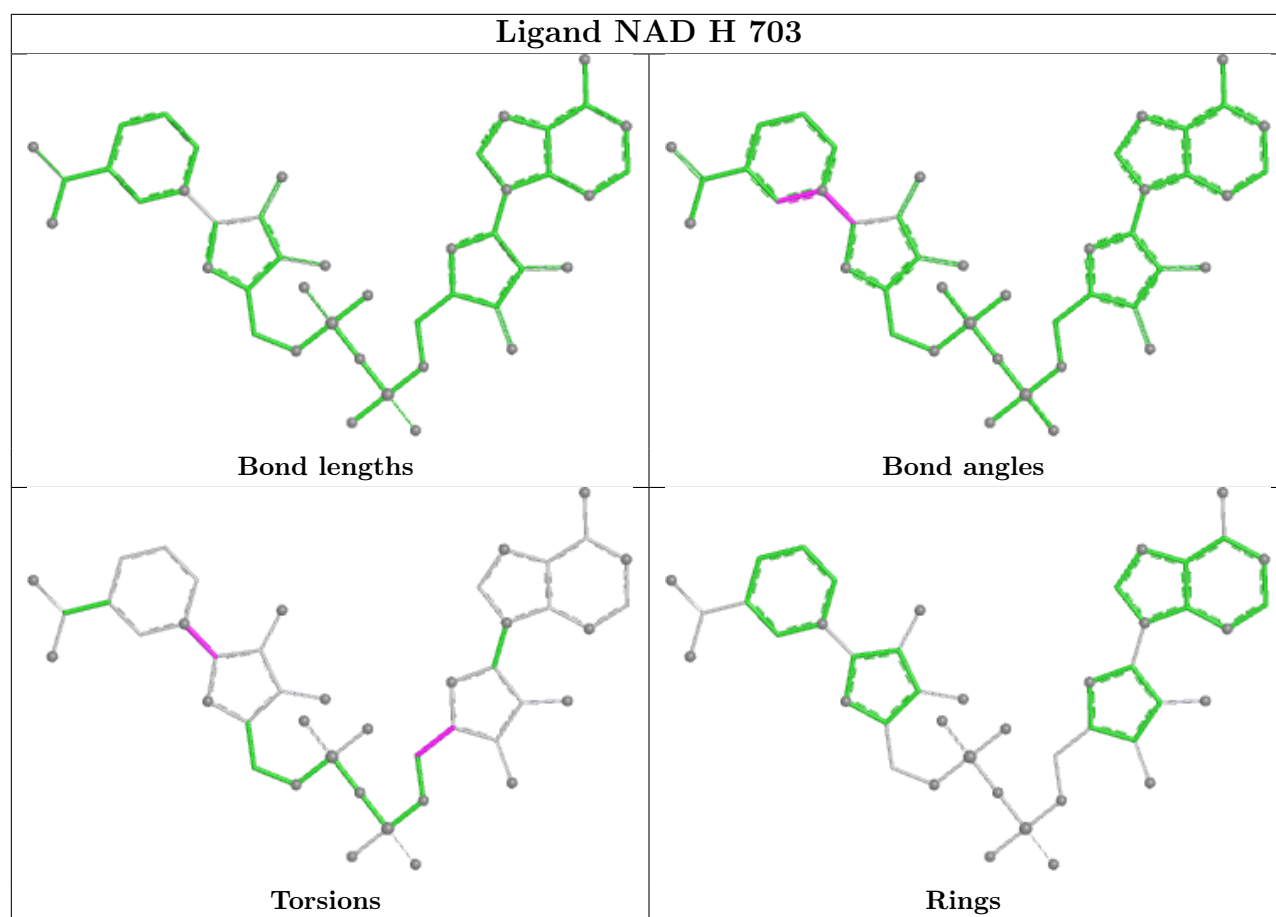












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	A	342/353 (96%)	-0.65	1 (0%) 90 91	18, 30, 54, 89	5 (1%)
1	B	342/353 (96%)	-0.63	3 (0%) 81 83	16, 30, 56, 89	4 (1%)
1	C	344/353 (97%)	-0.76	4 (1%) 76 78	14, 27, 43, 95	11 (3%)
1	D	343/353 (97%)	-0.59	2 (0%) 85 87	16, 31, 55, 91	3 (0%)
1	E	340/353 (96%)	-0.35	2 (0%) 85 87	15, 36, 77, 106	3 (0%)
1	F	343/353 (97%)	-0.58	2 (0%) 85 87	17, 33, 58, 86	4 (1%)
1	G	340/353 (96%)	-0.38	0 100 100	16, 36, 70, 83	1 (0%)
1	H	342/353 (96%)	-0.38	3 (0%) 81 83	18, 38, 64, 101	3 (0%)
1	I	341/353 (96%)	0.06	5 (1%) 72 74	29, 52, 87, 117	1 (0%)
1	J	343/353 (97%)	-0.37	3 (0%) 81 83	20, 40, 65, 86	3 (0%)
1	K	342/353 (96%)	-0.44	1 (0%) 90 91	21, 38, 62, 92	3 (0%)
1	L	340/353 (96%)	0.07	3 (0%) 81 83	32, 54, 89, 119	1 (0%)
All	All	4102/4236 (96%)	-0.42	29 (0%) 84 86	14, 36, 72, 119	42 (1%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	1	MET	3.9
1	D	1	MET	3.1
1	I	129	ILE	3.0
1	J	1	MET	2.9
1	H	341	ALA	2.9

