



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2025 – 04:27 PM EST

PDB ID : 9Z9C / pdb_00009z9c
Title : Crystal structure of a glyceraldehyde-3-phosphate dehydrogenase from
Neisseria gonorrhoeae in complex with NAD (P1 form)
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2025-11-18
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

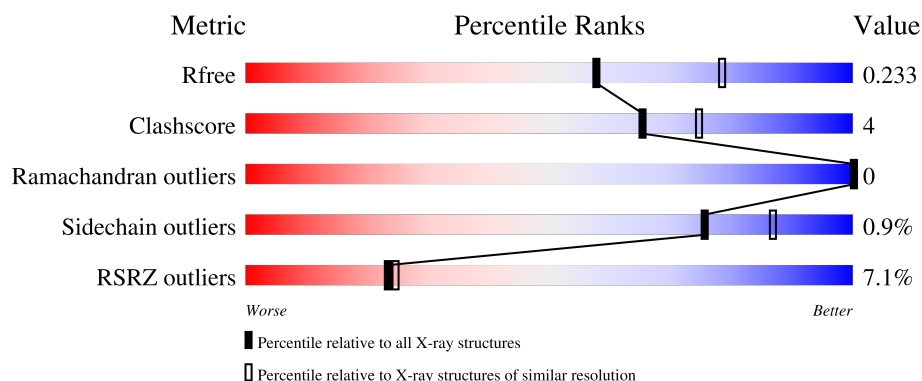
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



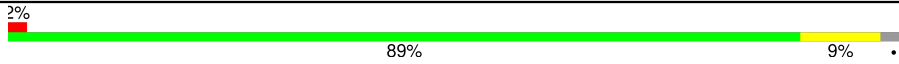
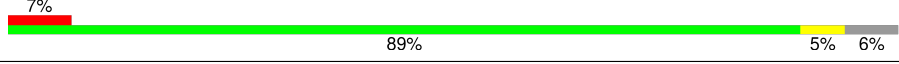
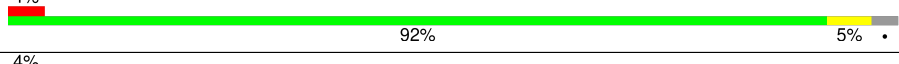
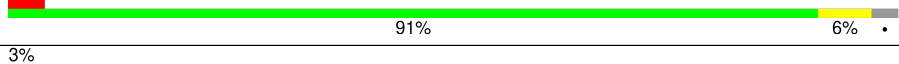

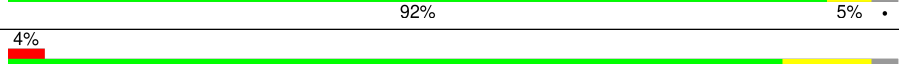
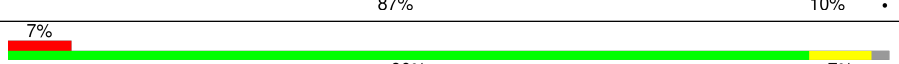
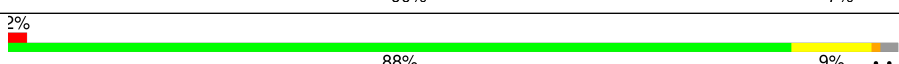
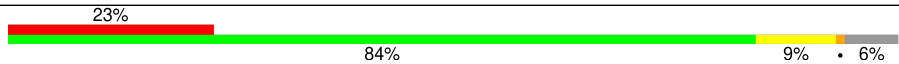

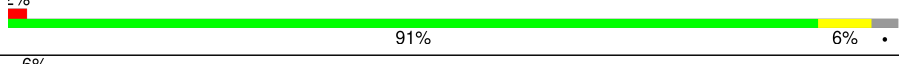
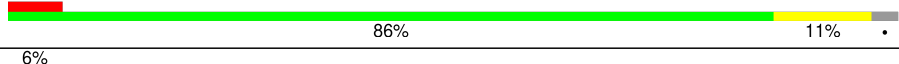
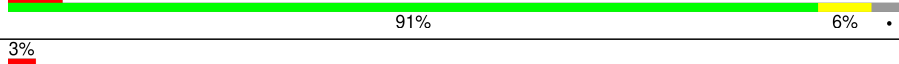
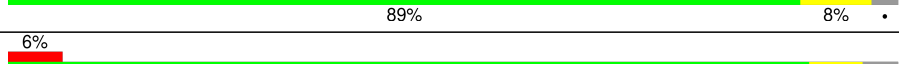





