



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 12:20 PM BST

PDB ID : 6N7L
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 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

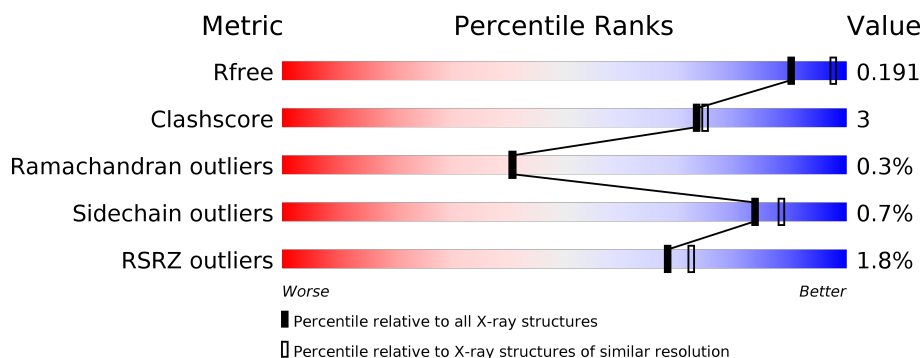
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on 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	<div> <div>90%</div> <div>7%</div> <div>•</div> </div>
1	B	353	<div> <div>91%</div> <div>6%</div> <div>•</div> </div>
1	C	353	<div> <div>90%</div> <div>7%</div> <div>•</div> </div>
1	D	353	<div> <div>92%</div> <div>5%</div> <div>•</div> </div>
1	E	353	<div> <div>86%</div> <div>10%</div> <div>• •</div> </div>
1	F	353	<div> <div>91%</div> <div>6%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	353	<div><div></div><div>90%</div><div>6%</div><div></div><div></div></div>
1	H	353	<div><div>%</div><div></div><div>90%</div><div>6%</div><div></div><div></div></div>
1	I	353	<div><div>5%</div><div></div><div>86%</div><div>10%</div><div></div><div></div></div>
1	J	353	<div><div></div><div>91%</div><div>6%</div><div></div><div></div></div>
1	K	353	<div><div>%</div><div></div><div>87%</div><div>9%</div><div></div><div></div></div>
1	L	353	<div><div>10%</div><div></div><div>89%</div><div>6%</div><div></div><div></div></div>

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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0

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

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Cl 1 1	0	0
5	J	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	K	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	I	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Cl 1	0	0
5	A	1	Total 1	Cl 1	0	0
5	L	1	Total 1	Cl 1	0	0
5	F	1	Total 1	Cl 1	0	0

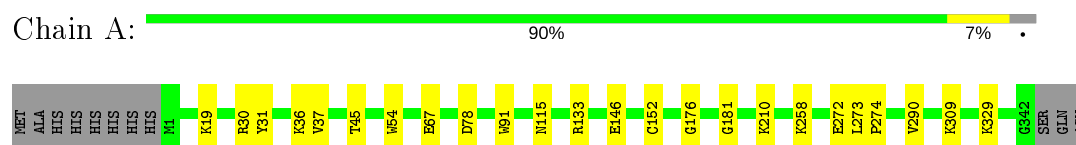
- Molecule 6 is water.

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

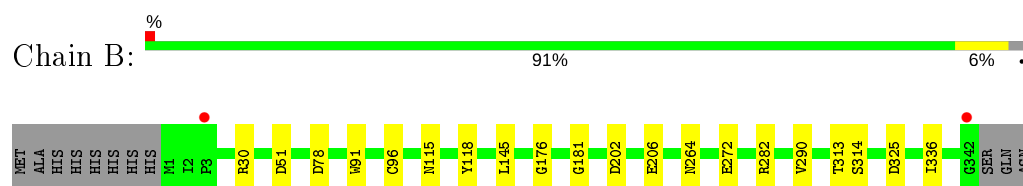
3 Residue-property plots [i](#)

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.

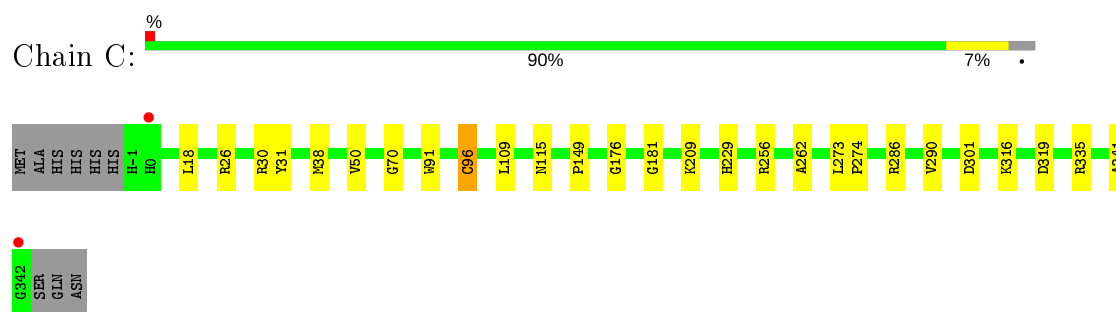
- Molecule 1: Alcohol dehydrogenase



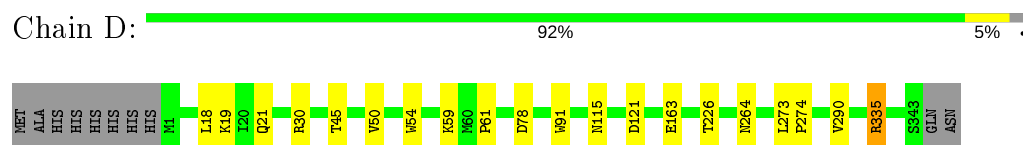
- Molecule 1: Alcohol dehydrogenase



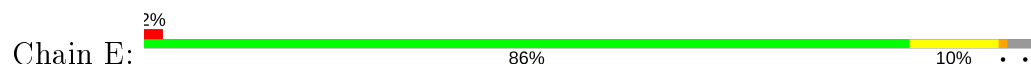
- Molecule 1: Alcohol dehydrogenase

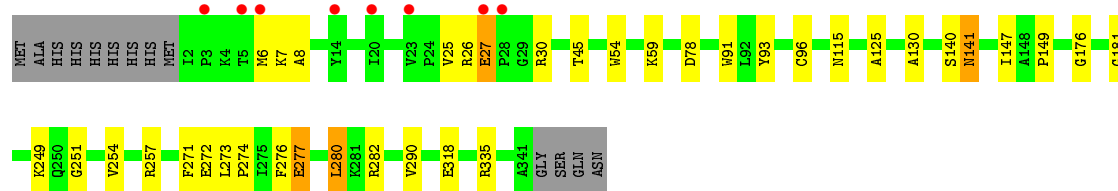


- Molecule 1: Alcohol dehydrogenase

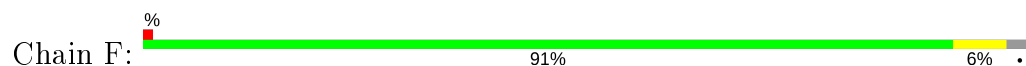


- Molecule 1: Alcohol dehydrogenase

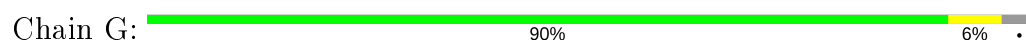




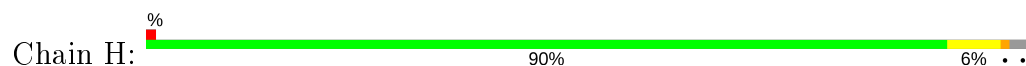
- Molecule 1: Alcohol dehydrogenase



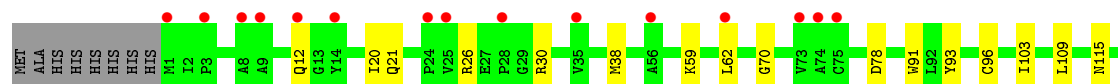
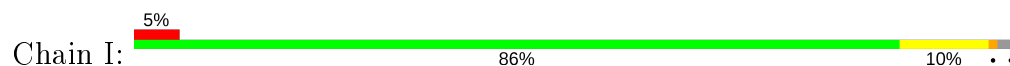
- Molecule 1: Alcohol dehydrogenase



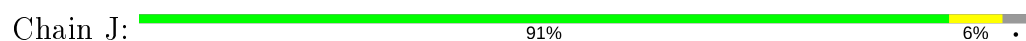
- Molecule 1: Alcohol dehydrogenase



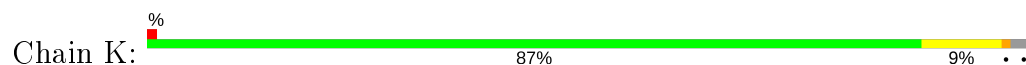
- Molecule 1: Alcohol dehydrogenase

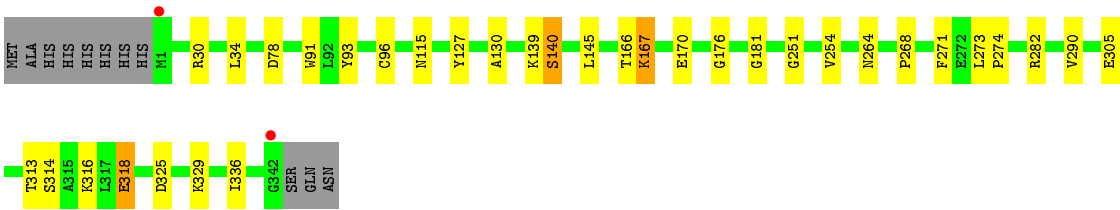


- Molecule 1: Alcohol dehydrogenase

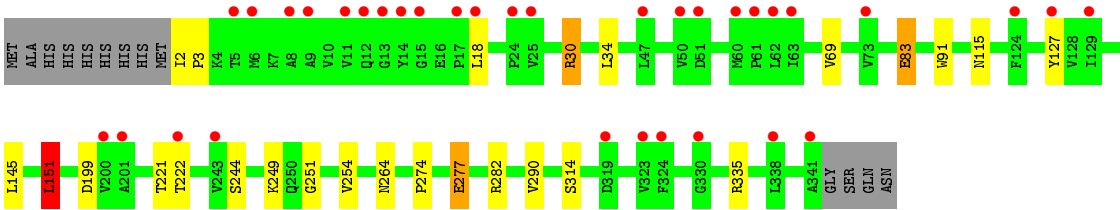
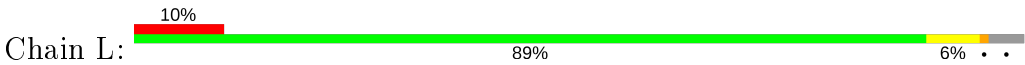


- Molecule 1: Alcohol dehydrogenase





● 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 0.149 , 0.191	Depositor DCC
R_{free} test set	15384 reflections (6.06%)	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 , 55.0	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: ZN, EDO, NAD, CL

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	0.42	2/2612 (0.1%)	0.57	2/3549 (0.1%)
1	B	0.39	0/2585	0.55	0/3518
1	C	0.39	0/2692	0.56	0/3649
1	D	0.37	0/2607	0.54	0/3541
1	E	0.47	3/2564 (0.1%)	0.68	10/3489 (0.3%)
1	F	0.47	3/2593 (0.1%)	0.60	3/3527 (0.1%)
1	G	0.45	2/2553 (0.1%)	0.61	3/3474 (0.1%)
1	H	0.49	3/2583 (0.1%)	0.70	8/3515 (0.2%)
1	I	0.37	0/2522	0.59	3/3438 (0.1%)
1	J	0.35	0/2575	0.56	2/3505 (0.1%)
1	K	0.43	2/2576 (0.1%)	0.67	6/3506 (0.2%)
1	L	0.44	3/2475 (0.1%)	0.58	3/3382 (0.1%)
All	All	0.42	18/30937 (0.1%)	0.60	40/42093 (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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	318	GLU	CD-OE2	10.83	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	83	GLU	CD-OE2	9.22	1.35	1.25
1	G	318	GLU	CG-CD	9.19	1.65	1.51
1	L	277	GLU	CD-OE2	8.78	1.35	1.25
1	K	318	GLU	CD-OE2	8.28	1.34	1.25
1	F	318	GLU	CD-OE2	7.92	1.34	1.25
1	F	318	GLU	CD-OE1	7.91	1.34	1.25
1	H	318	GLU	CB-CG	-7.72	1.37	1.52
1	F	7	LYS	CE-NZ	-7.54	1.30	1.49
1	E	27	GLU	CD-OE2	7.11	1.33	1.25
1	E	318	GLU	CD-OE2	6.83	1.33	1.25
1	E	318	GLU	CD-OE1	6.66	1.32	1.25
1	A	329	LYS	CB-CG	6.53	1.70	1.52
1	K	140	SER	CB-OG	6.49	1.50	1.42
1	L	277	GLU	CB-CG	-6.44	1.40	1.52
1	G	318	GLU	CD-OE1	5.89	1.32	1.25
1	A	329	LYS	CE-NZ	5.43	1.62	1.49
1	H	243	VAL	CB-CG1	5.27	1.64	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	318	GLU	CA-CB-CG	18.25	153.56	113.40
1	K	167	LYS	CD-CE-NZ	-14.14	79.17	111.70
1	K	167	LYS	CB-CG-CD	12.38	143.79	111.60
1	J	36	LYS	CG-CD-CE	-11.92	76.14	111.90
1	H	318	GLU	N-CA-CB	-9.80	92.96	110.60
1	L	277	GLU	CA-CB-CG	-9.19	93.19	113.40
1	I	277	GLU	CA-CB-CG	8.80	132.75	113.40
1	F	7	LYS	CD-CE-NZ	-8.04	93.22	111.70
1	H	318	GLU	CB-CA-C	7.95	126.31	110.40
1	H	243	VAL	CG1-CB-CG2	7.88	123.50	110.90
1	E	140	SER	C-N-CA	7.74	141.05	121.70
1	E	141	ASN	N-CA-CB	-7.73	96.69	110.60
1	L	151	LEU	CA-CB-CG	-7.60	97.81	115.30
1	I	244	SER	N-CA-CB	7.60	121.90	110.50
1	G	318	GLU	CG-CD-OE2	-7.51	103.27	118.30
1	G	318	GLU	CG-CD-OE1	7.19	132.68	118.30
1	H	318	GLU	CB-CG-CD	-7.11	95.00	114.20
1	I	277	GLU	N-CA-CB	7.04	123.28	110.60
1	E	318	GLU	CG-CD-OE2	7.02	132.35	118.30
1	K	167	LYS	CG-CD-CE	6.97	132.82	111.90
1	F	318	GLU	CA-CB-CG	-6.85	98.33	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	318	GLU	CA-CB-CG	6.57	127.85	113.40
1	E	27	GLU	CG-CD-OE2	-6.46	105.38	118.30
1	L	83	GLU	CG-CD-OE2	-6.42	105.46	118.30
1	K	318	GLU	N-CA-CB	-6.39	99.09	110.60
1	A	329	LYS	CG-CD-CE	6.39	131.08	111.90
1	E	280	LEU	CA-CB-CG	-6.35	100.70	115.30
1	J	36	LYS	CB-CA-C	-6.25	97.89	110.40
1	F	318	GLU	CB-CA-C	6.22	122.84	110.40
1	K	166	THR	C-N-CA	6.15	137.08	121.70
1	G	318	GLU	OE1-CD-OE2	-5.83	116.30	123.30
1	K	167	LYS	CA-CB-CG	5.74	126.02	113.40
1	E	141	ASN	CB-CA-C	5.63	121.65	110.40
1	E	277	GLU	CA-CB-CG	5.51	125.52	113.40
1	E	26	ARG	C-N-CA	-5.45	108.07	121.70
1	H	326	LYS	CB-CG-CD	5.43	125.71	111.60
1	H	317	LEU	C-N-CA	5.42	135.24	121.70
1	E	318	GLU	CG-CD-OE1	-5.33	107.64	118.30
1	H	220	LYS	CA-CB-CG	5.18	124.80	113.40
1	A	329	LYS	N-CA-CB	-5.10	101.42	110.60

There are no chirality outliers.

All (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
1	L	83	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2548	0	2552	17	0
1	B	2524	0	2511	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2610	0	2684	24	0
1	D	2549	0	2566	15	0
1	E	2506	0	2488	32	0
1	F	2532	0	2522	20	0
1	G	2501	0	2485	17	0
1	H	2525	0	2525	14	0
1	I	2470	0	2417	24	0
1	J	2517	0	2498	18	0
1	K	2518	0	2498	21	0
1	L	2423	0	2316	15	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	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1	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	3	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	0	0
All	All	33393	0	30920	203	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 3.