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 ⓘ

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
2	EDO	G	504	4/4	0.78	0.16	64,65,67,69	0
2	EDO	C	407	4/4	0.81	0.16	48,50,52,56	0
2	EDO	I	407	4/4	0.82	0.14	65,65,68,69	0
2	EDO	J	405	4/4	0.82	0.21	60,62,63,63	0
2	EDO	C	413	4/4	0.83	0.15	46,48,54,57	0
2	EDO	C	408	4/4	0.84	0.16	56,59,62,64	0
2	EDO	I	405	4/4	0.84	0.17	66,67,68,68	0
2	EDO	D	507	4/4	0.84	0.12	58,66,71,73	0
2	EDO	F	409	4/4	0.84	0.14	49,58,64,64	0
2	EDO	C	405	4/4	0.85	0.15	50,51,55,63	0
2	EDO	F	401	4/4	0.85	0.15	42,44,48,50	0
2	EDO	J	401	4/4	0.85	0.15	45,47,50,61	0
2	EDO	G	508	4/4	0.85	0.12	46,47,47,47	0
2	EDO	J	408	4/4	0.85	0.20	55,67,73,73	0
2	EDO	A	409[B]	4/4	0.86	0.14	28,34,36,36	4
2	EDO	B	405	4/4	0.86	0.14	59,60,62,63	0
2	EDO	A	408	4/4	0.86	0.15	49,51,56,57	0
2	EDO	A	409[A]	4/4	0.86	0.14	28,33,36,36	4
2	EDO	G	507	4/4	0.87	0.13	71,72,73,76	0
2	EDO	E	405	4/4	0.87	0.20	54,58,58,64	0
2	EDO	E	407	4/4	0.87	0.16	68,69,72,72	0
2	EDO	A	411	4/4	0.87	0.13	59,66,70,74	0
2	EDO	D	504	4/4	0.87	0.14	32,37,41,43	0
2	EDO	G	502	4/4	0.87	0.20	58,59,61,67	0
2	EDO	J	406	4/4	0.87	0.16	65,67,68,76	0
2	EDO	J	407	4/4	0.87	0.13	50,51,56,61	0
2	EDO	B	403	4/4	0.87	0.14	48,48,57,57	0
2	EDO	I	401	4/4	0.88	0.12	41,45,46,48	0
2	EDO	I	404	4/4	0.88	0.17	56,56,65,67	0
2	EDO	C	406	4/4	0.88	0.19	44,49,52,64	0
2	EDO	I	406	4/4	0.88	0.14	56,56,57,57	0
2	EDO	F	410	4/4	0.88	0.13	53,58,63,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	D	509	4/4	0.88	0.15	61,64,72,76	0
2	EDO	E	408	4/4	0.88	0.11	44,48,55,63	0
2	EDO	E	401	4/4	0.88	0.13	30,39,42,46	0
2	EDO	F	408	4/4	0.88	0.20	68,69,69,74	0
2	EDO	H	702	4/4	0.88	0.13	37,41,43,44	0
2	EDO	A	410	4/4	0.89	0.15	63,66,69,72	0
2	EDO	A	405	4/4	0.89	0.17	43,44,52,55	0
2	EDO	C	401	4/4	0.89	0.12	32,35,35,35	0
2	EDO	C	412	4/4	0.89	0.13	57,60,61,64	0
2	EDO	G	505	4/4	0.89	0.11	47,49,50,52	0
2	EDO	C	403	4/4	0.89	0.12	43,45,47,52	0
2	EDO	D	502	4/4	0.89	0.12	45,48,49,50	0
2	EDO	A	412	4/4	0.89	0.16	55,57,58,64	0
2	EDO	D	506	4/4	0.89	0.12	53,57,58,59	0
2	EDO	K	405	4/4	0.89	0.10	51,54,63,69	0
2	EDO	L	404	4/4	0.89	0.14	51,52,53,61	0
2	EDO	E	409	4/4	0.90	0.15	50,51,58,59	0
2	EDO	B	406	4/4	0.90	0.16	60,60,62,63	0
2	EDO	H	707	4/4	0.90	0.11	51,55,59,65	0
2	EDO	G	503	4/4	0.90	0.20	36,42,47,57	0
2	EDO	I	403	4/4	0.90	0.17	65,65,68,76	0
2	EDO	J	403	4/4	0.90	0.10	63,64,64,66	0
2	EDO	H	701	4/4	0.91	0.12	50,54,56,59	0
2	EDO	E	403	4/4	0.91	0.13	47,55,57,60	0
2	EDO	A	404	4/4	0.91	0.10	57,59,59,62	0