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	342	<div> <div>2%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	B	342	<div> <div>3%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	C	342	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	D	342	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	E	342	<div> <div>4%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	342	
1	G	342	
1	H	342	
1	I	342	
1	J	342	
1	K	342	
1	L	342	
1	M	342	
1	N	342	
1	O	342	
1	P	342	
1	Q	342	
1	R	342	
1	S	342	
1	T	342	
1	U	342	
1	V	342	
1	W	342	
1	X	342	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 60606 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2480	1554	428	488	10			
1	B	333	Total	C	N	O	S	0	0	0
			2478	1553	427	488	10			
1	C	332	Total	C	N	O	S	0	0	0
			2464	1547	426	481	10			
1	D	332	Total	C	N	O	S	0	0	0
			2490	1561	434	485	10			
1	E	333	Total	C	N	O	S	0	0	0
			2484	1558	429	486	11			
1	F	333	Total	C	N	O	S	0	0	0
			2491	1563	429	489	10			
1	G	323	Total	C	N	O	S	0	0	0
			2386	1498	413	465	10			
1	H	332	Total	C	N	O	S	0	0	0
			2488	1561	434	483	10			
1	I	333	Total	C	N	O	S	0	0	0
			2472	1550	428	483	11			
1	J	333	Total	C	N	O	S	0	0	0
			2489	1560	430	489	10			
1	K	332	Total	C	N	O	S	0	0	0
			2474	1552	429	483	10			
1	L	332	Total	C	N	O	S	0	0	0
			2470	1549	428	483	10			
1	M	334	Total	C	N	O	S	0	0	0
			2500	1569	435	485	11			
1	N	334	Total	C	N	O	S	0	0	0
			2497	1565	431	490	11			
1	O	321	Total	C	N	O	S	0	0	0
			2362	1479	411	462	10			
1	P	324	Total	C	N	O	S	0	0	0
			2367	1486	406	465	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	333	Total	C	N	O	S	0	0	0
			2491	1561	433	486	11			
1	R	333	Total	C	N	O	S	0	0	0
			2487	1561	429	487	10			
1	S	330	Total	C	N	O	S	0	0	0
			2443	1535	423	475	10			
1	T	332	Total	C	N	O	S	0	0	0
			2484	1557	430	487	10			
1	U	328	Total	C	N	O	S	0	0	0
			2441	1531	421	478	11			
1	V	331	Total	C	N	O	S	0	0	0
			2470	1552	432	476	10			
1	W	287	Total	C	N	O	S	0	0	0
			2128	1337	364	417	10			
1	X	329	Total	C	N	O	S	0	0	0
			2448	1537	425	475	11			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP B4RPP8
A	-6	ALA	-	expression tag	UNP B4RPP8
A	-5	HIS	-	expression tag	UNP B4RPP8
A	-4	HIS	-	expression tag	UNP B4RPP8
A	-3	HIS	-	expression tag	UNP B4RPP8
A	-2	HIS	-	expression tag	UNP B4RPP8
A	-1	HIS	-	expression tag	UNP B4RPP8
A	0	HIS	-	expression tag	UNP B4RPP8
B	-7	MET	-	initiating methionine	UNP B4RPP8
B	-6	ALA	-	expression tag	UNP B4RPP8
B	-5	HIS	-	expression tag	UNP B4RPP8
B	-4	HIS	-	expression tag	UNP B4RPP8
B	-3	HIS	-	expression tag	UNP B4RPP8
B	-2	HIS	-	expression tag	UNP B4RPP8
B	-1	HIS	-	expression tag	UNP B4RPP8
B	0	HIS	-	expression tag	UNP B4RPP8
C	-7	MET	-	initiating methionine	UNP B4RPP8
C	-6	ALA	-	expression tag	UNP B4RPP8
C	-5	HIS	-	expression tag	UNP B4RPP8
C	-4	HIS	-	expression tag	UNP B4RPP8
C	-3	HIS	-	expression tag	UNP B4RPP8
C	-2	HIS	-	expression tag	UNP B4RPP8
C	-1	HIS	-	expression tag	UNP B4RPP8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP B4RPP8
D	-7	MET	-	initiating methionine	UNP B4RPP8
D	-6	ALA	-	expression tag	UNP B4RPP8
D	-5	HIS	-	expression tag	UNP B4RPP8
D	-4	HIS	-	expression tag	UNP B4RPP8
D	-3	HIS	-	expression tag	UNP B4RPP8
D	-2	HIS	-	expression tag	UNP B4RPP8
D	-1	HIS	-	expression tag	UNP B4RPP8
D	0	HIS	-	expression tag	UNP B4RPP8
E	-7	MET	-	initiating methionine	UNP B4RPP8
E	-6	ALA	-	expression tag	UNP B4RPP8
E	-5	HIS	-	expression tag	UNP B4RPP8
E	-4	HIS	-	expression tag	UNP B4RPP8
E	-3	HIS	-	expression tag	UNP B4RPP8
E	-2	HIS	-	expression tag	UNP B4RPP8
E	-1	HIS	-	expression tag	UNP B4RPP8
E	0	HIS	-	expression tag	UNP B4RPP8
F	-7	MET	-	initiating methionine	UNP B4RPP8
F	-6	ALA	-	expression tag	UNP B4RPP8
F	-5	HIS	-	expression tag	UNP B4RPP8
F	-4	HIS	-	expression tag	UNP B4RPP8
F	-3	HIS	-	expression tag	UNP B4RPP8
F	-2	HIS	-	expression tag	UNP B4RPP8
F	-1	HIS	-	expression tag	UNP B4RPP8
F	0	HIS	-	expression tag	UNP B4RPP8
G	-7	MET	-	initiating methionine	UNP B4RPP8
G	-6	ALA	-	expression tag	UNP B4RPP8
G	-5	HIS	-	expression tag	UNP B4RPP8
G	-4	HIS	-	expression tag	UNP B4RPP8
G	-3	HIS	-	expression tag	UNP B4RPP8
G	-2	HIS	-	expression tag	UNP B4RPP8
G	-1	HIS	-	expression tag	UNP B4RPP8
G	0	HIS	-	expression tag	UNP B4RPP8
H	-7	MET	-	initiating methionine	UNP B4RPP8
H	-6	ALA	-	expression tag	UNP B4RPP8
H	-5	HIS	-	expression tag	UNP B4RPP8
H	-4	HIS	-	expression tag	UNP B4RPP8
H	-3	HIS	-	expression tag	UNP B4RPP8
H	-2	HIS	-	expression tag	UNP B4RPP8
H	-1	HIS	-	expression tag	UNP B4RPP8
H	0	HIS	-	expression tag	UNP B4RPP8
I	-7	MET	-	initiating methionine	UNP B4RPP8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	ALA	-	expression tag	UNP B4RPP8
I	-5	HIS	-	expression tag	UNP B4RPP8
I	-4	HIS	-	expression tag	UNP B4RPP8
I	-3	HIS	-	expression tag	UNP B4RPP8
I	-2	HIS	-	expression tag	UNP B4RPP8
I	-1	HIS	-	expression tag	UNP B4RPP8
I	0	HIS	-	expression tag	UNP B4RPP8
J	-7	MET	-	initiating methionine	UNP B4RPP8
J	-6	ALA	-	expression tag	UNP B4RPP8
J	-5	HIS	-	expression tag	UNP B4RPP8
J	-4	HIS	-	expression tag	UNP B4RPP8
J	-3	HIS	-	expression tag	UNP B4RPP8
J	-2	HIS	-	expression tag	UNP B4RPP8
J	-1	HIS	-	expression tag	UNP B4RPP8
J	0	HIS	-	expression tag	UNP B4RPP8
K	-7	MET	-	initiating methionine	UNP B4RPP8
K	-6	ALA	-	expression tag	UNP B4RPP8
K	-5	HIS	-	expression tag	UNP B4RPP8
K	-4	HIS	-	expression tag	UNP B4RPP8
K	-3	HIS	-	expression tag	UNP B4RPP8
K	-2	HIS	-	expression tag	UNP B4RPP8
K	-1	HIS	-	expression tag	UNP B4RPP8
K	0	HIS	-	expression tag	UNP B4RPP8
L	-7	MET	-	initiating methionine	UNP B4RPP8
L	-6	ALA	-	expression tag	UNP B4RPP8
L	-5	HIS	-	expression tag	UNP B4RPP8
L	-4	HIS	-	expression tag	UNP B4RPP8
L	-3	HIS	-	expression tag	UNP B4RPP8
L	-2	HIS	-	expression tag	UNP B4RPP8
L	-1	HIS	-	expression tag	UNP B4RPP8
L	0	HIS	-	expression tag	UNP B4RPP8
M	-7	MET	-	initiating methionine	UNP B4RPP8
M	-6	ALA	-	expression tag	UNP B4RPP8
M	-5	HIS	-	expression tag	UNP B4RPP8
M	-4	HIS	-	expression tag	UNP B4RPP8
M	-3	HIS	-	expression tag	UNP B4RPP8
M	-2	HIS	-	expression tag	UNP B4RPP8
M	-1	HIS	-	expression tag	UNP B4RPP8
M	0	HIS	-	expression tag	UNP B4RPP8
N	-7	MET	-	initiating methionine	UNP B4RPP8
N	-6	ALA	-	expression tag	UNP B4RPP8
N	-5	HIS	-	expression tag	UNP B4RPP8