All (203) 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:8:ALA:HB2	1.40	0.98
1:A:36:LYS:NZ	6:A:501:HOH:O	1.98	0.97
1:C:96:CYS:HB2	2:C:407:EDO:H22	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:PHE:HD1	1:H:275[A]:ILE:HD11	1.45	0.81
1:E:6:MET:CE	1:E:125:ALA:HB1	2.12	0.80
1:I:12:GLN:HE21	1:I:21:GLN:HE22	1.31	0.78
1:E:6:MET:HE3	1:E:125:ALA:HB1	1.68	0.75
1:E:249:LYS:HD3	2:E:406:EDO:H21	1.69	0.74
1:E:30:ARG:HH21	1:F:30:ARG:HH21	1.34	0.73
1:G:217:VAL:HA	2:G:508:EDO:H11	1.69	0.73
1:K:167:LYS:HG3	1:K:170:GLU:CD	2.07	0.73
1:K:167:LYS:HG3	1:K:170:GLU:OE2	1.89	0.72
1:E:257:ARG:H	2:H:701:EDO:H11	1.55	0.72
1:E:78:ASP:OD2	1:F:30:ARG:NH2	2.23	0.72
1:I:30:ARG:HH21	1:J:30:ARG:HH21	1.39	0.70
1:G:227:TYR:HB2	2:G:503:EDO:H22	1.71	0.70
1:G:273[A]:LEU:HD12	1:G:274:PRO:HD2	1.73	0.69
1:E:147:ILE:HD13	2:E:407:EDO:H22	1.76	0.67
1:F:210[B]:LYS:NZ	6:F:505:HOH:O	2.28	0.67
1:E:272:GLU:H	2:E:406:EDO:H22	1.60	0.66
1:F:322:ASP:OD1	6:F:501:HOH:O	2.14	0.66
1:A:273:LEU:HD12	1:A:274:PRO:HD2	1.76	0.66
1:K:305:GLU:OE1	6:K:501:HOH:O	2.14	0.65
1:C:319:ASP:OD2	6:C:501:HOH:O	2.15	0.65
1:F:273:LEU:HD12	1:F:274:PRO:HD2	1.79	0.64
1:A:37:VAL:O	6:A:501:HOH:O	2.15	0.64
1:E:6:MET:HG2	1:E:25:VAL:HG22	1.80	0.62
1:I:272:GLU:H	2:I:404:EDO:H12	1.65	0.62
1:K:273:LEU:HD12	1:K:274:PRO:HD2	1.79	0.62
1:E:30:ARG:NH2	1:F:30:ARG:HH21	1.97	0.62
1:F:163:GLU:HA	2:F:407:EDO:H21	1.82	0.60
1:B:272:GLU:H	2:B:404:EDO:H21	1.67	0.59
1:K:78:ASP:CG	1:L:30:ARG:HH22	2.06	0.59
1:F:319:ASP:OD2	6:F:502:HOH:O	2.17	0.58
1:I:12:GLN:NE2	1:I:21:GLN:HE22	2.02	0.57
1:A:133:ARG:HD2	2:A:409[B]:EDO:H12	1.87	0.57
1:E:30:ARG:HH21	1:F:30:ARG:NH2	2.01	0.57
1:F:272:GLU:HG3	2:F:404:EDO:H12	1.87	0.56
1:C:301:ASP:HB3	2:C:401:EDO:H11	1.87	0.56
1:I:30:ARG:HH21	1:J:30:ARG:NH2	2.03	0.56
1:C:30:ARG:HH21	1:D:30:ARG:HH21	1.52	0.56
1:J:323:VAL:HG13	1:J:336:ILE:HD12	1.88	0.56
1:C:229:HIS:HE1	2:C:406:EDO:H21	1.71	0.56
1:A:272:GLU:HB2	2:A:406:EDO:H11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ARG:NH2	1:D:30:ARG:HH21	2.07	0.53
1:C:30:ARG:NH2	1:D:78:ASP:OD2	2.42	0.53
1:E:78:ASP:CG	1:F:30:ARG:HH22	2.11	0.53
1:C:256:ARG:HA	2:C:406:EDO:H21	1.92	0.52
1:G:325:ASP:O	1:G:329:LYS:HG3	2.09	0.52
1:H:243:VAL:HG22	3:H:703:NAD:H52A	1.91	0.52
1:D:163:GLU:HA	2:D:508:EDO:H12	1.91	0.52
1:H:273[B]:LEU:HD12	1:H:274:PRO:HD2	1.91	0.52
1:K:145:LEU:HD21	1:K:314[A]:SER:HB2	1.91	0.52
1:E:271:PHE:CE1	1:H:273[B]:LEU:HD23	2.45	0.52
1:E:273:LEU:HD12	1:E:274:PRO:HD2	1.91	0.52
1:C:91:TRP:O	1:C:115:ASN:HA	2.10	0.51
1:D:18:LEU:HD11	1:D:50:VAL:HG21	1.91	0.51
1:F:91:TRP:O	1:F:115:ASN:HA	2.11	0.51
1:K:316:LYS:HB3	1:K:318:GLU:OE1	2.10	0.51
1:D:91:TRP:O	1:D:115:ASN:HA	2.12	0.50
2:A:401:EDO:H12	6:A:702:HOH:O	2.09	0.50
1:A:309:LYS:HG3	6:A:602:HOH:O	2.10	0.50
1:C:30:ARG:HH21	1:D:30:ARG:NH2	2.09	0.50
1:I:319:ASP:O	1:I:323:VAL:HG23	2.12	0.49
1:D:59:LYS:NZ	1:D:121:ASP:OD1	2.44	0.49
1:C:273:LEU:HD12	1:C:274:PRO:HD2	1.94	0.49
1:K:167:LYS:CG	1:K:170:GLU:CD	2.78	0.49
1:H:38:MET:HG2	1:H:70:GLY:HA2	1.95	0.49
1:A:78:ASP:CG	1:B:30:ARG:HH22	2.14	0.49
1:C:30:ARG:HD3	1:C:31:TYR:CE2	2.47	0.49
1:E:91:TRP:O	1:E:115:ASN:HA	2.13	0.48
1:G:91:TRP:O	1:G:115:ASN:HA	2.14	0.48
1:I:245:PRO:HB2	2:I:404:EDO:C2	2.43	0.48
1:I:59:LYS:HZ2	1:I:62:LEU:HD12	1.78	0.48
1:E:93:TYR:CE2	1:E:130:ALA:HA	2.47	0.48
1:E:277:GLU:HG3	6:E:637:HOH:O	2.14	0.48
1:I:91:TRP:O	1:I:115:ASN:HA	2.14	0.48
1:I:26:ARG:HH22	1:I:129:ILE:HD11	1.78	0.48
1:I:38:MET:HG2	1:I:70:GLY:HA2	1.96	0.48
2:C:401:EDO:H12	6:C:732:HOH:O	2.12	0.48
1:G:38:MET:HA	1:G:341:ALA:HB2	1.94	0.48
1:E:6:MET:HE1	1:E:8:ALA:CB	2.29	0.48
1:I:93:TYR:CE2	1:I:130:ALA:HA	2.49	0.47
1:J:93:TYR:CE2	1:J:130:ALA:HA	2.49	0.47
1:F:20:ILE:HG21	1:F:318:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:LYS:O	1:I:62:LEU:HB2	2.15	0.47
1:A:210:LYS:HB2	1:A:210:LYS:HE3	1.53	0.47
1:A:30:ARG:HD3	1:A:31:TYR:CE2	2.50	0.47
1:B:91:TRP:O	1:B:115:ASN:HA	2.15	0.47
1:C:18:LEU:HD11	1:C:50[B]:VAL:HG21	1.97	0.46
1:J:91:TRP:O	1:J:115:ASN:HA	2.16	0.46
1:D:61:PRO:HG2	2:D:505:EDO:H22	1.96	0.46
1:F:236:HIS:CD2	2:F:411:EDO:H21	2.50	0.46
1:E:273:LEU:HD23	1:H:271:PHE:CE1	2.50	0.46
1:I:12:GLN:HE21	1:I:21:GLN:NE2	2.07	0.46
1:L:145:LEU:HD21	1:L:314:SER:HB2	1.98	0.46
1:D:335[A]:ARG:NH1	3:D:501:NAD:O1N	2.41	0.46
1:I:217:VAL:HG11	1:I:224:PRO:HA	1.98	0.46
1:E:45:THR:HG23	1:E:54:TRP:CH2	2.51	0.46
1:H:91:TRP:O	1:H:115:ASN:HA	2.16	0.46
1:I:78:ASP:CG	1:J:30:ARG:HH22	2.19	0.46
1:J:273:LEU:HD12	1:J:274:PRO:HD2	1.98	0.46
1:L:264:ASN:O	3:L:402:NAD:H2N	2.16	0.46
1:K:91:TRP:O	1:K:115:ASN:HA	2.16	0.46
1:L:221:THR:OG1	1:L:222:THR:HG23	2.16	0.45
1:H:251:GLY:O	1:H:254:VAL:HG22	2.16	0.45
1:J:217:VAL:HA	2:J:407:EDO:C2	2.46	0.45
1:D:45:THR:HG23	1:D:54:TRP:CH2	2.51	0.45
1:I:264:ASN:O	3:I:402:NAD:H2N	2.16	0.45
1:E:6:MET:HE3	1:E:7:LYS:O	2.16	0.45
1:F:20:ILE:HG13	1:F:318:GLU:CG	2.46	0.45
1:L:34:LEU:HD11	1:L:127:TYR:HB3	1.97	0.45
1:A:91:TRP:O	1:A:115:ASN:HA	2.17	0.45
1:L:91:TRP:O	1:L:115:ASN:HA	2.17	0.45
1:E:30:ARG:NH2	1:F:30:ARG:HE	2.14	0.45
1:H:118:TYR:CE1	2:H:704:EDO:H12	2.52	0.45
1:I:78:ASP:OD1	1:J:30:ARG:NH2	2.50	0.45
1:F:20:ILE:HG13	1:F:318:GLU:HG2	1.99	0.44
1:J:217:VAL:HA	2:J:407:EDO:H22	2.00	0.44
1:F:257:ARG:HH21	2:F:409:EDO:H22	1.81	0.44
1:G:273[B]:LEU:HD22	1:G:274:PRO:HD2	1.99	0.44
1:C:176:GLY:O	1:C:181:GLY:HA3	2.17	0.44
1:K:264:ASN:O	3:K:402:NAD:H2N	2.17	0.44
1:B:282:ARG:HB2	1:C:109:LEU:HD21	2.00	0.44
1:L:18:LEU:HD12	1:L:18:LEU:H	1.82	0.44
1:F:145:LEU:HD21	1:F:314[B]:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:ASN:O	3:G:501:NAD:H2N	2.18	0.44
1:G:316:LYS:HE2	1:G:316:LYS:HB3	1.63	0.44
1:J:176:GLY:O	1:J:181:GLY:HA3	2.18	0.44
1:C:209:LYS:HG3	2:C:412:EDO:H11	1.99	0.43
1:A:45:THR:HG23	1:A:54:TRP:CH2	2.54	0.43
1:H:319:ASP:OD2	6:H:802:HOH:O	2.21	0.43
1:B:325:ASP:OD1	6:B:501:HOH:O	2.21	0.43
1:D:264:ASN:O	3:D:501:NAD:H2N	2.18	0.43
1:G:26:ARG:NH2	6:G:610:HOH:O	2.51	0.43
1:A:176:GLY:O	1:A:181:GLY:HA3	2.19	0.43
1:E:257:ARG:HG3	2:H:701:EDO:H11	2.00	0.43
1:C:149:PRO:HG3	1:C:335[B]:ARG:HG2	2.01	0.43
1:C:38[B]:MET:HG2	1:C:70:GLY:HA2	2.01	0.43
1:B:176:GLY:O	1:B:181:GLY:HA3	2.19	0.43
1:E:6:MET:HE3	1:E:8:ALA:HB2	1.86	0.43
1:B:145:LEU:HD21	1:B:314:SER:HB3	2.01	0.43
1:H:173:ALA:HB2	1:H:235:MET:HG3	2.01	0.43
1:J:109:LEU:HD21	1:K:282:ARG:HB2	2.01	0.43
1:B:313:THR:HB	1:B:336[A]:ILE:HD13	2.01	0.43
1:E:149:PRO:HG3	1:E:335[A]:ARG:HG2	2.01	0.42
1:K:251:GLY:O	1:K:254:VAL:HG22	2.19	0.42
1:K:325:ASP:OD2	1:K:329:LYS:HE3	2.19	0.42
1:I:277:GLU:HB3	1:I:281:LYS:HD3	2.00	0.42
1:L:199:ASP:OD1	3:L:402:NAD:O2B	2.25	0.42
1:B:51:ASP:HB3	1:G:230:LYS:HE3	2.02	0.42
1:K:30:ARG:HH11	1:L:30:ARG:CZ	2.33	0.42
1:C:96:CYS:CB	2:C:407:EDO:H22	2.40	0.42
1:E:282:ARG:HG2	1:H:287:GLY:O	2.20	0.42
1:J:38[A]:MET:HA	1:J:341:ALA:HB2	2.01	0.42
1:A:146:GLU:HB3	6:A:602:HOH:O	2.18	0.42
1:L:2:ILE:HA	1:L:3:PRO:HD3	1.91	0.42
1:A:67:GLU:OE2	1:A:152:CYS:HB3	2.19	0.42
1:B:202:ASP:O	1:B:206:GLU:HG2	2.19	0.42
1:C:316:LYS:HE2	1:C:319:ASP:OD2	2.20	0.42
1:H:248:PHE:CD2	1:H:263:LEU:HD22	2.53	0.42
1:K:176:GLY:O	1:K:181:GLY:HA3	2.20	0.42
1:B:118:TYR:CE2	2:B:403:EDO:H11	2.54	0.42
1:A:30:ARG:NH2	1:B:78:ASP:OD2	2.44	0.42
1:C:262:ALA:HA	1:C:286:ARG:O	2.19	0.42
1:C:26:ARG:HD3	2:C:404:EDO:O1	2.20	0.42
1:J:38[B]:MET:HA	1:J:341:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASP:OD2	1:B:30:ARG:NH2	2.43	0.41
1:L:274:PRO:HB2	1:L:277:GLU:OE1	2.20	0.41
1:E:251:GLY:O	1:E:254:VAL:HG22	2.20	0.41
1:F:38:MET:HA	1:F:341:ALA:HB2	2.00	0.41
1:J:264:ASN:O	3:J:402:NAD:H2N	2.21	0.41
1:L:251:GLY:O	1:L:254:VAL:HG22	2.20	0.41
1:B:264:ASN:O	3:B:402:NAD:H2N	2.20	0.41
1:I:109:LEU:HD21	1:L:282:ARG:HB2	2.01	0.41
1:I:103:ILE:O	1:J:105:GLY:HA2	2.20	0.41
1:I:205:LEU:HD22	1:I:216:THR:HB	2.02	0.41
1:D:19:LYS:HD3	1:D:21:GLN:HE21	1.86	0.41
1:G:176:GLY:O	1:G:181:GLY:HA3	2.20	0.41
1:C:38[A]:MET:HA	1:C:341:ALA:HB2	2.02	0.41
1:J:179:GLY:HA3	1:J:335[B]:ARG:NH1	2.36	0.41
1:K:93:TYR:CE2	1:K:130:ALA:HA	2.56	0.41
1:A:258:LYS:HE2	6:D:626:HOH:O	2.20	0.41
1:C:38[B]:MET:HA	1:C:341:ALA:HB2	2.02	0.41
1:H:220:LYS:HA	1:H:220:LYS:HE2	2.02	0.41
1:L:69:VAL:CG1	1:L:151:LEU:HD13	2.50	0.41
1:I:20:ILE:HD11	1:I:318:GLU:HA	2.01	0.41
1:D:273:LEU:HD12	1:D:274:PRO:HD2	2.02	0.40
1:G:38:MET:HG2	1:G:70:GLY:HA2	2.02	0.40
2:I:405:EDO:H12	6:I:543:HOH:O	2.20	0.40
1:E:276:PHE:O	1:E:280:LEU:HD12	2.21	0.40
2:E:410:EDO:H12	1:G:302:PHE:CD1	2.56	0.40
1:G:227:TYR:CB	2:G:503:EDO:H22	2.48	0.40
1:K:313:THR:HB	1:K:336:ILE:HD13	2.03	0.40
1:K:30:ARG:HH11	1:L:30:ARG:NH2	2.20	0.40
1:G:6:MET:HB3	1:G:25:VAL:CG2	2.52	0.40
1:E:176:GLY:O	1:E:181:GLY:HA3	2.21	0.40
1:I:59:LYS:NZ	1:I:121:ASP:OD1	2.50	0.40
1:J:273:LEU:HD23	1:K:271:PHE:CE1	2.57	0.40
1:K:34:LEU:HD11	1:K:127:TYR:HB3	2.03	0.40
1:D:226:THR:HG21	1:K:268:PRO:HG3	2.02	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	345/353 (98%)	335 (97%)	9 (3%)	1 (0%)	41	41
1	B	344/353 (98%)	333 (97%)	10 (3%)	1 (0%)	41	41
1	C	353/353 (100%)	342 (97%)	10 (3%)	1 (0%)	41	41
1	D	344/353 (98%)	333 (97%)	10 (3%)	1 (0%)	41	41
1	E	341/353 (97%)	331 (97%)	9 (3%)	1 (0%)	41	41
1	F	345/353 (98%)	335 (97%)	9 (3%)	1 (0%)	41	41
1	G	339/353 (96%)	328 (97%)	10 (3%)	1 (0%)	41	41
1	H	343/353 (97%)	333 (97%)	9 (3%)	1 (0%)	41	41
1	I	340/353 (96%)	329 (97%)	10 (3%)	1 (0%)	41	41
1	J	344/353 (98%)	332 (96%)	11 (3%)	1 (0%)	41	41
1	K	343/353 (97%)	332 (97%)	9 (3%)	2 (1%)	25	21
1	L	339/353 (96%)	327 (96%)	11 (3%)	1 (0%)	41	41
All	All	4120/4236 (97%)	3990 (97%)	117 (3%)	13 (0%)	41	41

All (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
1	E	290	VAL
1	F	290	VAL
1	G	290	VAL
1	H	290	VAL
1	I	290	VAL
1	J	290	VAL
1	K	290	VAL

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Mol	Chain	Res	Type
1	L	290	VAL