2	EDO	K	403	4/4	0.91	0.09	52,53,54,58	0
2	EDO	J	404	4/4	0.91	0.13	67,69,69,72	0
2	EDO	L	401	4/4	0.91	0.12	40,49,54,55	0
2	EDO	L	403	4/4	0.91	0.15	58,59,60,65	0
2	EDO	F	403	4/4	0.91	0.11	47,48,51,54	0
2	EDO	A	403	4/4	0.92	0.12	40,50,50,53	0
2	EDO	B	408	4/4	0.92	0.12	46,50,55,58	0
2	EDO	E	404	4/4	0.92	0.10	40,48,50,54	0
2	EDO	K	401	4/4	0.92	0.13	40,41,51,57	0
2	EDO	D	508	4/4	0.92	0.12	40,52,56,59	0
2	EDO	K	404	4/4	0.92	0.12	38,48,49,52	0
2	EDO	H	704	4/4	0.92	0.10	52,53,55,57	0
2	EDO	F	407	4/4	0.92	0.11	49,53,53,54	0
2	EDO	D	505	4/4	0.92	0.13	50,54,55,57	0
2	EDO	G	506	4/4	0.92	0.10	63,68,71,74	0
5	CL	K	408	1/1	0.92	0.12	60,60,60,60	0
2	EDO	C	411	4/4	0.93	0.12	43,55,56,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	F	405	4/4	0.93	0.11	38,38,41,41	0
2	EDO	F	406	4/4	0.93	0.09	53,55,59,59	0
2	EDO	D	503	4/4	0.93	0.14	50,52,55,69	0
2	EDO	A	401	4/4	0.93	0.11	34,35,36,40	0
2	EDO	H	705	4/4	0.93	0.08	43,45,48,51	0
5	CL	F	414	1/1	0.93	0.10	56,56,56,56	0
5	CL	I	410	1/1	0.93	0.10	80,80,80,80	0
2	EDO	C	409	4/4	0.93	0.10	56,58,61,64	0
5	CL	L	407	1/1	0.93	0.10	64,64,64,64	0
2	EDO	B	401	4/4	0.94	0.10	33,47,51,54	0
2	EDO	E	410	4/4	0.94	0.14	35,36,43,51	0
2	EDO	H	706	4/4	0.94	0.09	50,51,54,55	0
2	EDO	F	411	4/4	0.94	0.14	40,45,47,47	0
2	EDO	B	404	4/4	0.95	0.11	23,28,43,55	0
2	EDO	A	406	4/4	0.95	0.13	26,39,44,56	0
5	CL	J	411	1/1	0.95	0.09	56,56,56,56	0
3	NAD	I	402	44/44	0.95	0.07	35,44,50,63	0
3	NAD	L	402	44/44	0.95	0.07	34,50,59,67	0
2	EDO	C	410	4/4	0.96	0.09	32,40,44,47	0
2	EDO	F	404	4/4	0.96	0.13	22,29,38,44	0
3	NAD	H	703	44/44	0.96	0.06	22,34,39,41	0
5	CL	G	511	1/1	0.96	0.09	54,54,54,54	0
5	CL	A	415	1/1	0.97	0.06	48,48,48,48	0
5	CL	B	411	1/1	0.97	0.08	49,49,49,49	0
5	CL	C	416	1/1	0.97	0.07	54,54,54,54	0
5	CL	D	512	1/1	0.97	0.06	53,53,53,53	0
5	CL	E	413	1/1	0.97	0.07	55,55,55,55	0
2	EDO	C	404	4/4	0.97	0.07	37,37,41,41	0
3	NAD	E	402	44/44	0.97	0.05	24,31,37,42	0
5	CL	H	710	1/1	0.97	0.09	54,54,54,54	0
3	NAD	G	501	44/44	0.97	0.06	22,31,36,37	0
2	EDO	E	406	4/4	0.97	0.07	21,30,42,43	0
2	EDO	B	407	4/4	0.97	0.06	27,35,38,39	0
2	EDO	A	407	4/4	0.97	0.06	31,36,38,39	0
3	NAD	D	501	44/44	0.98	0.04	19,28,31,32	0
4	ZN	I	408	1/1	0.98	0.04	50,50,50,50	0
4	ZN	I	409	1/1	0.98	0.13	70,70,70,70	0
4	ZN	L	405	1/1	0.98	0.04	57,57,57,57	0
3	NAD	A	402	44/44	0.98	0.04	18,25,30,31	0
3	NAD	F	402	44/44	0.98	0.05	19,28,32,37	0
3	NAD	J	402	44/44	0.98	0.05	22,34,40,44	0
3	NAD	K	402	44/44	0.98	0.05	21,31,38,39	0