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-4	HIS	-	expression tag	UNP B4RPP8
N	-3	HIS	-	expression tag	UNP B4RPP8
N	-2	HIS	-	expression tag	UNP B4RPP8
N	-1	HIS	-	expression tag	UNP B4RPP8
N	0	HIS	-	expression tag	UNP B4RPP8
O	-7	MET	-	initiating methionine	UNP B4RPP8
O	-6	ALA	-	expression tag	UNP B4RPP8
O	-5	HIS	-	expression tag	UNP B4RPP8
O	-4	HIS	-	expression tag	UNP B4RPP8
O	-3	HIS	-	expression tag	UNP B4RPP8
O	-2	HIS	-	expression tag	UNP B4RPP8
O	-1	HIS	-	expression tag	UNP B4RPP8
O	0	HIS	-	expression tag	UNP B4RPP8
P	-7	MET	-	initiating methionine	UNP B4RPP8
P	-6	ALA	-	expression tag	UNP B4RPP8
P	-5	HIS	-	expression tag	UNP B4RPP8
P	-4	HIS	-	expression tag	UNP B4RPP8
P	-3	HIS	-	expression tag	UNP B4RPP8
P	-2	HIS	-	expression tag	UNP B4RPP8
P	-1	HIS	-	expression tag	UNP B4RPP8
P	0	HIS	-	expression tag	UNP B4RPP8
Q	-7	MET	-	initiating methionine	UNP B4RPP8
Q	-6	ALA	-	expression tag	UNP B4RPP8
Q	-5	HIS	-	expression tag	UNP B4RPP8
Q	-4	HIS	-	expression tag	UNP B4RPP8
Q	-3	HIS	-	expression tag	UNP B4RPP8
Q	-2	HIS	-	expression tag	UNP B4RPP8
Q	-1	HIS	-	expression tag	UNP B4RPP8
Q	0	HIS	-	expression tag	UNP B4RPP8
R	-7	MET	-	initiating methionine	UNP B4RPP8
R	-6	ALA	-	expression tag	UNP B4RPP8
R	-5	HIS	-	expression tag	UNP B4RPP8
R	-4	HIS	-	expression tag	UNP B4RPP8
R	-3	HIS	-	expression tag	UNP B4RPP8
R	-2	HIS	-	expression tag	UNP B4RPP8
R	-1	HIS	-	expression tag	UNP B4RPP8
R	0	HIS	-	expression tag	UNP B4RPP8
S	-7	MET	-	initiating methionine	UNP B4RPP8
S	-6	ALA	-	expression tag	UNP B4RPP8
S	-5	HIS	-	expression tag	UNP B4RPP8
S	-4	HIS	-	expression tag	UNP B4RPP8
S	-3	HIS	-	expression tag	UNP B4RPP8