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	267/278 (96%)	266 (100%)	1 (0%)	91	94
1	B	261/278 (94%)	260 (100%)	1 (0%)	91	94
1	C	278/278 (100%)	277 (100%)	1 (0%)	91	94
1	D	266/278 (96%)	264 (99%)	2 (1%)	81	86
1	E	258/278 (93%)	256 (99%)	2 (1%)	81	86
1	F	261/278 (94%)	258 (99%)	3 (1%)	73	79
1	G	258/278 (93%)	257 (100%)	1 (0%)	91	94
1	H	262/278 (94%)	261 (100%)	1 (0%)	91	94
1	I	247/278 (89%)	242 (98%)	5 (2%)	55	60
1	J	258/278 (93%)	256 (99%)	2 (1%)	81	86
1	K	259/278 (93%)	258 (100%)	1 (0%)	91	94
1	L	235/278 (84%)	229 (97%)	6 (3%)	46	50
All	All	3110/3336 (93%)	3084 (99%)	26 (1%)	84	86

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	B	96	CYS
1	C	96	CYS
1	D	335[A]	ARG
1	D	335[B]	ARG
1	E	59	LYS
1	E	96	CYS
1	F	96	CYS
1	F	335[A]	ARG

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Mol	Chain	Res	Type
1	F	335[B]	ARG
1	G	96	CYS
1	H	96	CYS
1	I	96	CYS
1	I	231	GLU
1	I	314	SER
1	I	335[A]	ARG
1	I	335[B]	ARG
1	J	335[A]	ARG
1	J	335[B]	ARG
1	K	96	CYS
1	L	30	ARG
1	L	151	LEU
1	L	244	SER
1	L	249	LYS
1	L	335[A]	ARG
1	L	335[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	12	GLN
1	B	21	GLN
1	B	264	ASN
1	C	229	HIS
1	C	264	ASN
1	D	21	GLN
1	D	114	GLN
1	E	12	GLN
1	H	21	GLN
1	I	12	GLN
1	I	264	ASN
1	J	21	GLN
1	K	264	ASN
1	L	304	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 monosaccharides 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	F	411	-	3,3,3	0.51	0	2,2,2	0.16	0
2	EDO	F	406	-	3,3,3	0.48	0	2,2,2	0.35	0
2	EDO	J	407	-	3,3,3	0.46	0	2,2,2	0.57	0
2	EDO	K	405	-	3,3,3	0.46	0	2,2,2	0.49	0
2	EDO	D	502	-	3,3,3	0.48	0	2,2,2	0.22	0
2	EDO	F	408	-	3,3,3	0.42	0	2,2,2	0.53	0
3	NAD	K	402	-	42,48,48	0.54	0	50,73,73	0.67	2 (4%)
2	EDO	H	704	-	3,3,3	0.50	0	2,2,2	0.28	0
2	EDO	C	406	-	3,3,3	0.57	0	2,2,2	0.11	0
2	EDO	C	403	-	3,3,3	0.50	0	2,2,2	0.37	0
2	EDO	D	504	-	3,3,3	0.76	0	2,2,2	0.35	0
2	EDO	F	403	-	3,3,3	0.47	0	2,2,2	0.45	0
2	EDO	A	409[A]	-	3,3,3	0.52	0	2,2,2	0.19	0
2	EDO	I	406	-	3,3,3	0.42	0	2,2,2	0.61	0
2	EDO	H	705	-	3,3,3	0.48	0	2,2,2	0.17	0
2	EDO	K	401	-	3,3,3	0.55	0	2,2,2	0.20	0
2	EDO	D	506	-	3,3,3	0.47	0	2,2,2	0.27	0
2	EDO	A	407	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	B	401	-	3,3,3	0.58	0	2,2,2	0.21	0
2	EDO	C	409	-	3,3,3	0.46	0	2,2,2	0.39	0
2	EDO	C	408	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	F	404	-	3,3,3	0.39	0	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	G	507	-	3,3,3	0.48	0	2,2,2	0.27	0
2	EDO	C	407	-	3,3,3	0.49	0	2,2,2	0.45	0
2	EDO	F	409	-	3,3,3	0.49	0	2,2,2	0.33	0
2	EDO	K	403	-	3,3,3	0.41	0	2,2,2	0.50	0
2	EDO	D	509	-	3,3,3	0.43	0	2,2,2	0.27	0
3	NAD	G	501	-	42,48,48	0.55	0	50,73,73	0.70	2 (4%)
3	NAD	C	402	-	42,48,48	0.58	0	50,73,73	0.78	2 (4%)
2	EDO	A	406	-	3,3,3	0.37	0	2,2,2	0.86	0
2	EDO	H	702	-	3,3,3	0.69	0	2,2,2	0.23	0
2	EDO	G	502	-	3,3,3	0.44	0	2,2,2	0.38	0
2	EDO	E	403	-	3,3,3	0.42	0	2,2,2	0.46	0
2	EDO	F	401	-	3,3,3	0.60	0	2,2,2	0.13	0
3	NAD	F	402	-	42,48,48	0.52	0	50,73,73	0.72	2 (4%)
2	EDO	G	504	-	3,3,3	0.50	0	2,2,2	0.28	0
2	EDO	E	408	-	3,3,3	0.48	0	2,2,2	0.56	0
2	EDO	B	403	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	L	404	-	3,3,3	0.44	0	2,2,2	0.41	0
2	EDO	E	404	-	3,3,3	0.41	0	2,2,2	0.48	0
2	EDO	J	408	-	3,3,3	0.44	0	2,2,2	0.49	0
2	EDO	B	408	-	3,3,3	0.49	0	2,2,2	0.43	0
2	EDO	E	409	-	3,3,3	0.36	0	2,2,2	0.70	0
2	EDO	B	407	-	3,3,3	0.52	0	2,2,2	0.07	0
2	EDO	A	401	-	3,3,3	0.70	0	2,2,2	0.62	0
2	EDO	I	405	-	3,3,3	0.49	0	2,2,2	0.27	0
2	EDO	I	401	-	3,3,3	0.66	0	2,2,2	0.21	0
3	NAD	L	402	-	42,48,48	0.51	0	50,73,73	0.73	2 (4%)
2	EDO	F	410	-	3,3,3	0.53	0	2,2,2	0.13	0
2	EDO	J	401	-	3,3,3	0.60	0	2,2,2	0.11	0
2	EDO	E	401	-	3,3,3	0.68	0	2,2,2	0.17	0
3	NAD	J	402	-	42,48,48	0.57	0	50,73,73	0.74	3 (6%)
2	EDO	E	406	-	3,3,3	0.42	0	2,2,2	0.47	0
2	EDO	F	407	-	3,3,3	0.47	0	2,2,2	0.15	0
2	EDO	C	401	-	3,3,3	0.71	0	2,2,2	0.59	0
2	EDO	A	412	-	3,3,3	0.37	0	2,2,2	0.78	0
2	EDO	F	405	-	3,3,3	0.50	0	2,2,2	0.12	0
2	EDO	A	408	-	3,3,3	0.44	0	2,2,2	0.49	0
2	EDO	A	409[B]	-	3,3,3	0.49	0	2,2,2	0.28	0
2	EDO	E	405	-	3,3,3	0.48	0	2,2,2	0.24	0
2	EDO	G	505	-	3,3,3	0.47	0	2,2,2	0.35	0
2	EDO	A	403	-	3,3,3	0.48	0	2,2,2	0.30	0
2	EDO	I	407	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	J	405	-	3,3,3	0.54	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	A	402	-	42,48,48	0.56	0	50,73,73	0.76	2 (4%)
2	EDO	C	412	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	A	404	-	3,3,3	0.49	0	2,2,2	0.26	0
2	EDO	B	404	-	3,3,3	0.41	0	2,2,2	0.52	0
2	EDO	C	404	-	3,3,3	0.37	0	2,2,2	0.64	0
2	EDO	D	508	-	3,3,3	0.47	0	2,2,2	0.10	0
2	EDO	E	410	-	3,3,3	0.41	0	2,2,2	0.23	0
2	EDO	C	410	-	3,3,3	0.47	0	2,2,2	0.35	0
2	EDO	B	406	-	3,3,3	0.40	0	2,2,2	0.63	0
2	EDO	A	411	-	3,3,3	0.47	0	2,2,2	0.41	0
3	NAD	D	501	-	42,48,48	0.57	0	50,73,73	0.72	3 (6%)
2	EDO	G	503	-	3,3,3	0.42	0	2,2,2	0.36	0
3	NAD	E	402	-	42,48,48	0.55	0	50,73,73	0.74	3 (6%)
2	EDO	K	404	-	3,3,3	0.51	0	2,2,2	0.16	0
2	EDO	A	410	-	3,3,3	0.49	0	2,2,2	0.31	0
3	NAD	B	402	-	42,48,48	0.52	0	50,73,73	0.72	2 (4%)
2	EDO	D	503	-	3,3,3	0.47	0	2,2,2	0.38	0
2	EDO	J	406	-	3,3,3	0.41	0	2,2,2	0.60	0
2	EDO	J	403	-	3,3,3	0.44	0	2,2,2	0.48	0
2	EDO	G	506	-	3,3,3	0.45	0	2,2,2	0.38	0
2	EDO	E	407	-	3,3,3	0.49	0	2,2,2	0.16	0
2	EDO	C	411	-	3,3,3	0.46	0	2,2,2	0.23	0
2	EDO	L	401	-	3,3,3	0.57	0	2,2,2	0.05	0
2	EDO	H	706	1	3,3,3	0.49	0	2,2,2	0.41	0
2	EDO	G	508	-	3,3,3	0.43	0	2,2,2	0.59	0
2	EDO	I	404	-	3,3,3	0.37	0	2,2,2	0.38	0
2	EDO	C	413	-	3,3,3	0.63	0	2,2,2	0.11	0
2	EDO	B	405	-	3,3,3	0.44	0	2,2,2	0.48	0
3	NAD	I	402	-	42,48,48	0.54	0	50,73,73	0.65	2 (4%)
2	EDO	H	707	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	C	405	-	3,3,3	0.50	0	2,2,2	0.28	0
2	EDO	A	405	-	3,3,3	0.52	0	2,2,2	0.29	0
2	EDO	D	507	-	3,3,3	0.49	0	2,2,2	0.33	0
2	EDO	H	701	-	3,3,3	0.46	0	2,2,2	0.32	0
3	NAD	H	703	-	42,48,48	0.51	0	50,73,73	0.71	1 (2%)
2	EDO	D	505	-	3,3,3	0.43	0	2,2,2	0.50	0
2	EDO	I	403	-	3,3,3	0.46	0	2,2,2	0.38	0
2	EDO	L	403	-	3,3,3	0.44	0	2,2,2	0.34	0
2	EDO	J	404	-	3,3,3	0.48	0	2,2,2	0.32	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	F	411	-	-	0/1/1/1	-
2	EDO	F	406	-	-	0/1/1/1	-
2	EDO	J	407	-	-	1/1/1/1	-
2	EDO	K	405	-	-	0/1/1/1	-
2	EDO	D	502	-	-	0/1/1/1	-
2	EDO	F	408	-	-	0/1/1/1	-
3	NAD	K	402	-	-	5/26/62/62	0/5/5/5
2	EDO	H	704	-	-	0/1/1/1	-
2	EDO	C	406	-	-	1/1/1/1	-
2	EDO	C	403	-	-	1/1/1/1	-
2	EDO	D	504	-	-	0/1/1/1	-
2	EDO	F	403	-	-	0/1/1/1	-
2	EDO	A	409[A]	-	-	0/1/1/1	-
2	EDO	I	406	-	-	1/1/1/1	-
2	EDO	H	705	-	-	0/1/1/1	-
2	EDO	K	401	-	-	1/1/1/1	-
2	EDO	D	506	-	-	0/1/1/1	-
2	EDO	A	407	-	-	0/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	C	409	-	-	0/1/1/1	-
2	EDO	C	408	-	-	0/1/1/1	-
2	EDO	F	404	-	-	0/1/1/1	-
2	EDO	G	507	-	-	0/1/1/1	-
2	EDO	C	407	-	-	0/1/1/1	-
2	EDO	F	409	-	-	0/1/1/1	-
2	EDO	K	403	-	-	1/1/1/1	-
2	EDO	D	509	-	-	0/1/1/1	-
3	NAD	G	501	-	-	5/26/62/62	0/5/5/5
3	NAD	C	402	-	-	5/26/62/62	0/5/5/5
2	EDO	A	406	-	-	1/1/1/1	-
2	EDO	H	702	-	-	0/1/1/1	-
2	EDO	G	502	-	-	0/1/1/1	-
2	EDO	E	403	-	-	0/1/1/1	-
2	EDO	F	401	-	-	0/1/1/1	-
3	NAD	F	402	-	-	5/26/62/62	0/5/5/5
2	EDO	G	504	-	-	1/1/1/1	-
2	EDO	E	408	-	-	1/1/1/1	-
2	EDO	B	403	-	-	0/1/1/1	-
2	EDO	L	404	-	-	1/1/1/1	-
2	EDO	E	404	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	J	408	-	-	1/1/1/1	-
2	EDO	B	408	-	-	1/1/1/1	-
2	EDO	E	409	-	-	0/1/1/1	-
2	EDO	B	407	-	-	0/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	I	405	-	-	0/1/1/1	-
2	EDO	I	401	-	-	0/1/1/1	-
3	NAD	L	402	-	-	5/26/62/62	0/5/5/5
2	EDO	F	410	-	-	0/1/1/1	-
2	EDO	J	401	-	-	0/1/1/1	-
2	EDO	E	401	-	-	0/1/1/1	-
3	NAD	J	402	-	-	5/26/62/62	0/5/5/5
2	EDO	E	406	-	-	1/1/1/1	-
2	EDO	F	407	-	-	0/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	A	412	-	-	1/1/1/1	-
2	EDO	F	405	-	-	0/1/1/1	-
2	EDO	A	408	-	-	0/1/1/1	-
2	EDO	A	409[B]	-	-	0/1/1/1	-
2	EDO	E	405	-	-	0/1/1/1	-
2	EDO	G	505	-	-	0/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	I	407	-	-	1/1/1/1	-
2	EDO	J	405	-	-	1/1/1/1	-
3	NAD	A	402	-	-	5/26/62/62	0/5/5/5
2	EDO	C	412	-	-	1/1/1/1	-
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	B	404	-	-	0/1/1/1	-
2	EDO	C	404	-	-	0/1/1/1	-
2	EDO	D	508	-	-	0/1/1/1	-
2	EDO	E	410	-	-	0/1/1/1	-
2	EDO	C	410	-	-	0/1/1/1	-
2	EDO	B	406	-	-	1/1/1/1	-
2	EDO	A	411	-	-	1/1/1/1	-
3	NAD	D	501	-	-	5/26/62/62	0/5/5/5
2	EDO	G	503	-	-	0/1/1/1	-
3	NAD	E	402	-	-	5/26/62/62	0/5/5/5
2	EDO	K	404	-	-	0/1/1/1	-
2	EDO	A	410	-	-	0/1/1/1	-
3	NAD	B	402	-	-	5/26/62/62	0/5/5/5
2	EDO	D	503	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	J	406	-	-	1/1/1/1	-
2	EDO	J	403	-	-	1/1/1/1	-
2	EDO	G	506	-	-	0/1/1/1	-
2	EDO	E	407	-	-	0/1/1/1	-
2	EDO	C	411	-	-	0/1/1/1	-
2	EDO	L	401	-	-	0/1/1/1	-
2	EDO	H	706	1	-	0/1/1/1	-
2	EDO	G	508	-	-	0/1/1/1	-
2	EDO	I	404	-	-	1/1/1/1	-
2	EDO	C	413	-	-	1/1/1/1	-
2	EDO	B	405	-	-	0/1/1/1	-
3	NAD	I	402	-	-	5/26/62/62	0/5/5/5
2	EDO	H	707	-	-	0/1/1/1	-
2	EDO	C	405	-	-	0/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-
2	EDO	D	507	-	-	0/1/1/1	-
2	EDO	H	701	-	-	0/1/1/1	-
3	NAD	H	703	-	-	5/26/62/62	0/5/5/5
2	EDO	D	505	-	-	0/1/1/1	-
2	EDO	I	403	-	-	0/1/1/1	-
2	EDO	L	403	-	-	1/1/1/1	-
2	EDO	J	404	-	-	1/1/1/1	-

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAD	C5A-C6A-N6A	2.46	124.10	120.35
3	C	402	NAD	O4B-C1B-C2B	-2.41	103.41	106.93
3	C	402	NAD	C5A-C6A-N6A	2.40	124.00	120.35
3	F	402	NAD	C5A-C6A-N6A	2.39	123.99	120.35
3	B	402	NAD	C5A-C6A-N6A	2.37	123.96	120.35
3	E	402	NAD	C5A-C6A-N6A	2.37	123.95	120.35
3	L	402	NAD	C5A-C6A-N6A	2.37	123.95	120.35
3	G	501	NAD	C5A-C6A-N6A	2.35	123.92	120.35
3	J	402	NAD	C5A-C6A-N6A	2.35	123.92	120.35
3	H	703	NAD	C5A-C6A-N6A	2.30	123.84	120.35
3	L	402	NAD	C2N-N1N-C1D	-2.30	114.02	119.14
3	D	501	NAD	C5A-C6A-N6A	2.24	123.76	120.35
3	I	402	NAD	C5A-C6A-N6A	2.21	123.71	120.35
3	E	402	NAD	C2N-N1N-C1D	-2.17	114.30	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	402	NAD	C2N-N1N-C1D	-2.17	114.31	119.14
3	D	501	NAD	C2N-N1N-C1D	-2.16	114.33	119.14
3	F	402	NAD	O4B-C1B-C2B	-2.15	103.79	106.93
3	A	402	NAD	C2N-N1N-C1D	-2.13	114.38	119.14
3	J	402	NAD	O4B-C1B-C2B	-2.09	103.87	106.93
3	K	402	NAD	C5A-C6A-N6A	2.07	123.49	120.35
3	D	501	NAD	O4B-C1B-C2B	-2.04	103.95	106.93
3	I	402	NAD	C2N-N1N-C1D	-2.04	114.60	119.14
3	E	402	NAD	O4B-C1B-C2B	-2.03	103.97	106.93
3	B	402	NAD	O4B-C1B-C2B	-2.02	103.97	106.93
3	K	402	NAD	O4B-C1B-C2B	-2.02	103.97	106.93
3	G	501	NAD	C2N-N1N-C1D	-2.01	114.66	119.14