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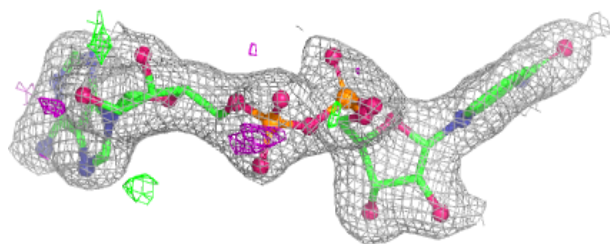
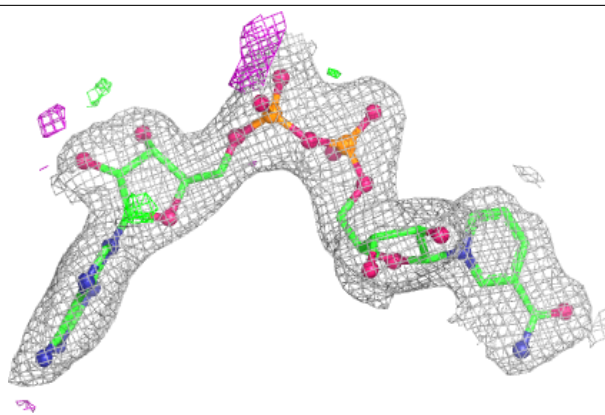
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	D	511	1/1	0.99	0.02	26,26,26,26	0
4	ZN	E	411	1/1	0.99	0.04	35,35,35,35	0
4	ZN	G	509	1/1	0.99	0.02	33,33,33,33	0
4	ZN	H	708	1/1	0.99	0.03	34,34,34,34	0
4	ZN	H	709	1/1	0.99	0.01	32,32,32,32	0
3	NAD	C	402	44/44	0.99	0.04	15,22,27,30	0
3	NAD	B	402	44/44	0.99	0.04	15,23,29,30	0
4	ZN	J	409	1/1	0.99	0.04	38,38,38,38	0
4	ZN	J	410	1/1	0.99	0.03	38,38,38,38	0
4	ZN	K	406	1/1	0.99	0.03	36,36,36,36	0
4	ZN	K	407	1/1	0.99	0.02	37,37,37,37	0
4	ZN	A	413	1/1	0.99	0.01	29,29,29,29	0
4	ZN	C	414	1/1	1.00	0.01	27,27,27,27	0
4	ZN	C	415	1/1	1.00	0.03	29,29,29,29	0
4	ZN	D	510	1/1	1.00	0.02	31,31,31,31	0
4	ZN	A	414	1/1	1.00	0.01	25,25,25,25	0
4	ZN	B	409	1/1	1.00	0.01	29,29,29,29	0
4	ZN	E	412	1/1	1.00	0.02	29,29,29,29	0
4	ZN	F	412	1/1	1.00	0.02	30,30,30,30	0
4	ZN	F	413	1/1	1.00	0.03	30,30,30,30	0
4	ZN	B	410	1/1	1.00	0.01	27,27,27,27	0
4	ZN	L	406	1/1	1.00	0.01	39,39,39,39	0
4	ZN	G	510	1/1	1.00	0.02	32,32,32,32	0