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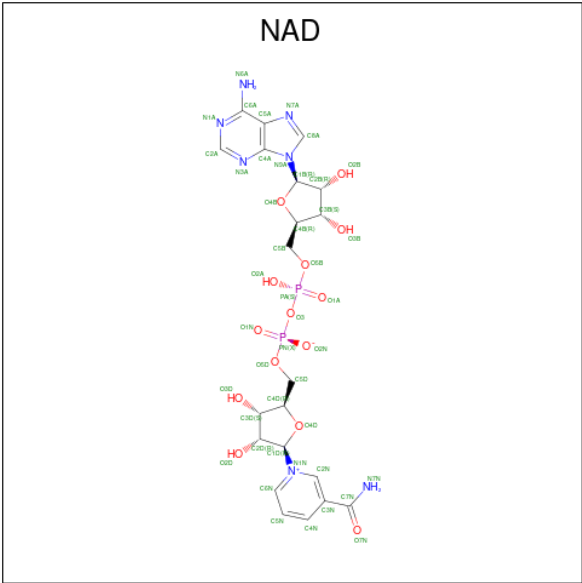
Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	HIS	-	expression tag	UNP B4RPP8
S	-1	HIS	-	expression tag	UNP B4RPP8
S	0	HIS	-	expression tag	UNP B4RPP8
T	-7	MET	-	initiating methionine	UNP B4RPP8
T	-6	ALA	-	expression tag	UNP B4RPP8
T	-5	HIS	-	expression tag	UNP B4RPP8
T	-4	HIS	-	expression tag	UNP B4RPP8
T	-3	HIS	-	expression tag	UNP B4RPP8
T	-2	HIS	-	expression tag	UNP B4RPP8
T	-1	HIS	-	expression tag	UNP B4RPP8
T	0	HIS	-	expression tag	UNP B4RPP8
U	-7	MET	-	initiating methionine	UNP B4RPP8
U	-6	ALA	-	expression tag	UNP B4RPP8
U	-5	HIS	-	expression tag	UNP B4RPP8
U	-4	HIS	-	expression tag	UNP B4RPP8
U	-3	HIS	-	expression tag	UNP B4RPP8
U	-2	HIS	-	expression tag	UNP B4RPP8
U	-1	HIS	-	expression tag	UNP B4RPP8
U	0	HIS	-	expression tag	UNP B4RPP8
V	-7	MET	-	initiating methionine	UNP B4RPP8
V	-6	ALA	-	expression tag	UNP B4RPP8
V	-5	HIS	-	expression tag	UNP B4RPP8
V	-4	HIS	-	expression tag	UNP B4RPP8
V	-3	HIS	-	expression tag	UNP B4RPP8
V	-2	HIS	-	expression tag	UNP B4RPP8
V	-1	HIS	-	expression tag	UNP B4RPP8
V	0	HIS	-	expression tag	UNP B4RPP8
W	-7	MET	-	initiating methionine	UNP B4RPP8
W	-6	ALA	-	expression tag	UNP B4RPP8
W	-5	HIS	-	expression tag	UNP B4RPP8
W	-4	HIS	-	expression tag	UNP B4RPP8
W	-3	HIS	-	expression tag	UNP B4RPP8
W	-2	HIS	-	expression tag	UNP B4RPP8
W	-1	HIS	-	expression tag	UNP B4RPP8
W	0	HIS	-	expression tag	UNP B4RPP8
X	-7	MET	-	initiating methionine	UNP B4RPP8
X	-6	ALA	-	expression tag	UNP B4RPP8
X	-5	HIS	-	expression tag	UNP B4RPP8
X	-4	HIS	-	expression tag	UNP B4RPP8
X	-3	HIS	-	expression tag	UNP B4RPP8
X	-2	HIS	-	expression tag	UNP B4RPP8
X	-1	HIS	-	expression tag	UNP B4RPP8