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	402	NAD	O4D-C1D-N1N-C2N
3	K	402	NAD	O4D-C1D-N1N-C6N
3	K	402	NAD	C2D-C1D-N1N-C2N
3	K	402	NAD	C2D-C1D-N1N-C6N
3	G	501	NAD	O4D-C1D-N1N-C2N
3	G	501	NAD	O4D-C1D-N1N-C6N
3	G	501	NAD	C2D-C1D-N1N-C2N
3	G	501	NAD	C2D-C1D-N1N-C6N
3	C	402	NAD	O4D-C1D-N1N-C2N
3	C	402	NAD	O4D-C1D-N1N-C6N
3	C	402	NAD	C2D-C1D-N1N-C2N
3	C	402	NAD	C2D-C1D-N1N-C6N
3	F	402	NAD	O4D-C1D-N1N-C2N
3	F	402	NAD	O4D-C1D-N1N-C6N
3	F	402	NAD	C2D-C1D-N1N-C2N
3	F	402	NAD	C2D-C1D-N1N-C6N
3	L	402	NAD	O4D-C1D-N1N-C2N
3	L	402	NAD	O4D-C1D-N1N-C6N
3	L	402	NAD	C2D-C1D-N1N-C2N
3	L	402	NAD	C2D-C1D-N1N-C6N
3	J	402	NAD	O4D-C1D-N1N-C2N
3	J	402	NAD	O4D-C1D-N1N-C6N
3	J	402	NAD	C2D-C1D-N1N-C2N
3	J	402	NAD	C2D-C1D-N1N-C6N
3	A	402	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	A	402	NAD	O4D-C1D-N1N-C6N
3	A	402	NAD	C2D-C1D-N1N-C2N
3	A	402	NAD	C2D-C1D-N1N-C6N
3	D	501	NAD	O4D-C1D-N1N-C2N
3	D	501	NAD	O4D-C1D-N1N-C6N
3	D	501	NAD	C2D-C1D-N1N-C2N
3	D	501	NAD	C2D-C1D-N1N-C6N
3	E	402	NAD	O4D-C1D-N1N-C2N
3	E	402	NAD	O4D-C1D-N1N-C6N
3	E	402	NAD	C2D-C1D-N1N-C2N
3	E	402	NAD	C2D-C1D-N1N-C6N
3	B	402	NAD	O4D-C1D-N1N-C2N
3	B	402	NAD	O4D-C1D-N1N-C6N
3	B	402	NAD	C2D-C1D-N1N-C2N
3	B	402	NAD	C2D-C1D-N1N-C6N
3	I	402	NAD	O4D-C1D-N1N-C2N
3	I	402	NAD	O4D-C1D-N1N-C6N
3	I	402	NAD	C2D-C1D-N1N-C2N
3	I	402	NAD	C2D-C1D-N1N-C6N
3	H	703	NAD	O4D-C1D-N1N-C2N
3	H	703	NAD	O4D-C1D-N1N-C6N
3	H	703	NAD	C2D-C1D-N1N-C2N
3	H	703	NAD	C2D-C1D-N1N-C6N
2	C	403	EDO	O1-C1-C2-O2
2	A	406	EDO	O1-C1-C2-O2
2	E	406	EDO	O1-C1-C2-O2
2	C	401	EDO	O1-C1-C2-O2
2	C	406	EDO	O1-C1-C2-O2
2	J	407	EDO	O1-C1-C2-O2
3	H	703	NAD	O4B-C4B-C5B-O5B
2	A	401	EDO	O1-C1-C2-O2
2	J	405	EDO	O1-C1-C2-O2
2	C	412	EDO	O1-C1-C2-O2
2	J	406	EDO	O1-C1-C2-O2
2	L	404	EDO	O1-C1-C2-O2
2	J	408	EDO	O1-C1-C2-O2
2	A	411	EDO	O1-C1-C2-O2
2	I	406	EDO	O1-C1-C2-O2
2	K	401	EDO	O1-C1-C2-O2
2	E	408	EDO	O1-C1-C2-O2
2	A	412	EDO	O1-C1-C2-O2
3	L	402	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	E	402	NAD	O4B-C4B-C5B-O5B
2	G	504	EDO	O1-C1-C2-O2
2	B	408	EDO	O1-C1-C2-O2
2	I	407	EDO	O1-C1-C2-O2
2	B	406	EDO	O1-C1-C2-O2
2	J	403	EDO	O1-C1-C2-O2
2	C	413	EDO	O1-C1-C2-O2
2	J	404	EDO	O1-C1-C2-O2
3	C	402	NAD	O4B-C4B-C5B-O5B
3	F	402	NAD	O4B-C4B-C5B-O5B
3	D	501	NAD	O4B-C4B-C5B-O5B
3	B	402	NAD	O4B-C4B-C5B-O5B
3	I	402	NAD	O4B-C4B-C5B-O5B
3	K	402	NAD	O4B-C4B-C5B-O5B
3	G	501	NAD	O4B-C4B-C5B-O5B
3	J	402	NAD	O4B-C4B-C5B-O5B
3	A	402	NAD	O4B-C4B-C5B-O5B
2	K	403	EDO	O1-C1-C2-O2
2	I	404	EDO	O1-C1-C2-O2
2	L	403	EDO	O1-C1-C2-O2

There are no ring outliers.

34 monomers are involved in 44 short contacts:

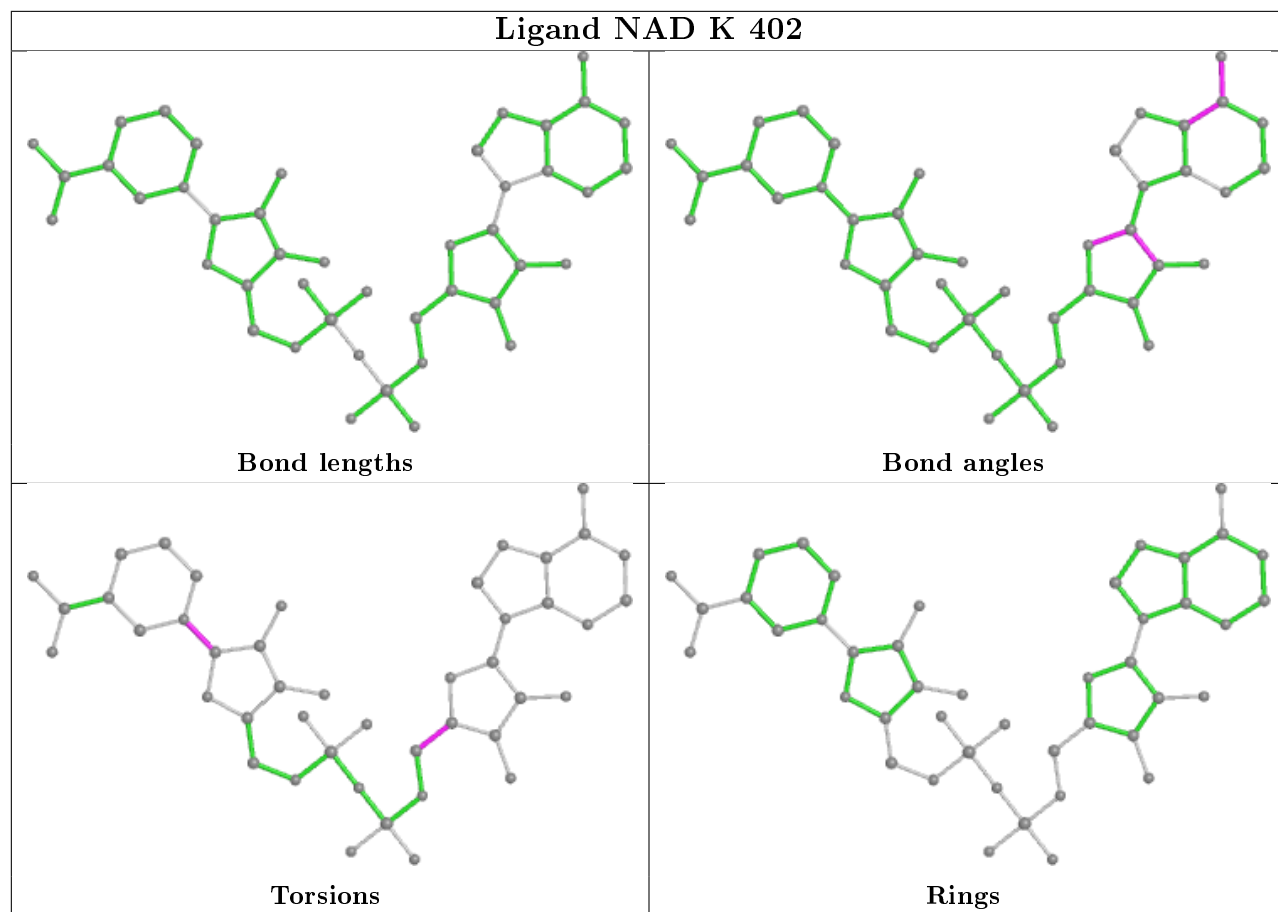
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	411	EDO	1	0
2	J	407	EDO	2	0
3	K	402	NAD	1	0
2	H	704	EDO	1	0
2	C	406	EDO	2	0
2	F	404	EDO	1	0
2	C	407	EDO	2	0
2	F	409	EDO	1	0
3	G	501	NAD	1	0
2	A	406	EDO	1	0
2	B	403	EDO	1	0
2	A	401	EDO	1	0
2	I	405	EDO	1	0
3	L	402	NAD	2	0
3	J	402	NAD	1	0
2	E	406	EDO	2	0
2	F	407	EDO	1	0

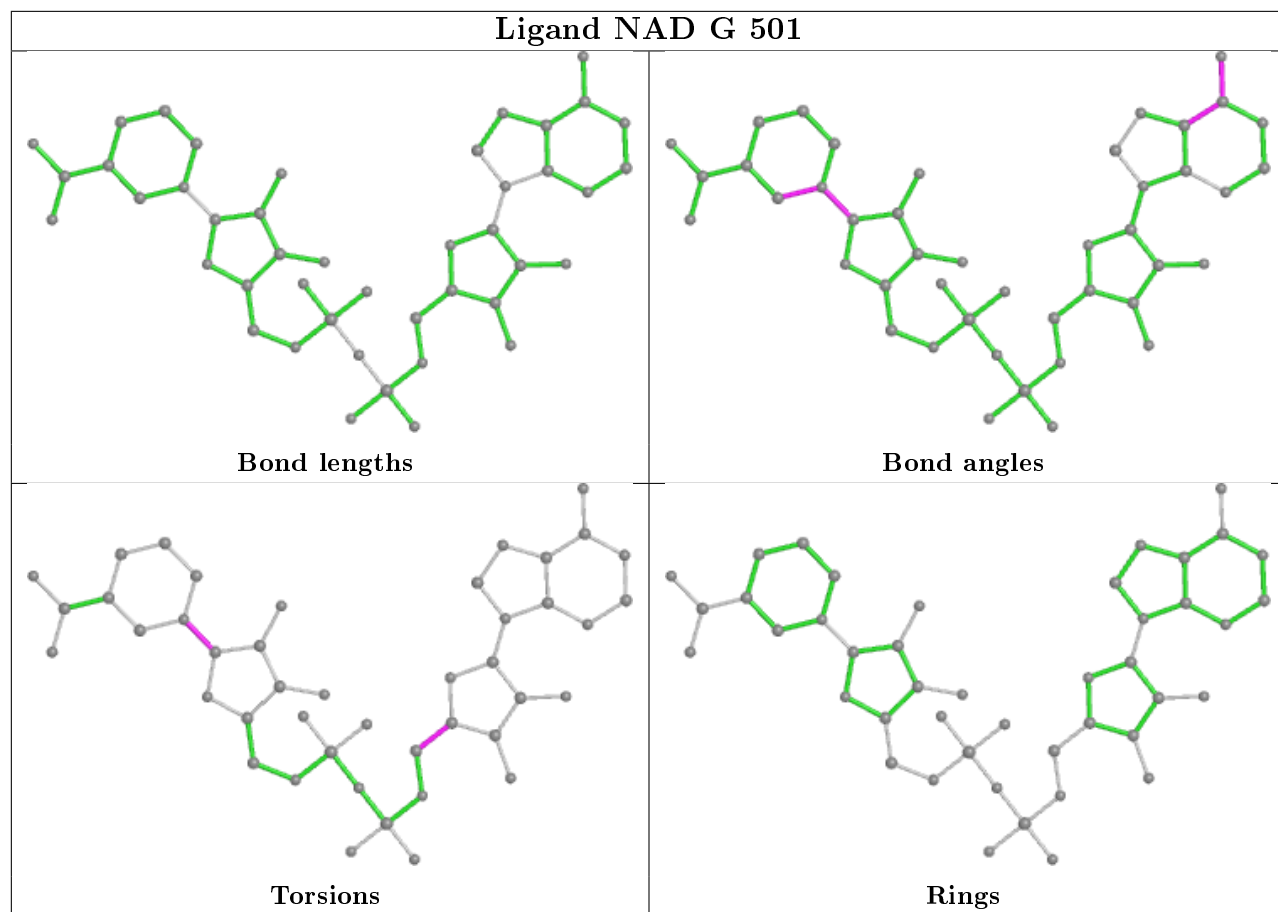
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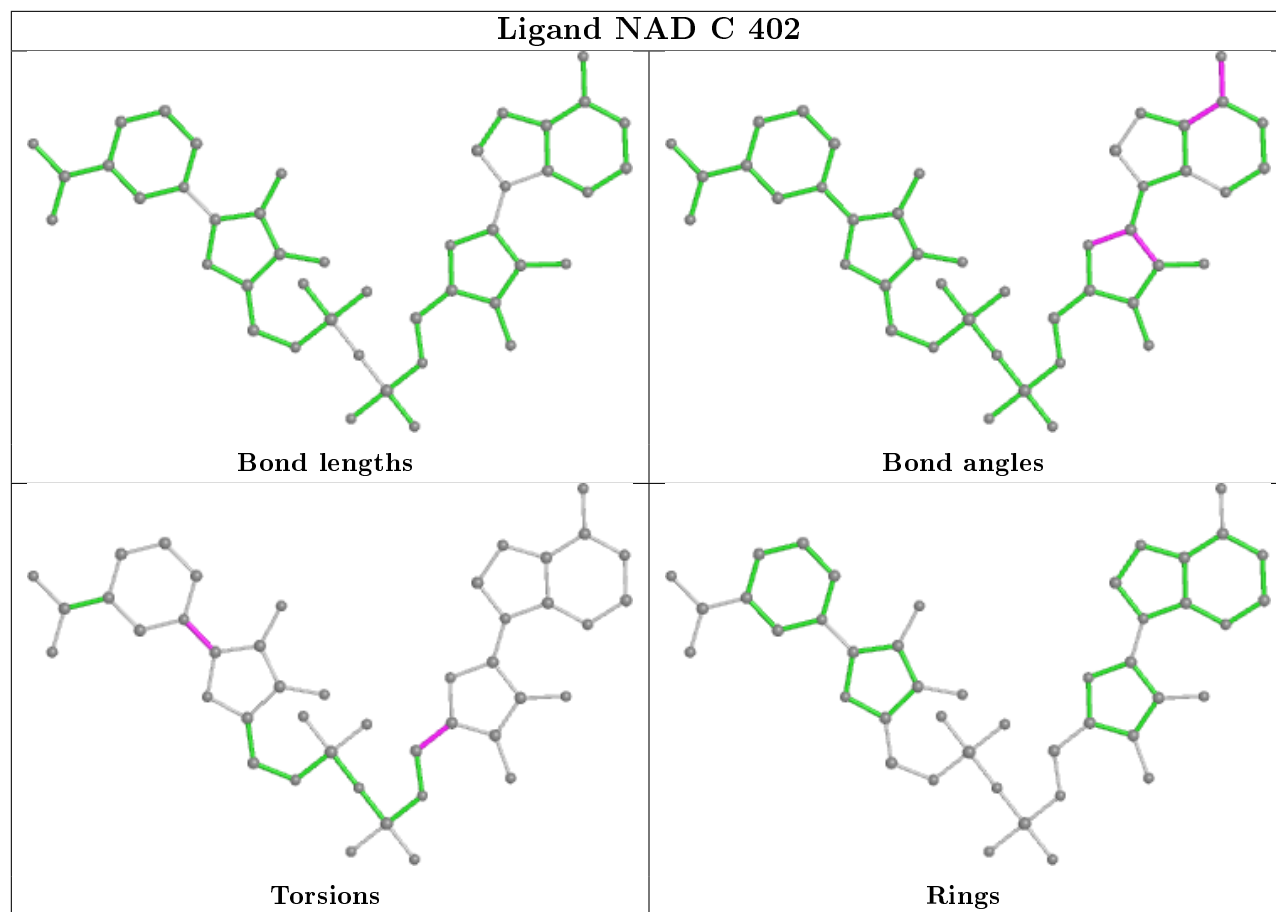
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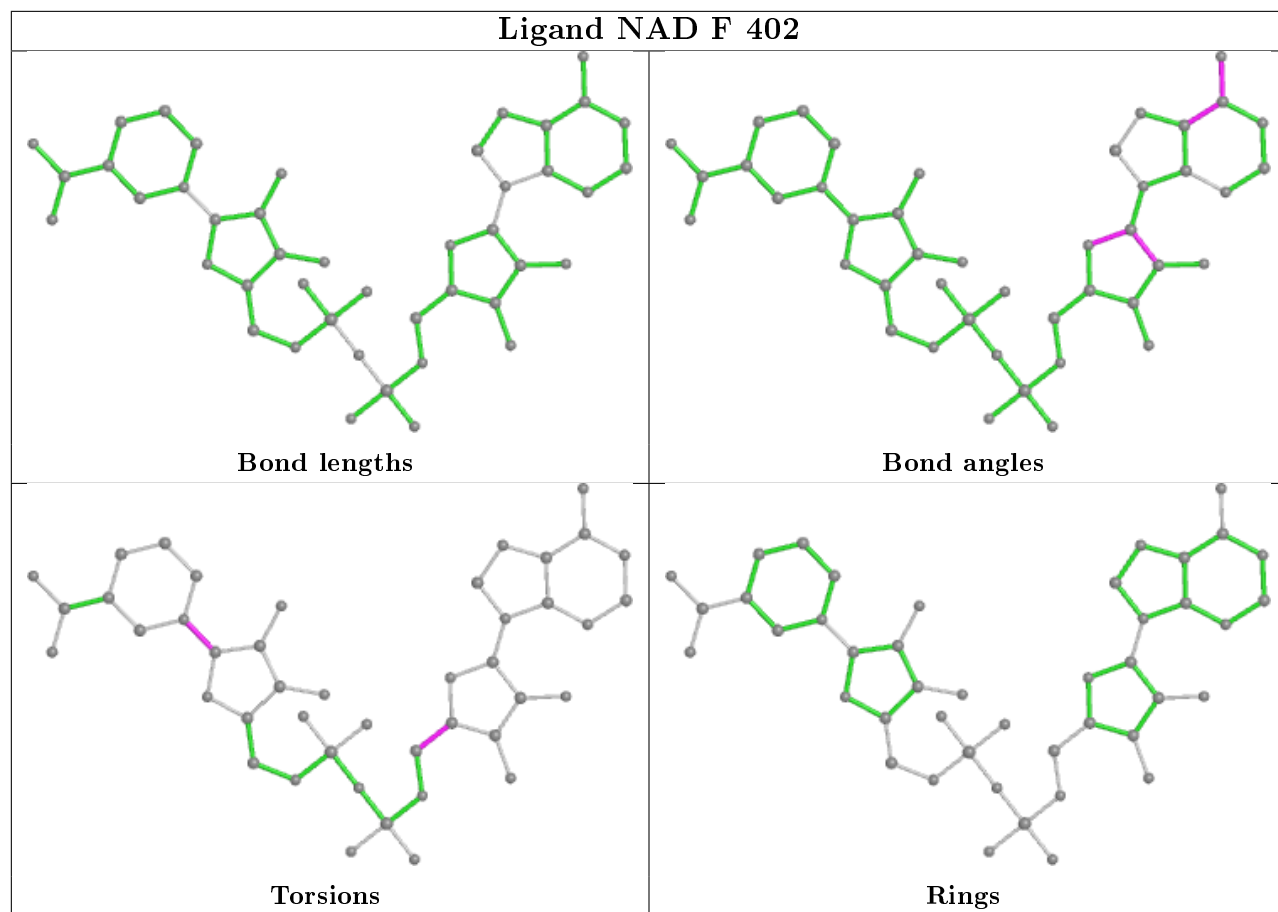
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	EDO	2	0
2	A	409[B]	EDO	1	0
2	C	412	EDO	1	0
2	B	404	EDO	1	0
2	C	404	EDO	1	0
2	D	508	EDO	1	0
2	E	410	EDO	1	0
3	D	501	NAD	2	0
2	G	503	EDO	2	0
3	B	402	NAD	1	0
2	E	407	EDO	1	0
2	G	508	EDO	1	0
2	I	404	EDO	2	0
3	I	402	NAD	1	0
2	H	701	EDO	2	0
3	H	703	NAD	1	0
2	D	505	EDO	1	0