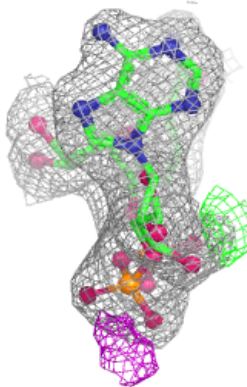
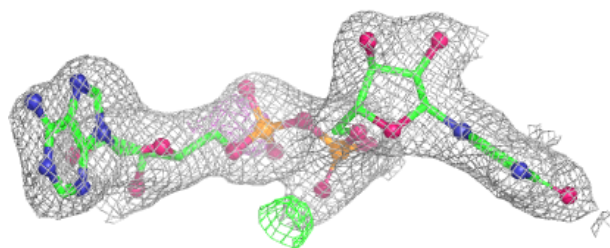
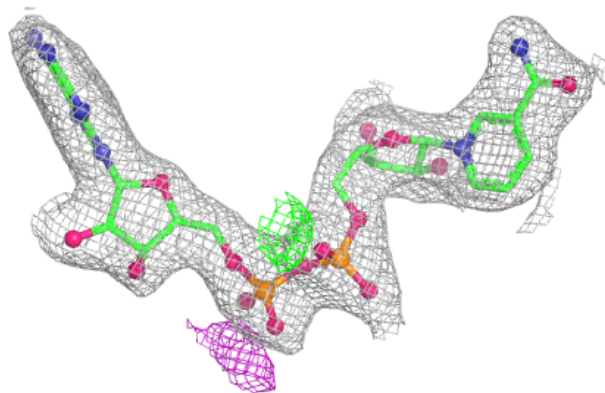
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD I 402:

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

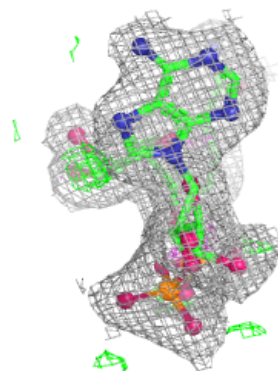
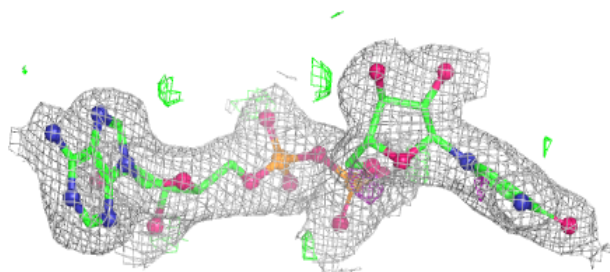
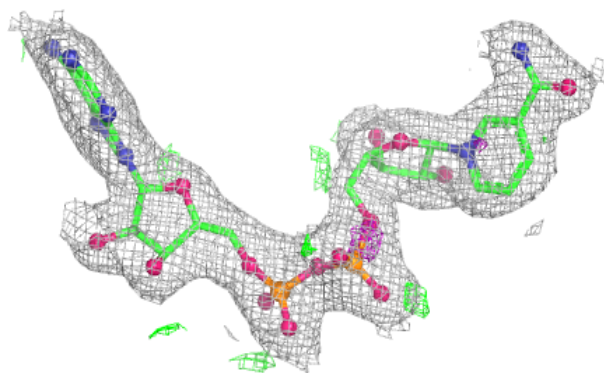
**Electron density around NAD L 402:**

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

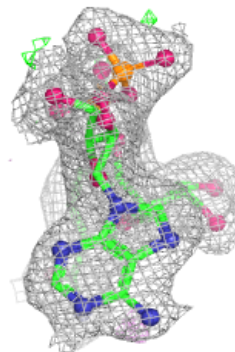
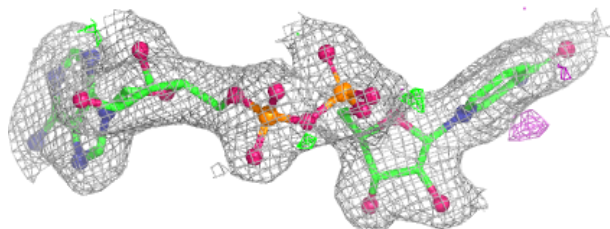
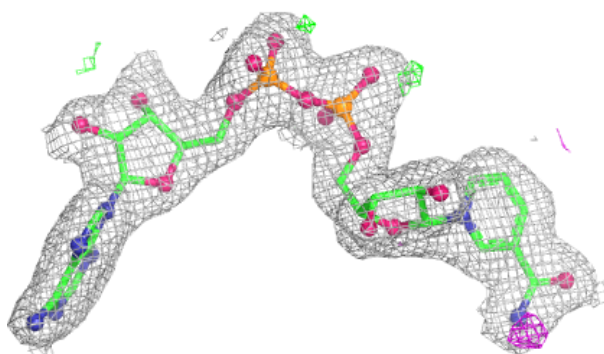