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Chain	Residue	Modelled	Actual	Comment	Reference
X	0	HIS	-	expression tag	UNP B4RPP8

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



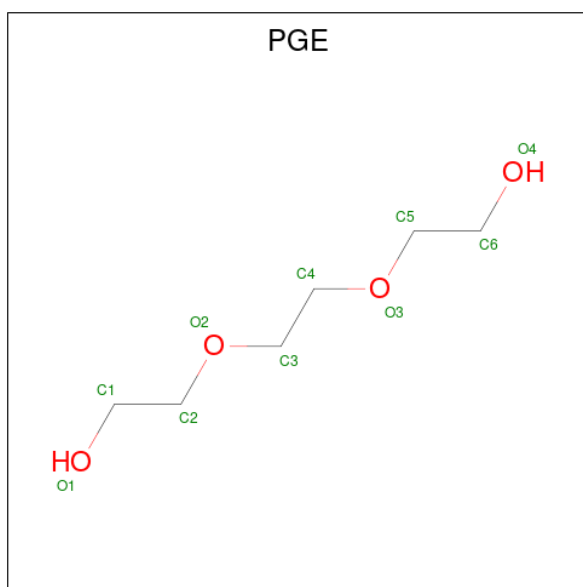
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	K	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	L	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	M	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	N	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	O	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	P	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	Q	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	R	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	S	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	T	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	U	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	V	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	W	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	X	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	41	Total	O	0	0
			41	41		
4	C	37	Total	O	0	0
			37	37		
4	D	64	Total	O	0	0
			64	64		
4	E	39	Total	O	0	0
			39	39		
4	F	35	Total	O	0	0
			35	35		
4	G	25	Total	O	0	0
			25	25		
4	H	44	Total	O	0	0
			44	44		
4	I	38	Total	O	0	0
			38	38		
4	J	33	Total	O	0	0
			33	33		
4	K	39	Total	O	0	0
			39	39		

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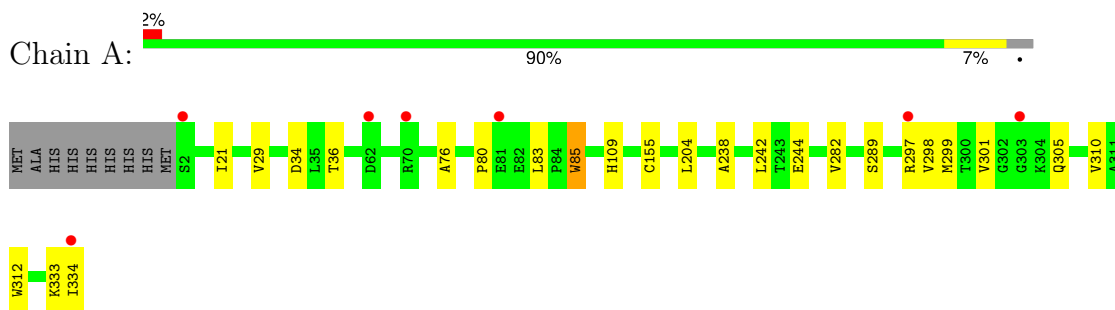
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	37	Total 37	O 37	0	0
4	M	34	Total 34	O 34	0	0
4	N	43	Total 43	O 43	0	0
4	O	3	Total 3	O 3	0	0
4	P	12	Total 12	O 12	0	0
4	Q	28	Total 28	O 28	0	0
4	R	19	Total 19	O 19	0	0
4	S	21	Total 21	O 21	0	0
4	T	45	Total 45	O 45	0	0
4	U	35	Total 35	O 35	0	0
4	V	22	Total 22	O 22	0	0
4	W	3	Total 3	O 3	0	0
4	X	17	Total 17	O 17	0	0

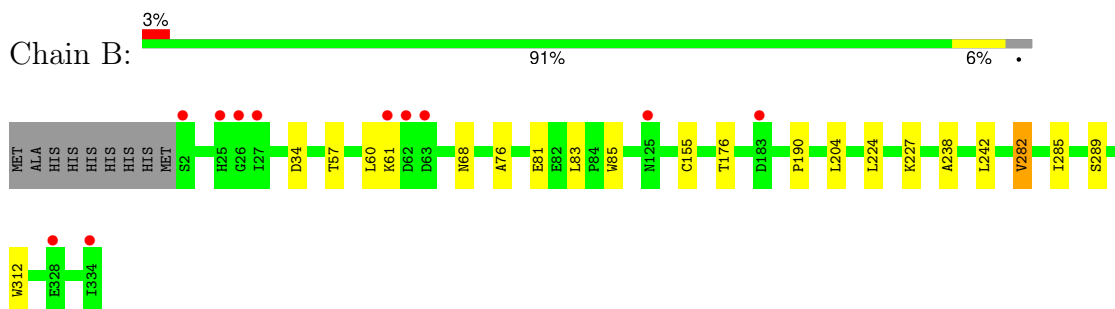
3 Residue-property plots [i](#)

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.