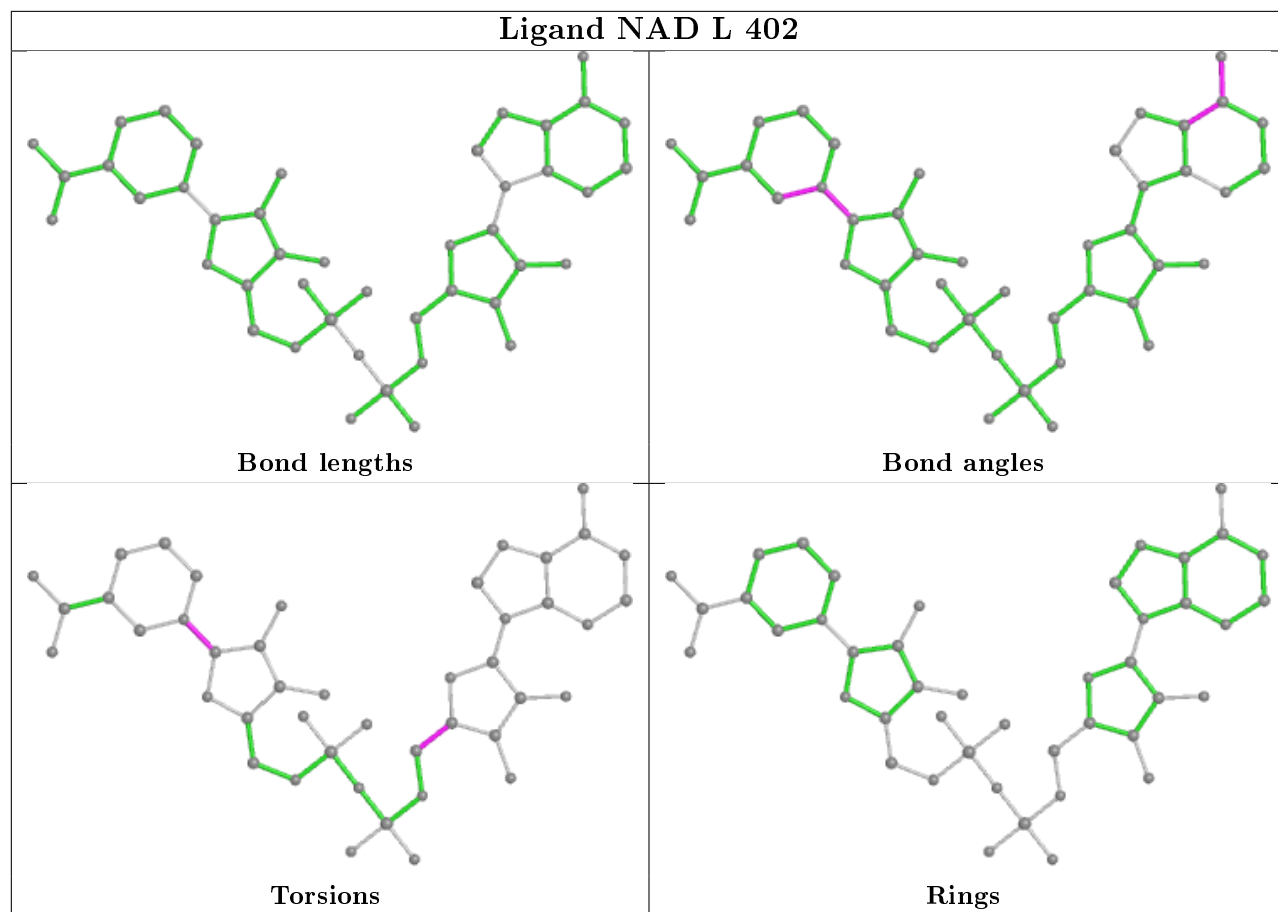
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