Electron density around NAD H 703:

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

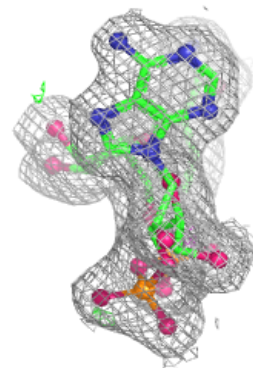
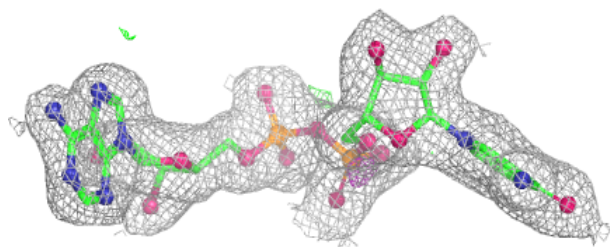
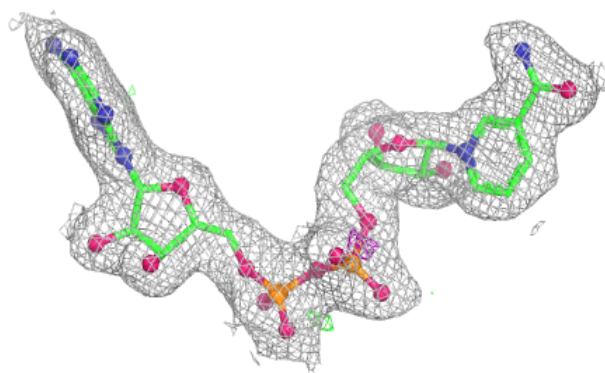
**Electron density around NAD E 402:**

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

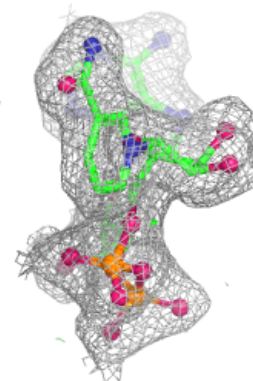
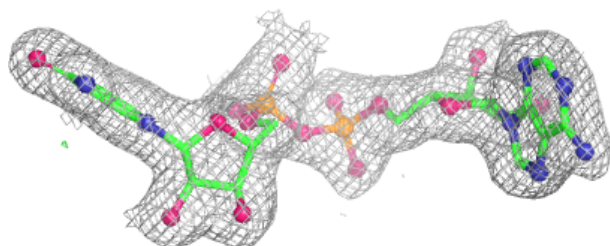
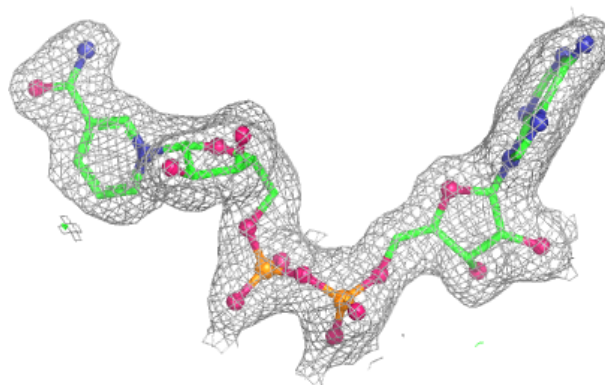


Electron density around NAD G 501:

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

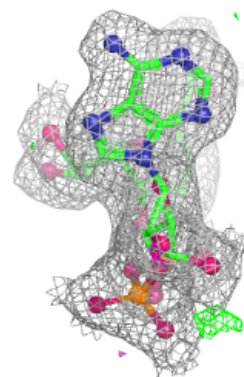
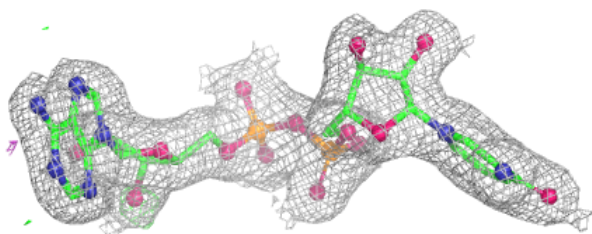
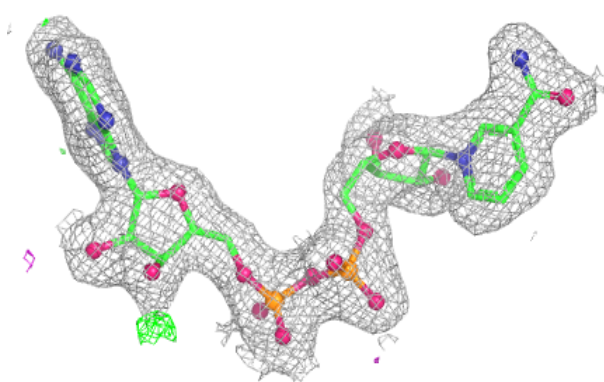
**Electron density around NAD D 501:**