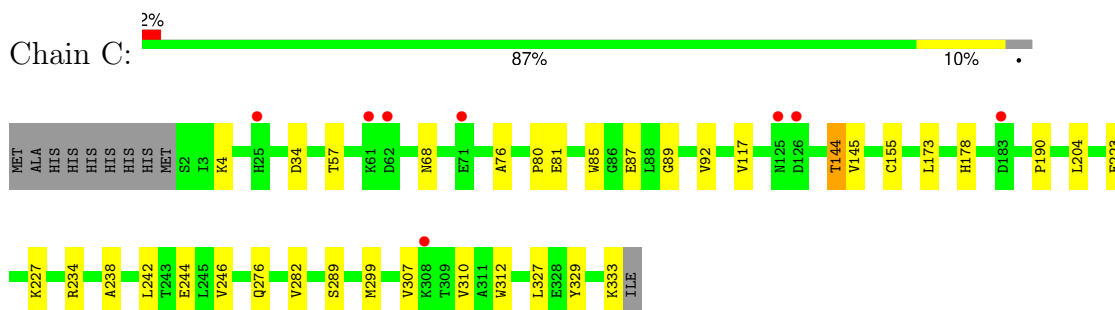
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



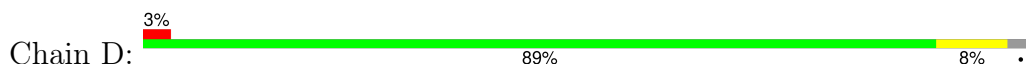
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

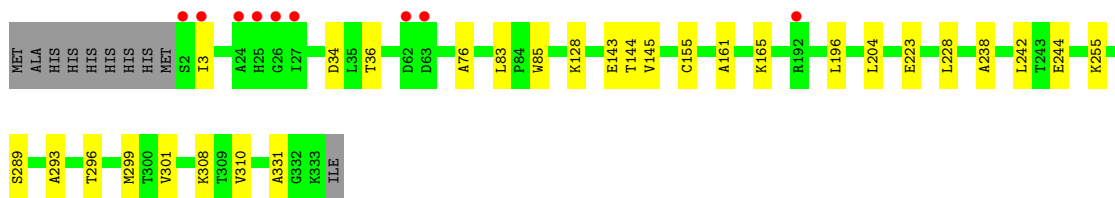


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

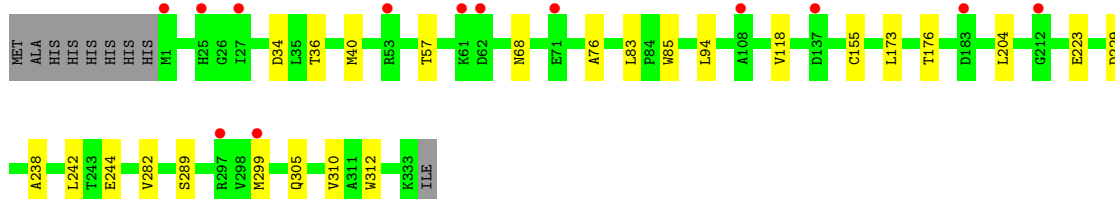
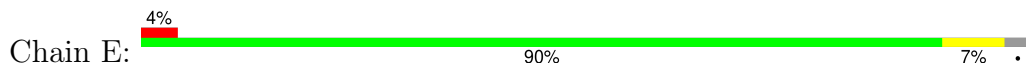


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

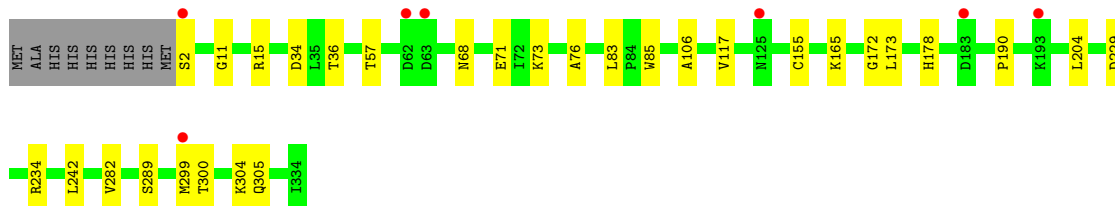
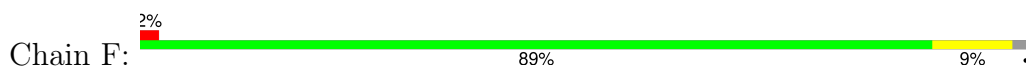




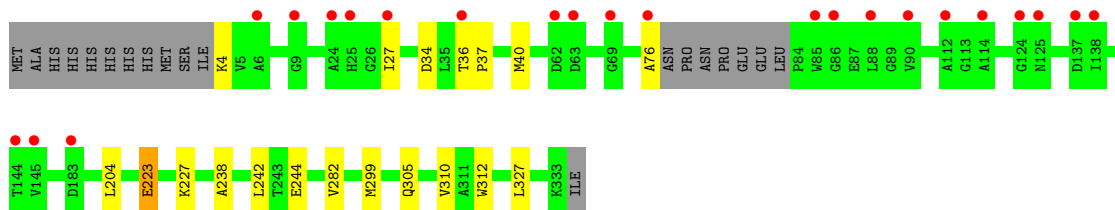
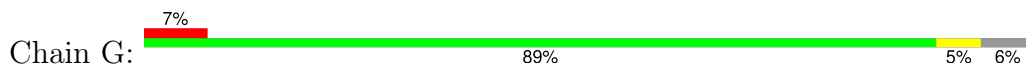
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