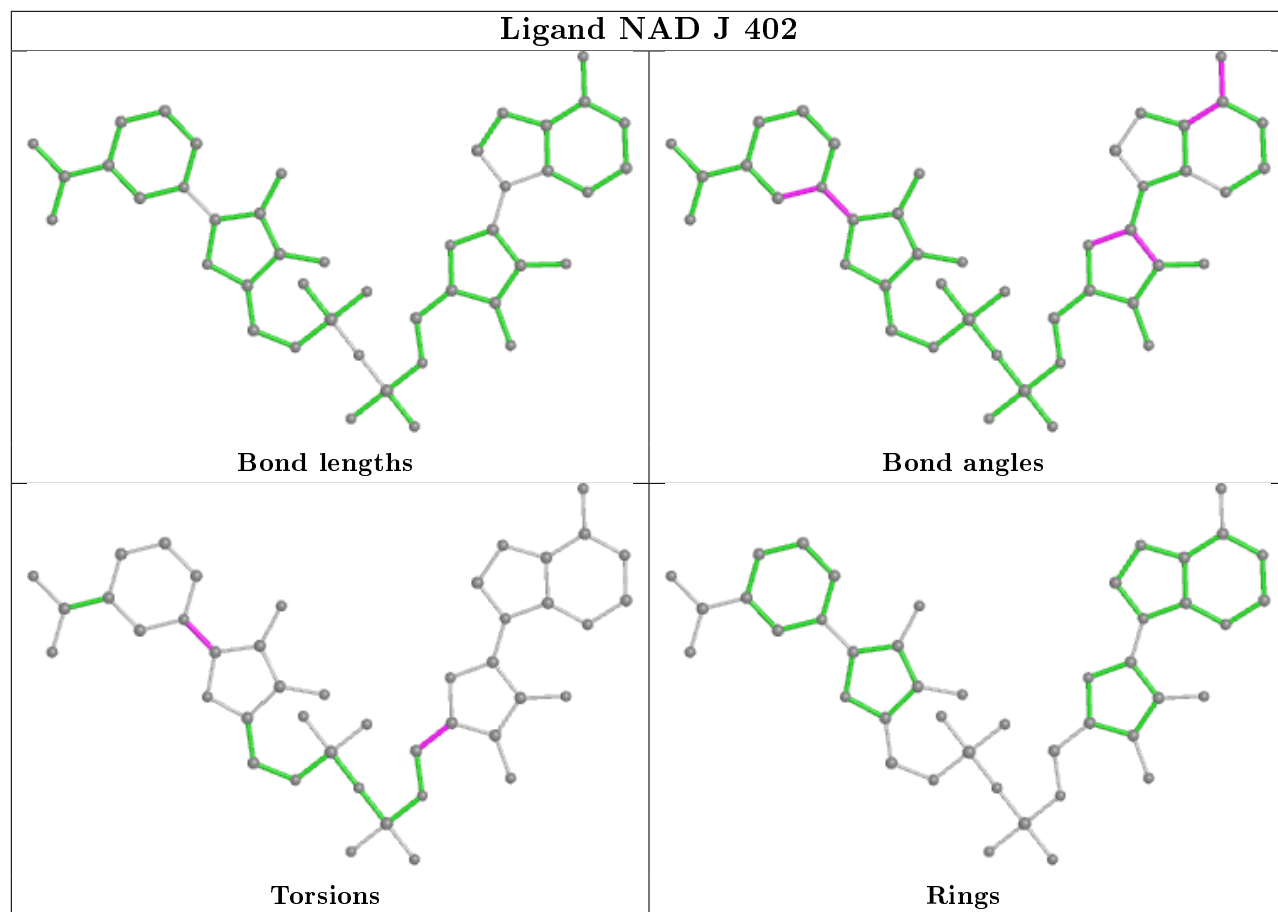


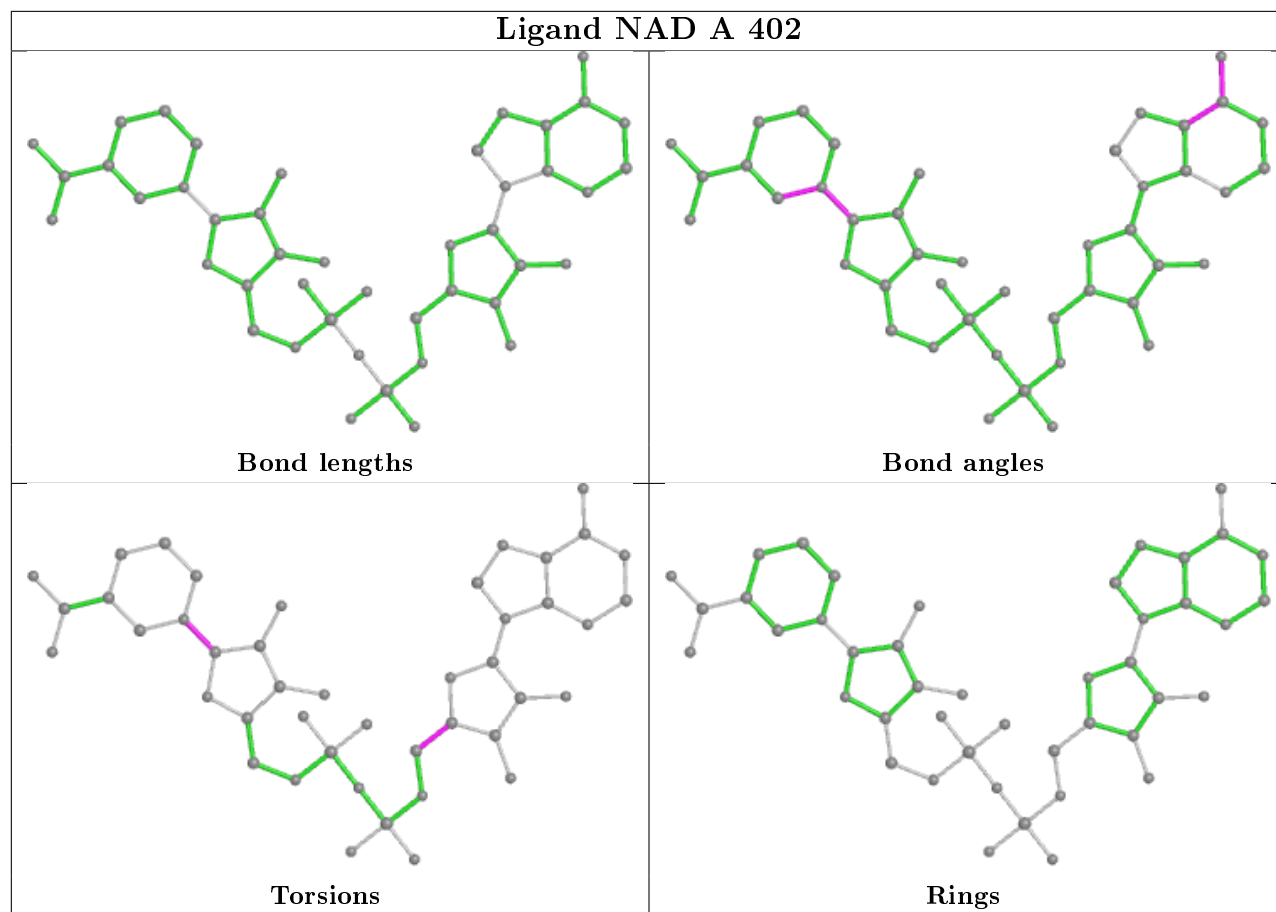


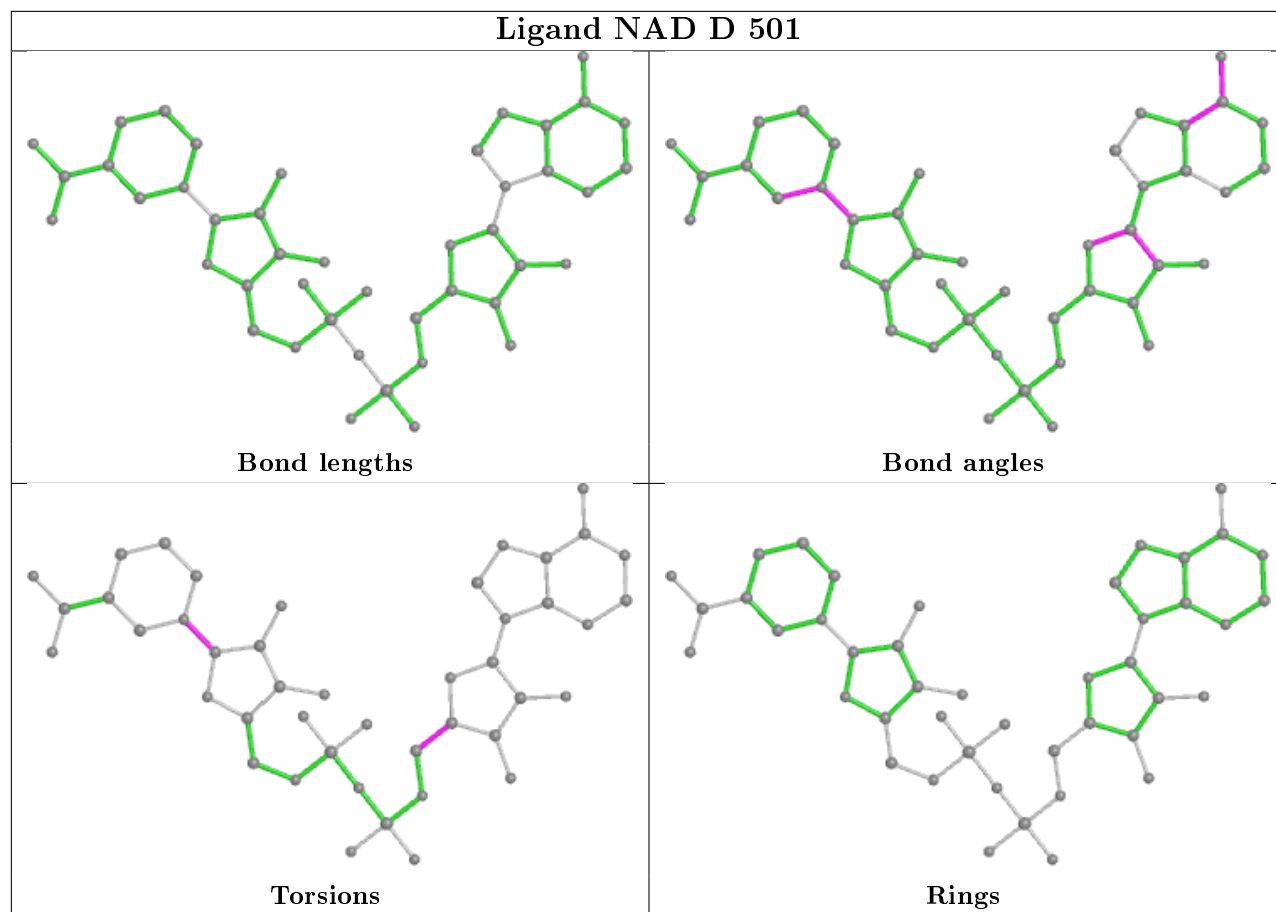


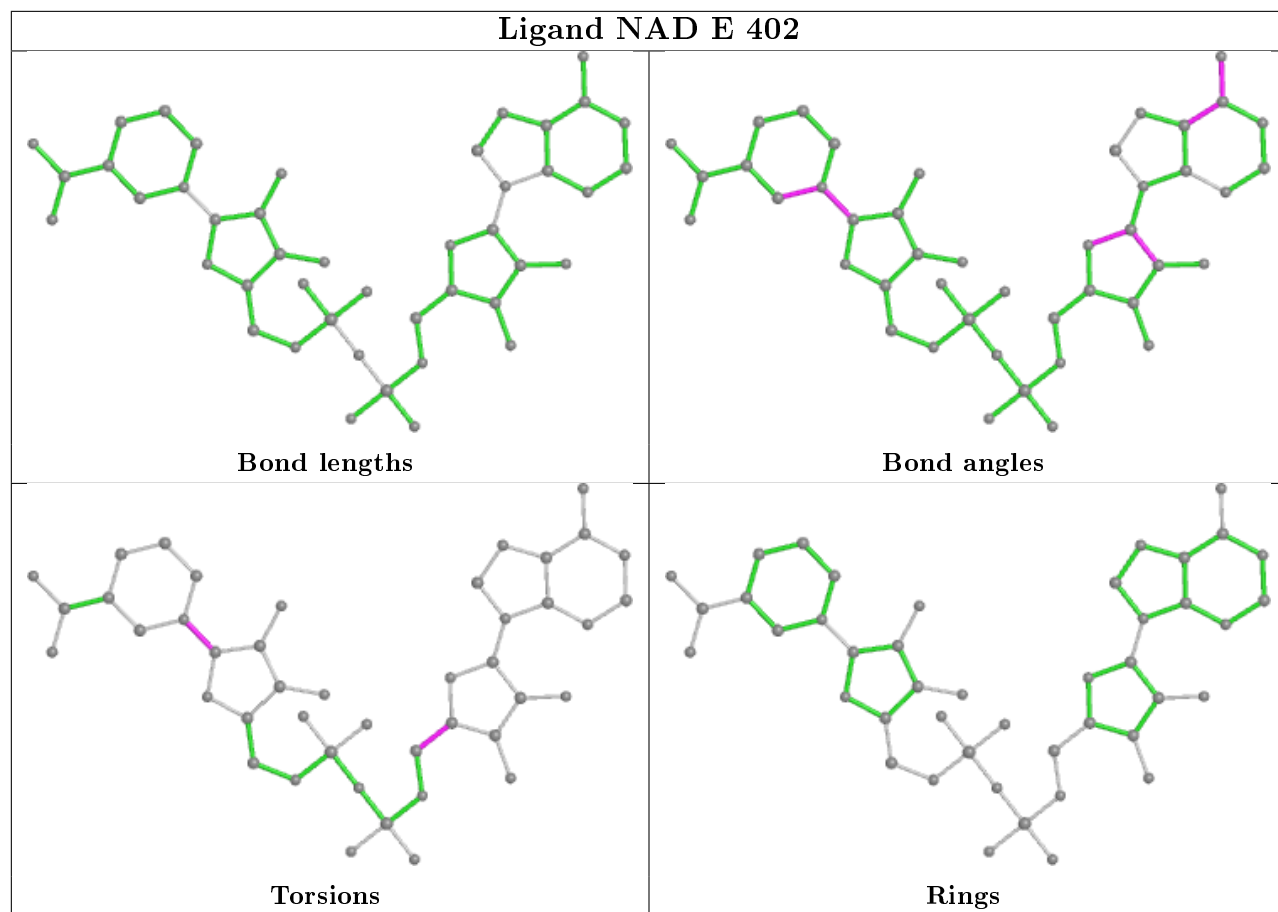


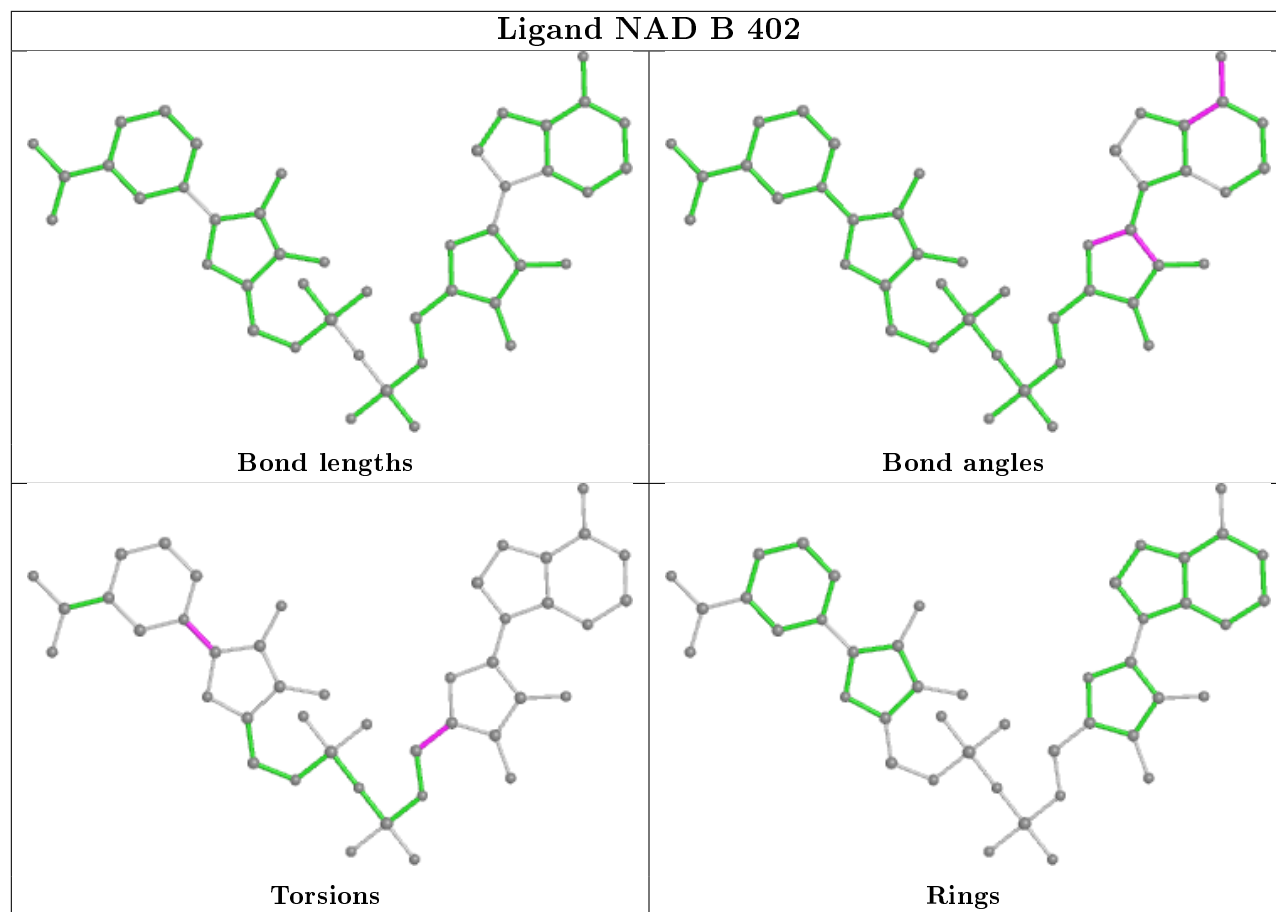


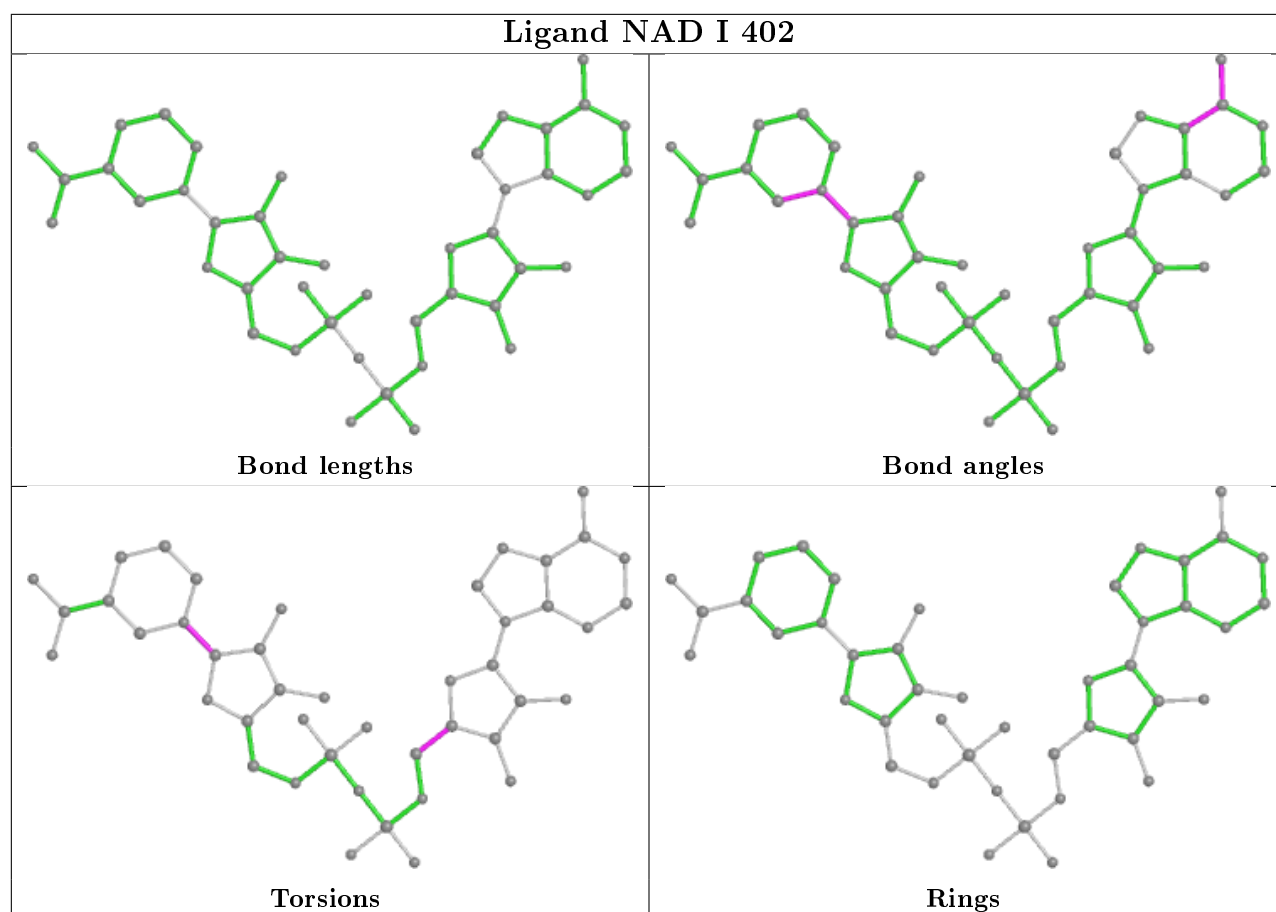


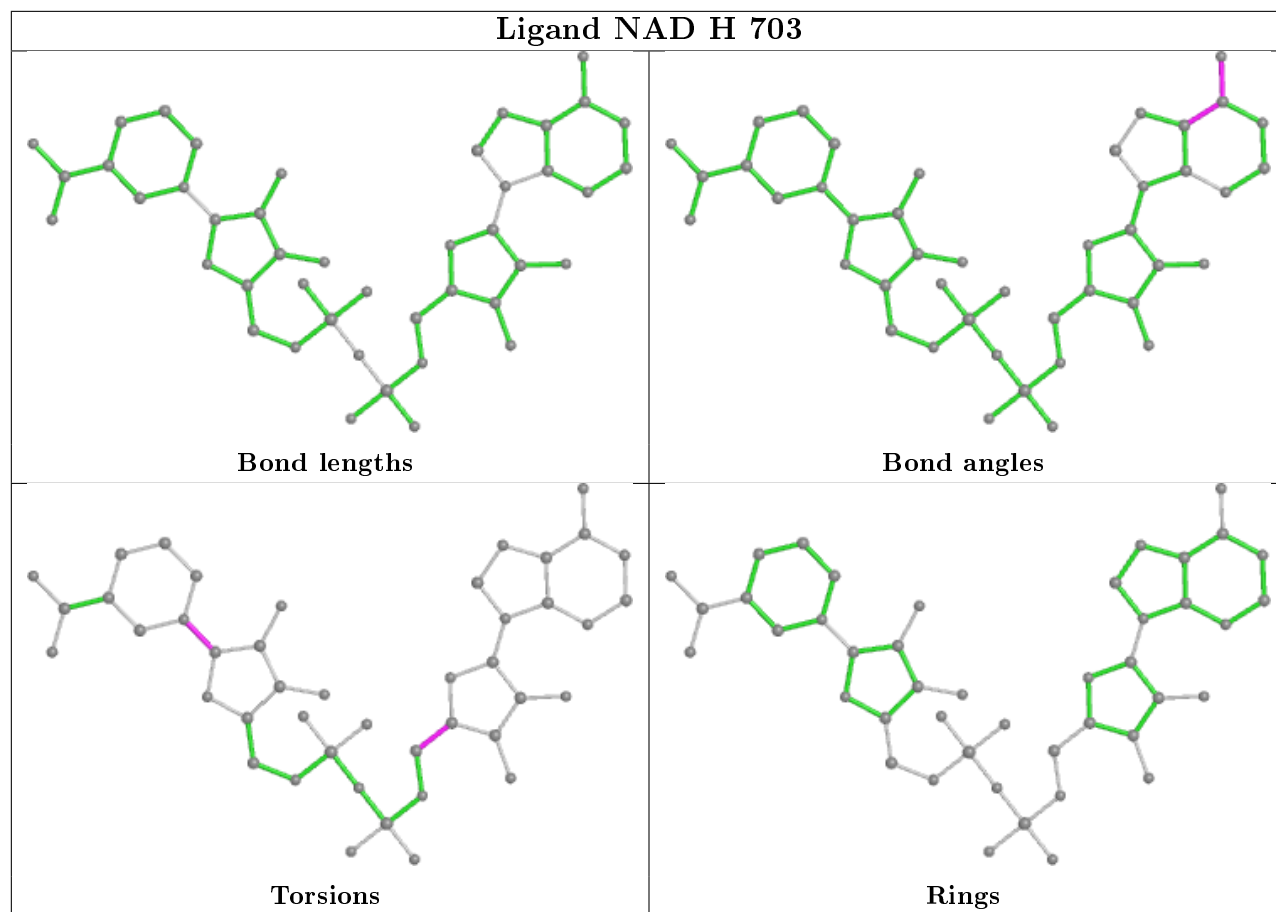












5.7 Other polymers [i](#)

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

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	342/353 (96%)	-0.53	0 100 100	19, 30, 54, 89	0
1	B	342/353 (96%)	-0.46	2 (0%) 89 91	18, 30, 56, 89	0
1	C	344/353 (97%)	-0.45	2 (0%) 89 91	18, 27, 43, 95	0
1	D	343/353 (97%)	-0.34	0 100 100	20, 31, 55, 91	0
1	E	340/353 (96%)	-0.24	8 (2%) 59 64	22, 36, 77, 106	0
1	F	343/353 (97%)	-0.38	5 (1%) 73 77	22, 33, 58, 86	0
1	G	340/353 (96%)	-0.29	1 (0%) 94 94	19, 36, 70, 83	0
1	H	342/353 (96%)	-0.37	2 (0%) 89 91	23, 38, 64, 101	0
1	I	341/353 (96%)	0.17	17 (4%) 28 34	30, 52, 87, 117	0
1	J	343/353 (97%)	-0.29	0 100 100	23, 40, 65, 86	0
1	K	342/353 (96%)	-0.42	2 (0%) 89 91	26, 39, 62, 92	0
1	L	340/353 (96%)	0.40	34 (10%) 7 9	32, 54, 89, 119	0
All	All	4102/4236 (96%)	-0.27	73 (1%) 68 72	18, 36, 72, 119	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	18	LEU	6.2
1	F	1	MET	4.8
1	L	62	LEU	4.4
1	L	14	TYR	4.2
1	B	342	GLY	4.0
1	F	342	GLY	3.7
1	I	1	MET	3.6
1	H	342	GLY	3.6
1	L	50	VAL	3.5
1	F	2	ILE	3.5
1	L	8	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	5	THR	3.4
1	E	23	VAL	3.3
1	L	200	VAL	3.1
1	I	14	TYR	3.1
1	L	338	LEU	3.0
1	L	15	GLY	3.0
1	I	24	PRO	3.0
1	L	63	ILE	3.0
1	E	28	PRO	2.9
1	L	341	ALA	2.9
1	I	74	ALA	2.9
1	L	9	ALA	2.9
1	C	0	HIS	2.8
1	B	3	PRO	2.8
1	L	324	PHE	2.8
1	E	3	PRO	2.8
1	L	51	ASP	2.8
1	I	3	PRO	2.8
1	H	1	MET	2.7
1	I	129	ILE	2.7
1	I	9	ALA	2.7
1	I	62	LEU	2.7
1	G	73	VAL	2.6
1	L	222	THR	2.6
1	L	11	VAL	2.6
1	L	24	PRO	2.6
1	L	61	PRO	2.6
1	I	35	VAL	2.5
1	I	340	ILE	2.5
1	I	28	PRO	2.5
1	C	342	GLY	2.5
1	L	60	MET	2.5
1	I	25	VAL	2.5
1	L	323	VAL	2.5
1	L	17	PRO	2.5
1	E	20	ILE	2.4
1	L	13	GLY	2.4
1	E	27	GLU	2.4
1	F	0	HIS	2.3
1	L	5	THR	2.3
1	E	14	TYR	2.3
1	L	124	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	243	VAL	2.2
1	I	75	CYS	2.2
1	L	201	ALA	2.2
1	I	12	GLN	2.2
1	K	342	GLY	2.2
1	L	73	VAL	2.2
1	L	330	GLY	2.2
1	L	47	LEU	2.2
1	L	127	TYR	2.2
1	I	73	VAL	2.1
1	L	25	VAL	2.1
1	E	6	MET	2.1
1	I	56	ALA	2.1
1	L	12	GLN	2.1
1	K	1	MET	2.1
1	I	8	ALA	2.0
1	L	319	ASP	2.0
1	F	24	PRO	2.0
1	L	6	MET	2.0
1	L	129	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	E	405	4/4	0.77	0.24	54,58,58,64	0
2	EDO	I	407	4/4	0.78	0.22	65,65,68,69	0
2	EDO	J	407	4/4	0.79	0.16	50,51,56,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	I	405	4/4	0.79	0.34	66,67,68,68	0
2	EDO	J	401	4/4	0.81	0.20	45,47,50,61	0
2	EDO	F	409	4/4	0.82	0.17	49,58,64,64	0
2	EDO	C	408	4/4	0.83	0.29	56,59,62,64	0
2	EDO	G	504	4/4	0.84	0.27	64,65,67,69	0
2	EDO	D	504	4/4	0.85	0.17	32,37,41,43	0
2	EDO	J	405	4/4	0.85	0.20	60,62,63,63	0
2	EDO	E	407	4/4	0.85	0.20	68,69,72,72	0
2	EDO	D	509	4/4	0.86	0.23	61,64,72,76	0
2	EDO	F	410	4/4	0.86	0.19	53,58,63,68	0
2	EDO	J	408	4/4	0.86	0.24	55,67,73,73	0
2	EDO	C	401	4/4	0.86	0.14	32,35,35,35	0
2	EDO	C	413	4/4	0.86	0.17	46,48,54,57	0
2	EDO	C	405	4/4	0.86	0.14	50,51,55,63	0
2	EDO	D	507	4/4	0.86	0.26	58,66,71,73	0
2	EDO	G	508	4/4	0.87	0.15	46,47,47,47	0
2	EDO	G	505	4/4	0.87	0.23	47,49,50,52	0
2	EDO	C	406	4/4	0.88	0.21	44,49,52,64	0
2	EDO	I	401	4/4	0.88	0.13	41,45,46,48	0
2	EDO	E	401	4/4	0.88	0.14	30,39,42,46	0
2	EDO	L	401	4/4	0.88	0.16	40,49,54,55	0
2	EDO	I	403	4/4	0.88	0.18	65,65,68,76	0
2	EDO	F	408	4/4	0.89	0.25	68,69,69,74	0
2	EDO	H	702	4/4	0.89	0.13	37,41,43,44	0
2	EDO	K	401	4/4	0.89	0.17	40,41,51,57	0
2	EDO	D	508	4/4	0.90	0.30	40,52,56,59	0
2	EDO	F	401	4/4	0.90	0.15	42,44,48,50	0
2	EDO	G	507	4/4	0.90	0.24	71,72,73,76	0
2	EDO	E	408	4/4	0.90	0.19	44,48,55,63	0
2	EDO	C	407	4/4	0.90	0.22	48,50,52,56	0
2	EDO	D	506	4/4	0.90	0.18	53,57,58,59	0
2	EDO	A	405	4/4	0.90	0.19	43,44,52,55	0
2	EDO	B	401	4/4	0.90	0.15	33,47,51,54	0
2	EDO	D	505	4/4	0.90	0.24	50,54,55,57	0
2	EDO	I	406	4/4	0.90	0.19	56,56,57,57	0
2	EDO	L	403	4/4	0.90	0.19	58,59,60,65	0
2	EDO	J	404	4/4	0.90	0.21	67,69,69,72	0
2	EDO	A	410	4/4	0.91	0.18	63,66,69,72	0
2	EDO	A	401	4/4	0.91	0.15	34,35,36,40	0
5	CL	I	410	1/1	0.91	0.07	80,80,80,80	0
2	EDO	H	706	4/4	0.91	0.12	50,51,54,55	0
2	EDO	G	502	4/4	0.91	0.22	58,59,61,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	B	408	4/4	0.91	0.26	46,50,55,58	0