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

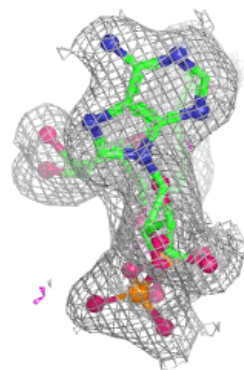
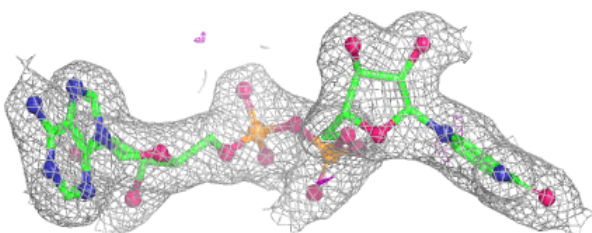
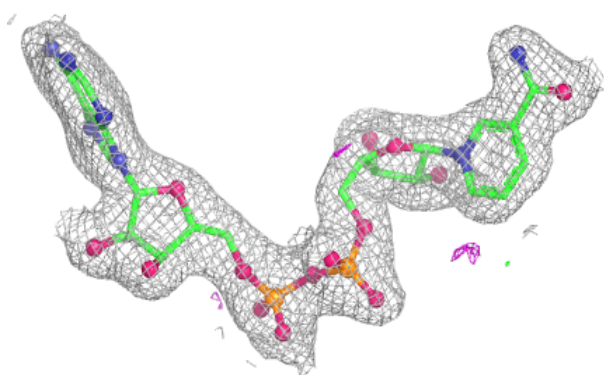


Electron density around NAD A 402:

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

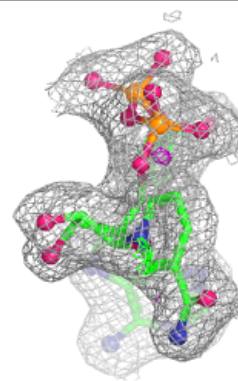
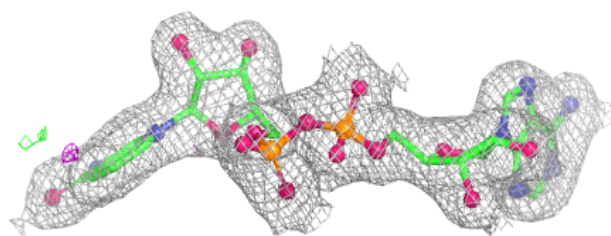
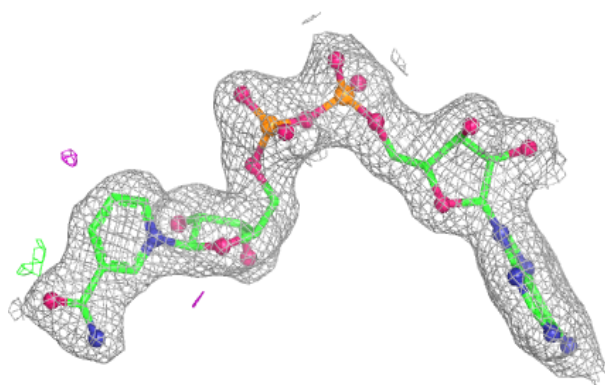
**Electron density around NAD F 402:**