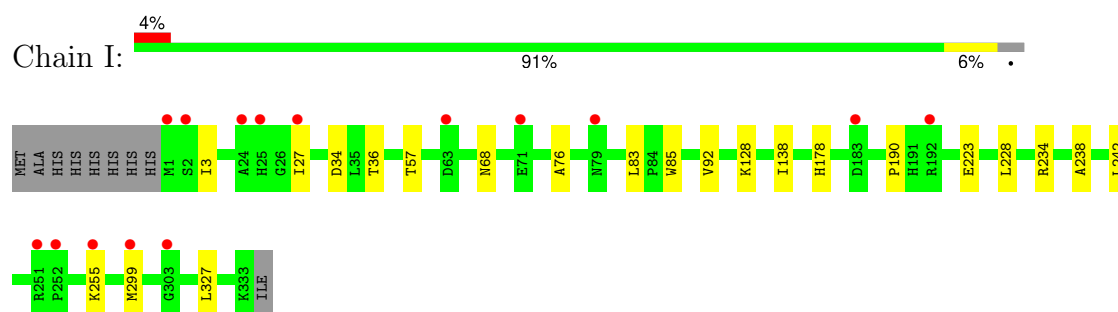
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



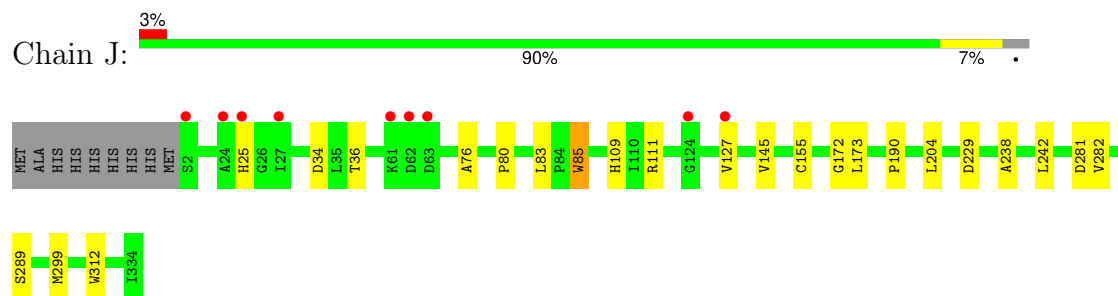
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



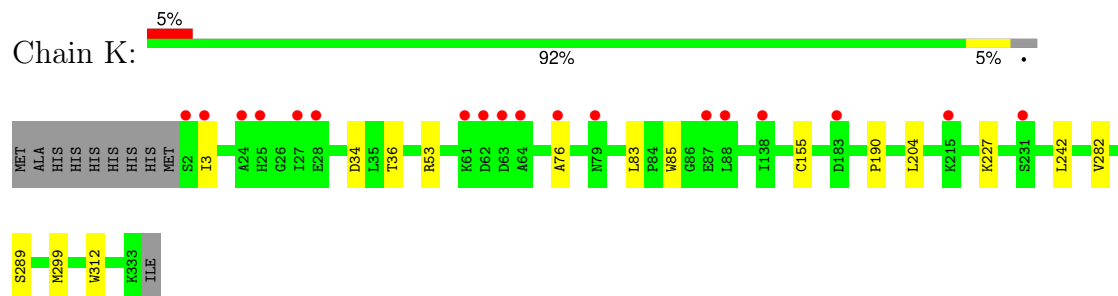
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



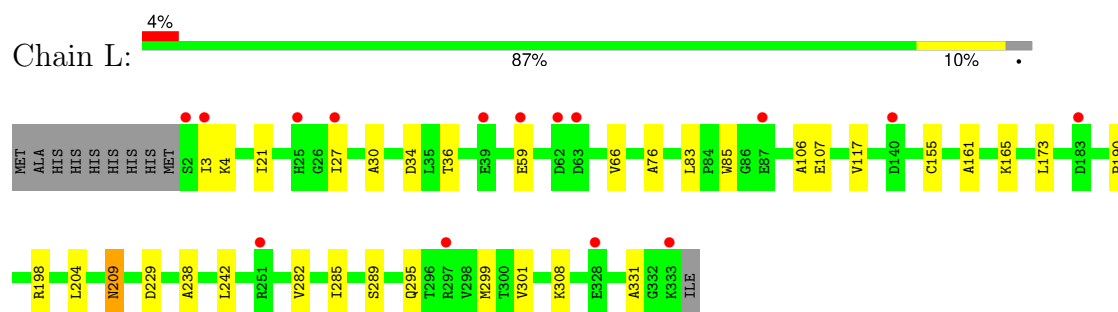
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