2	EDO	H	707	4/4	0.91	0.14	51,55,59,65	0
2	EDO	B	406	4/4	0.92	0.17	60,60,62,63	0
2	EDO	A	411	4/4	0.92	0.30	59,66,70,74	0
2	EDO	A	409[A]	4/4	0.92	0.17	28,33,36,36	4
2	EDO	J	406	4/4	0.92	0.18	65,67,68,76	0
2	EDO	G	506	4/4	0.92	0.32	63,68,71,74	0
2	EDO	A	403	4/4	0.92	0.19	40,50,50,53	0
2	EDO	F	405	4/4	0.92	0.15	38,38,41,41	0
2	EDO	A	409[B]	4/4	0.92	0.17	28,34,36,36	4
2	EDO	L	404	4/4	0.92	0.34	51,52,53,61	0
2	EDO	F	403	4/4	0.93	0.15	47,48,51,54	0
2	EDO	B	403	4/4	0.93	0.19	48,48,57,57	0
2	EDO	I	404	4/4	0.93	0.26	56,56,65,67	0
2	EDO	A	404	4/4	0.93	0.10	57,59,59,62	0
2	EDO	D	502	4/4	0.93	0.11	45,48,49,50	0
2	EDO	F	407	4/4	0.93	0.19	49,53,53,54	0
2	EDO	C	409	4/4	0.93	0.20	56,58,61,64	0
5	CL	G	511	1/1	0.93	0.07	54,54,54,54	0
2	EDO	E	409	4/4	0.93	0.19	50,51,58,59	0
2	EDO	C	403	4/4	0.93	0.16	43,45,47,52	0
2	EDO	H	705	4/4	0.93	0.13	43,45,48,51	0
2	EDO	F	406	4/4	0.93	0.20	53,55,59,59	0
2	EDO	C	412	4/4	0.94	0.09	57,60,61,64	0
2	EDO	K	405	4/4	0.94	0.21	51,54,63,69	0
2	EDO	A	412	4/4	0.94	0.21	55,57,58,64	0
2	EDO	A	406	4/4	0.94	0.19	26,39,44,56	0
2	EDO	B	405	4/4	0.94	0.34	59,60,62,63	0
5	CL	L	407	1/1	0.94	0.07	64,64,64,64	0
5	CL	E	413	1/1	0.94	0.10	55,55,55,55	0
2	EDO	G	503	4/4	0.94	0.24	36,42,47,57	0
2	EDO	K	404	4/4	0.94	0.21	38,48,49,52	0
2	EDO	H	704	4/4	0.94	0.10	52,53,55,57	0
2	EDO	H	701	4/4	0.94	0.13	50,54,56,59	0
5	CL	D	512	1/1	0.94	0.06	53,53,53,53	0
5	CL	K	408	1/1	0.94	0.09	60,60,60,60	0
2	EDO	F	411	4/4	0.94	0.15	40,45,47,47	0
5	CL	F	414	1/1	0.94	0.10	56,56,56,56	0
2	EDO	B	404	4/4	0.95	0.18	23,28,43,55	0
2	EDO	D	503	4/4	0.95	0.17	50,52,55,69	0
2	EDO	K	403	4/4	0.95	0.09	52,53,54,58	0
2	EDO	A	408	4/4	0.95	0.20	49,51,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	F	404	4/4	0.95	0.18	22,29,38,44	0
4	ZN	I	409	1/1	0.95	0.21	70,70,70,70	0
2	EDO	E	403	4/4	0.95	0.17	47,55,57,60	0
5	CL	J	411	1/1	0.96	0.06	56,56,56,56	0
3	NAD	I	402	44/44	0.96	0.09	35,44,50,63	0
2	EDO	J	403	4/4	0.96	0.14	63,64,64,66	0
3	NAD	L	402	44/44	0.96	0.10	34,50,59,67	0
2	EDO	C	410	4/4	0.96	0.10	32,40,44,47	0
2	EDO	C	411	4/4	0.96	0.23	43,55,56,62	0
2	EDO	E	406	4/4	0.97	0.13	21,30,42,43	0
5	CL	C	416	1/1	0.97	0.09	54,54,54,54	0
5	CL	B	411	1/1	0.97	0.07	49,49,49,49	0
5	CL	H	710	1/1	0.97	0.07	54,54,54,54	0
3	NAD	H	703	44/44	0.97	0.09	22,34,39,41	0
2	EDO	A	407	4/4	0.97	0.13	31,36,38,39	0
2	EDO	B	407	4/4	0.97	0.09	27,35,38,39	0
4	ZN	J	410	1/1	0.97	0.06	38,38,38,38	0
2	EDO	E	404	4/4	0.97	0.08	40,48,50,54	0
3	NAD	K	402	44/44	0.98	0.08	21,31,38,39	0
3	NAD	D	501	44/44	0.98	0.09	19,28,31,32	0
2	EDO	E	410	4/4	0.98	0.23	35,36,43,51	0
3	NAD	E	402	44/44	0.98	0.08	24,31,37,42	0
3	NAD	A	402	44/44	0.98	0.08	18,25,30,31	0
3	NAD	G	501	44/44	0.98	0.08	22,31,36,37	0
4	ZN	I	408	1/1	0.98	0.07	50,50,50,50	0
3	NAD	B	402	44/44	0.98	0.08	15,23,29,30	0
4	ZN	L	405	1/1	0.98	0.06	57,57,57,57	0
4	ZN	D	510	1/1	0.99	0.10	31,31,31,31	0
2	EDO	C	404	4/4	0.99	0.11	37,37,41,41	0
4	ZN	K	406	1/1	0.99	0.07	36,36,36,36	0
4	ZN	E	411	1/1	0.99	0.06	35,35,35,35	0
4	ZN	F	412	1/1	0.99	0.07	30,30,30,30	0
5	CL	A	415	1/1	0.99	0.09	48,48,48,48	0
3	NAD	C	402	44/44	0.99	0.09	15,22,27,30	0
4	ZN	G	509	1/1	0.99	0.07	33,33,33,33	0
3	NAD	J	402	44/44	0.99	0.08	22,34,40,44	0
4	ZN	J	409	1/1	0.99	0.05	38,38,38,38	0
4	ZN	K	407	1/1	0.99	0.09	37,37,37,37	0
4	ZN	H	709	1/1	0.99	0.09	32,32,32,32	0
3	NAD	F	402	44/44	0.99	0.08	19,28,32,37	0
4	ZN	H	708	1/1	0.99	0.06	34,34,34,34	0
4	ZN	G	510	1/1	1.00	0.06	32,32,32,32	0

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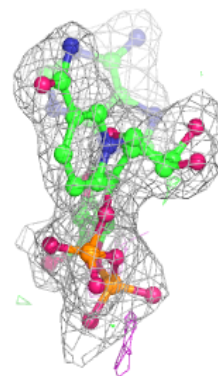
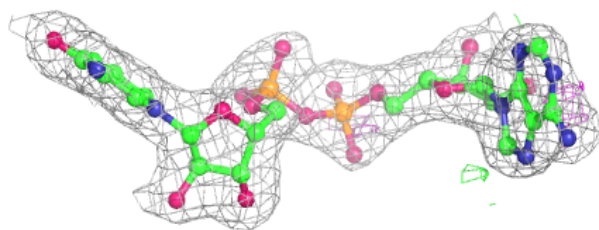
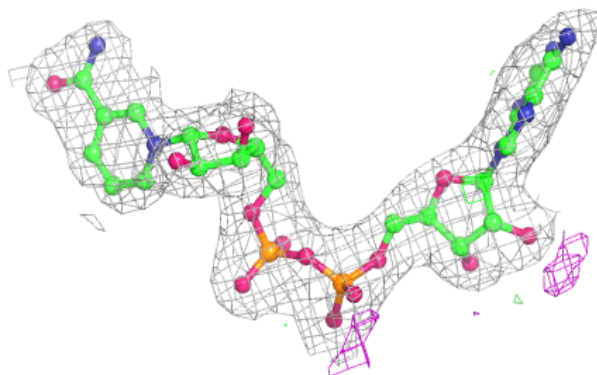
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	D	511	1/1	1.00	0.10	26,26,26,26	0
4	ZN	C	415	1/1	1.00	0.10	29,29,29,29	0
4	ZN	A	413	1/1	1.00	0.09	29,29,29,29	0
4	ZN	F	413	1/1	1.00	0.11	30,30,30,30	0
4	ZN	E	412	1/1	1.00	0.09	29,29,29,29	0
4	ZN	B	409	1/1	1.00	0.08	29,29,29,29	0
4	ZN	B	410	1/1	1.00	0.10	27,27,27,27	0
4	ZN	A	414	1/1	1.00	0.08	25,25,25,25	0
4	ZN	C	414	1/1	1.00	0.09	27,27,27,27	0
4	ZN	L	406	1/1	1.00	0.08	39,39,39,39	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.

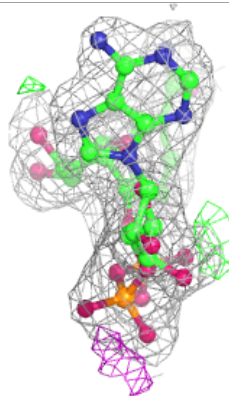
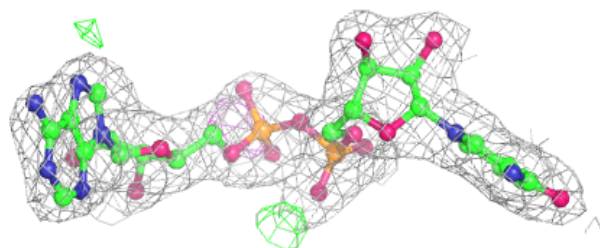
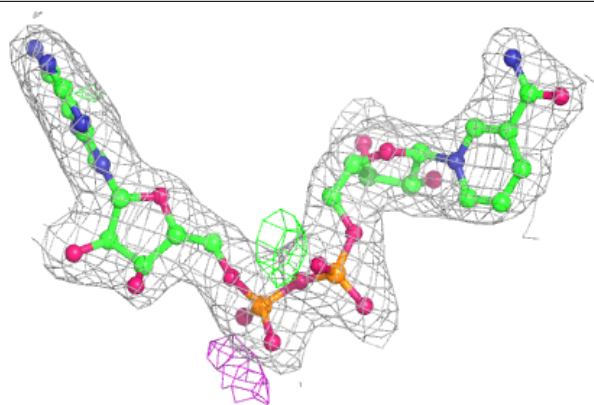
Electron density around NAD I 402:

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

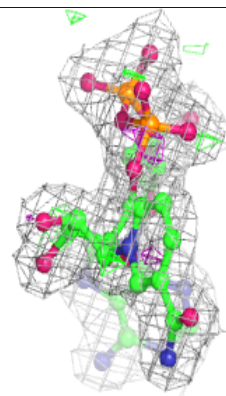
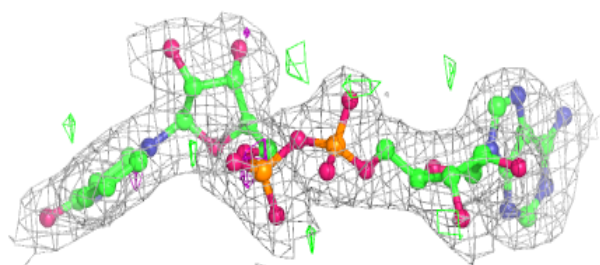
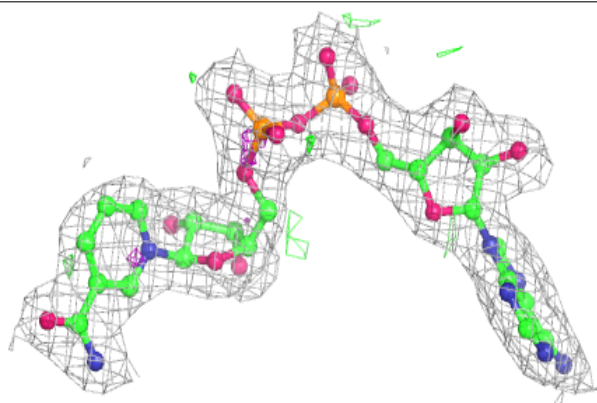