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

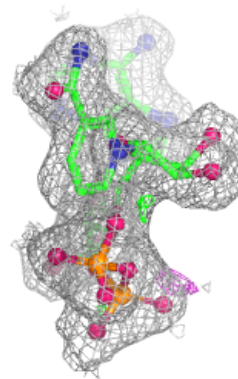
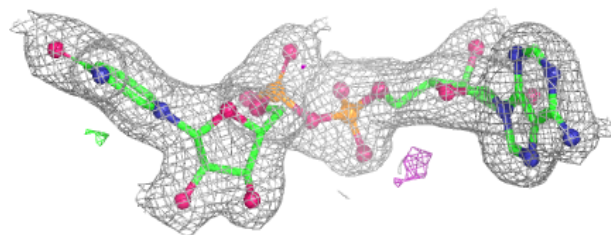
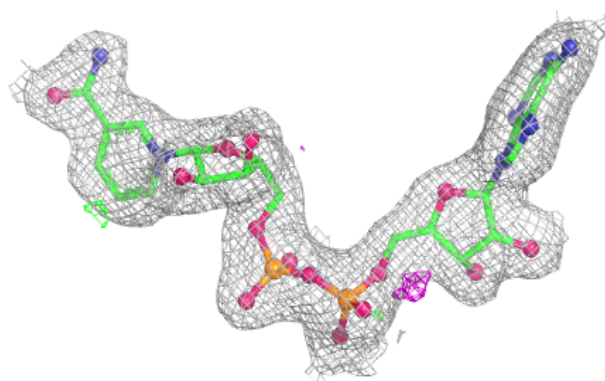


Electron density around NAD J 402:

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

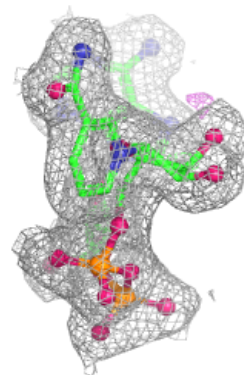
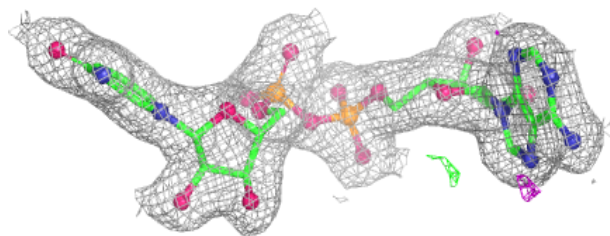
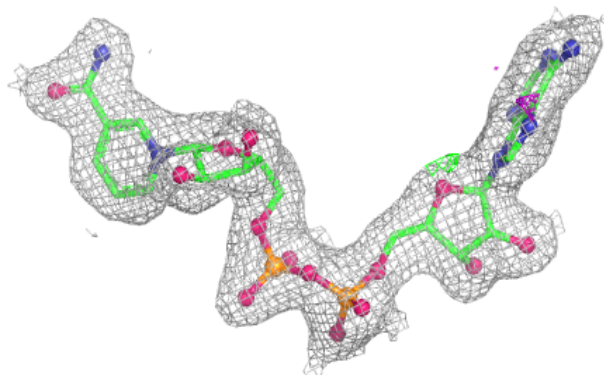
**Electron density around NAD K 402:**

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

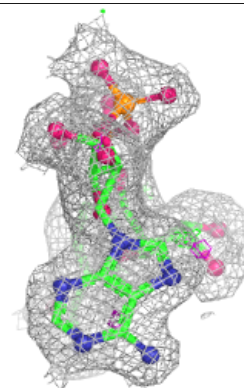
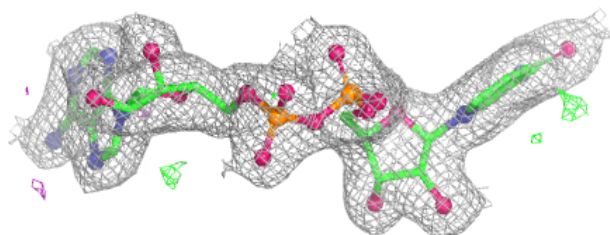
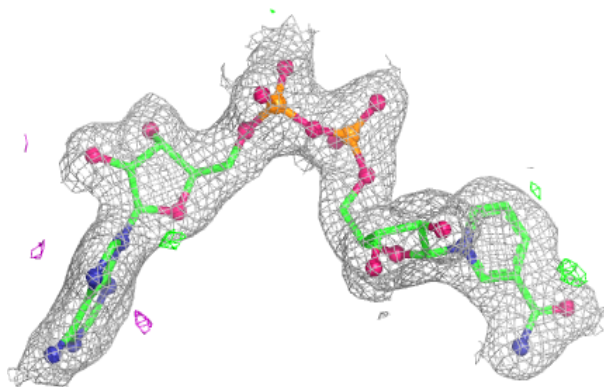


Electron density around NAD C 402:

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

**Electron density around NAD B 402:**

$2mF_o-DF_c$ (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.