Electron density around NAD L 402:

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

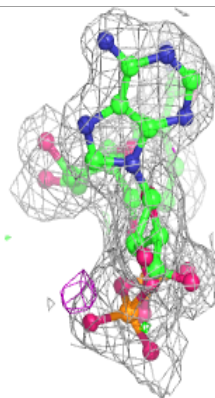
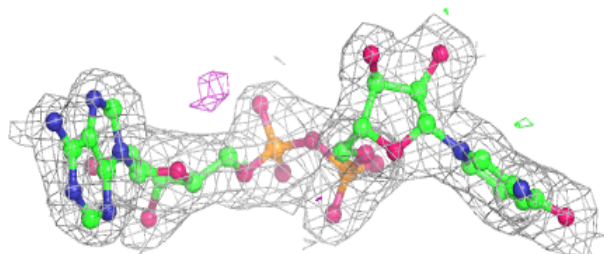
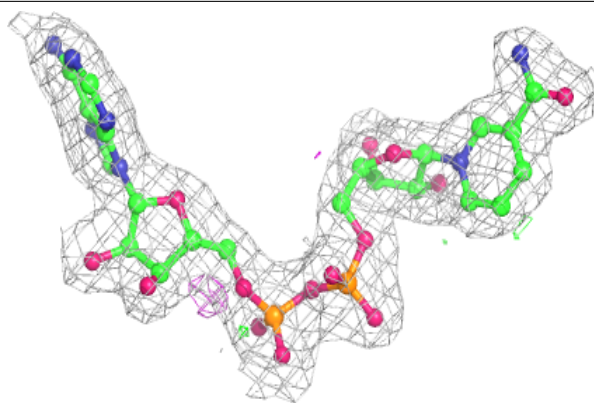
**Electron density around NAD H 703:**

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

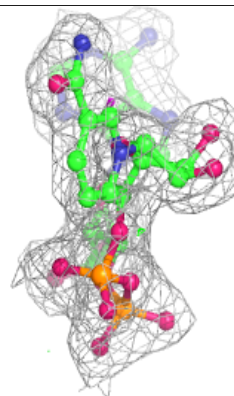
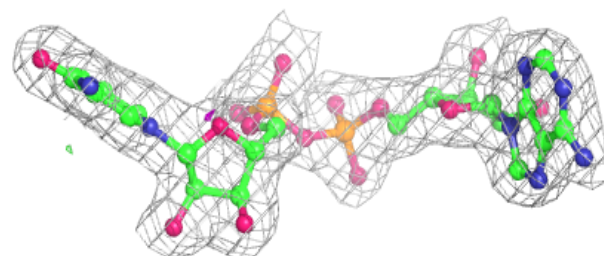
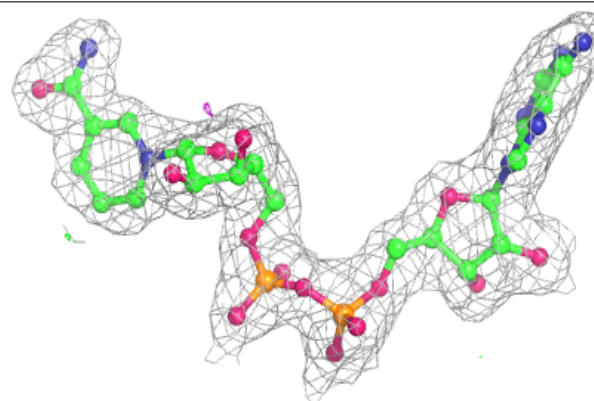


Electron density around NAD K 402:

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

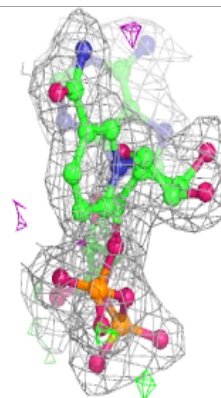
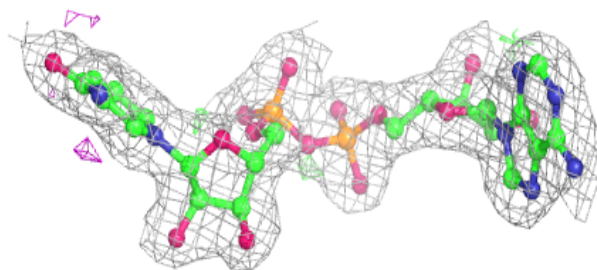
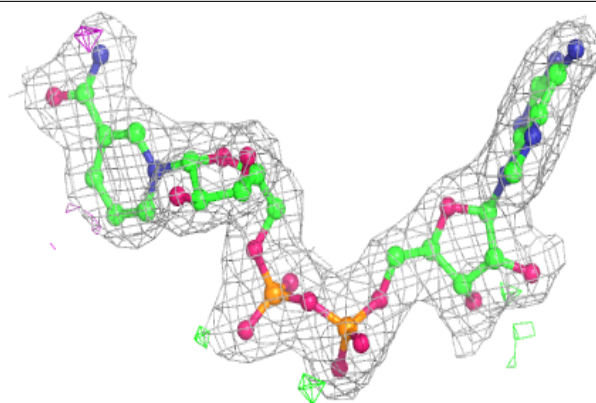
**Electron density around NAD D 501:**

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

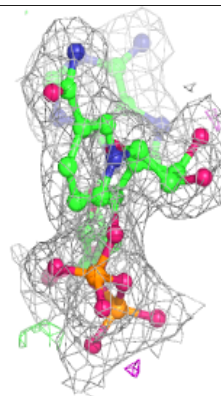
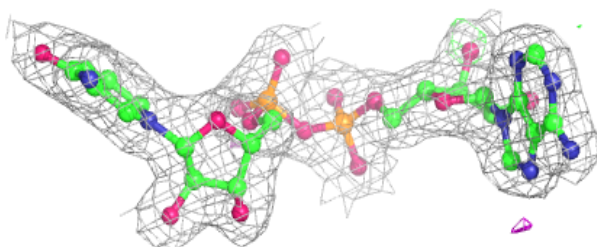
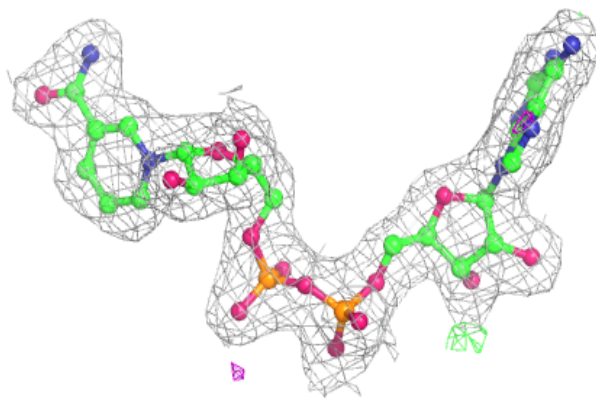


Electron density around NAD E 402:

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

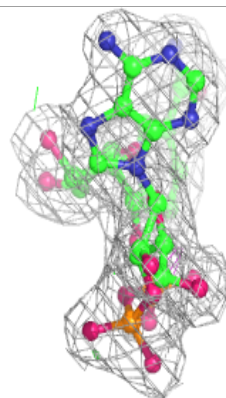
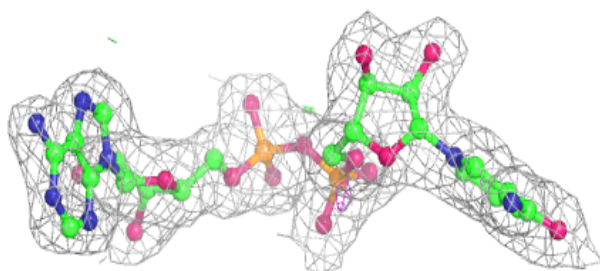
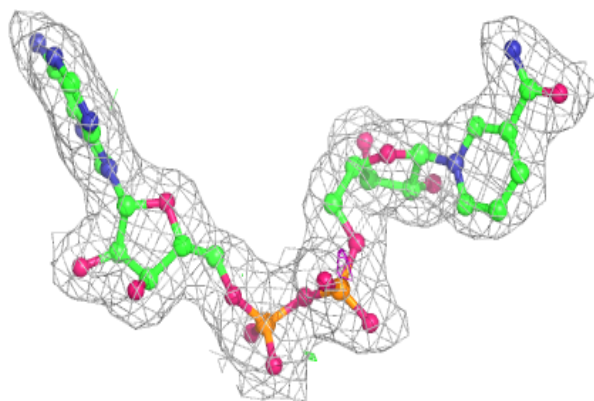
**Electron density around NAD A 402:**

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

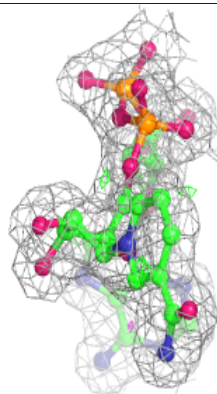
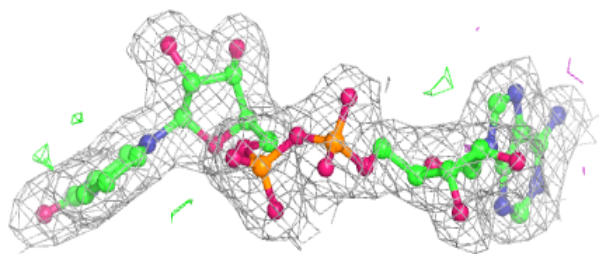
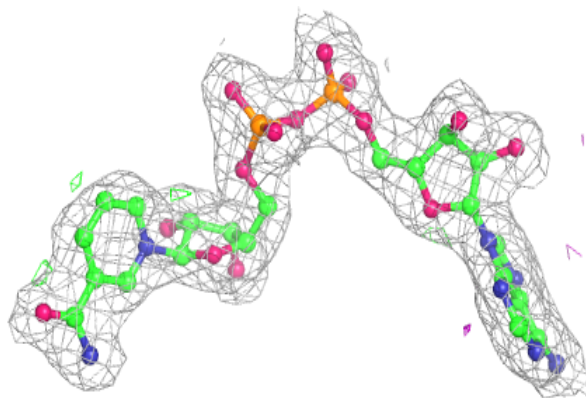


Electron density around NAD G 501:

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

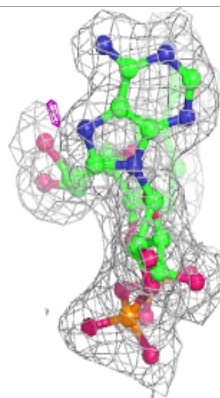
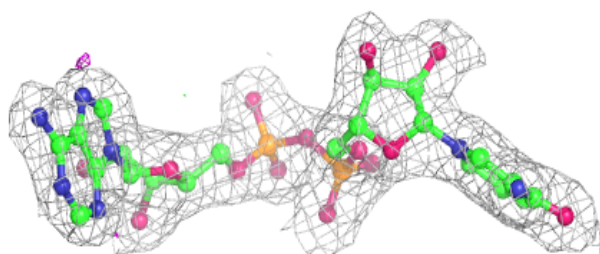
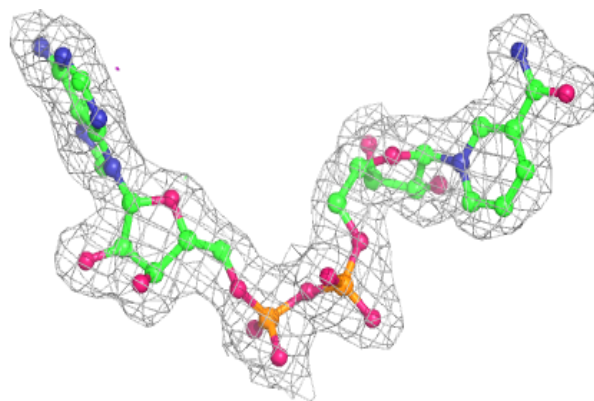
**Electron density around NAD B 402:**

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

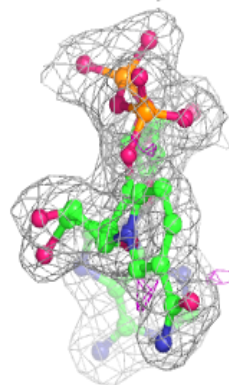
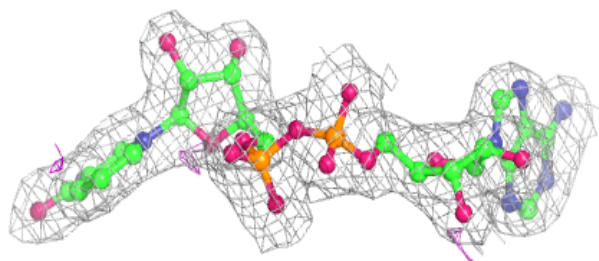
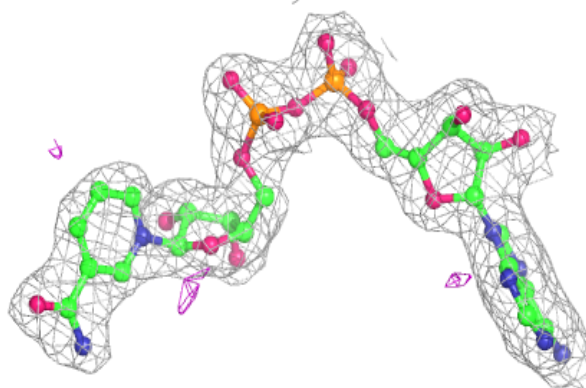


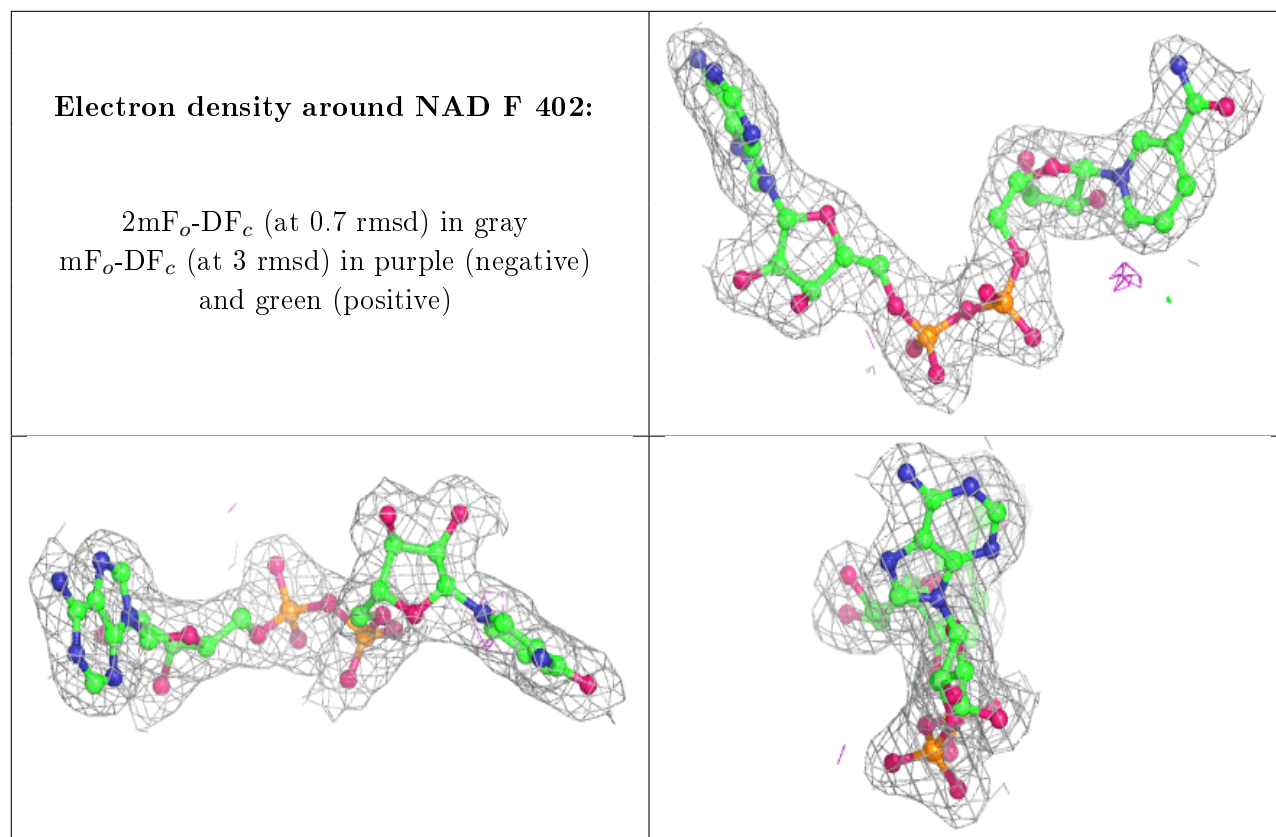
Electron density around NAD C 402:

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

**Electron density around NAD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.