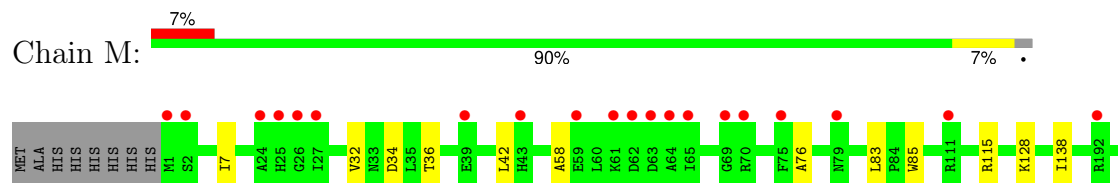
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

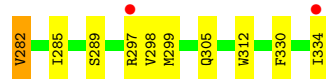
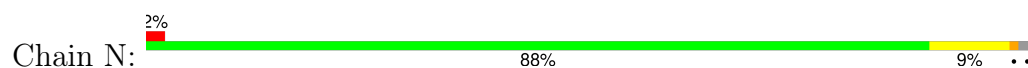


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

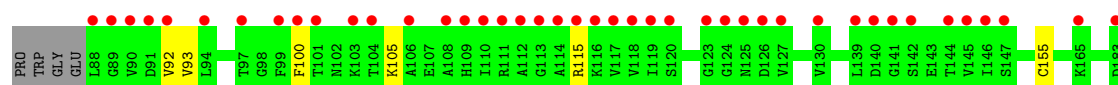
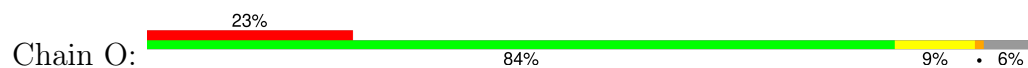




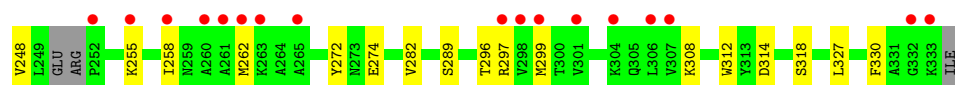
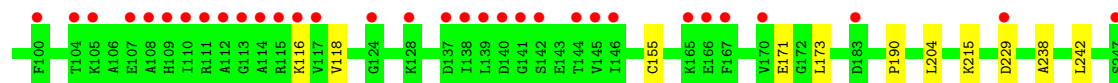
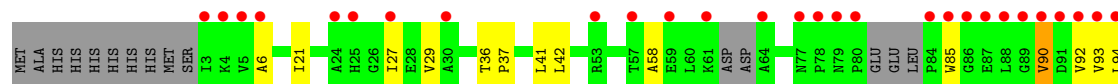
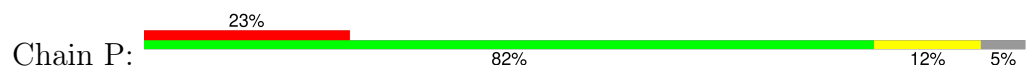
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



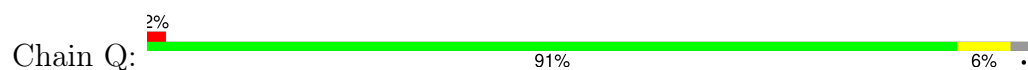
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

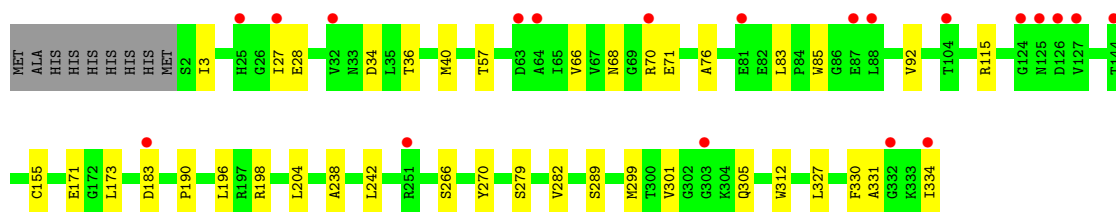
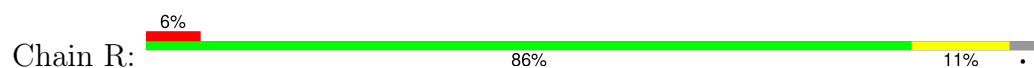


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

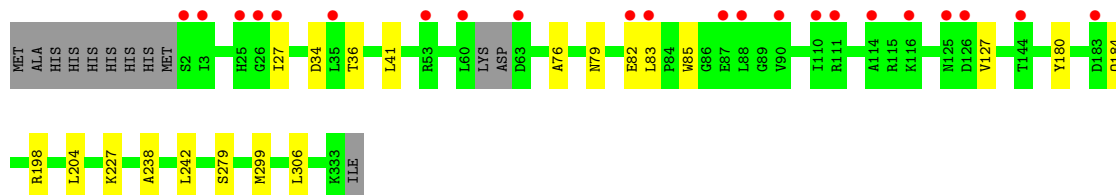
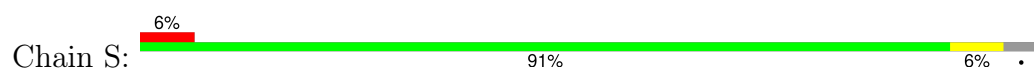




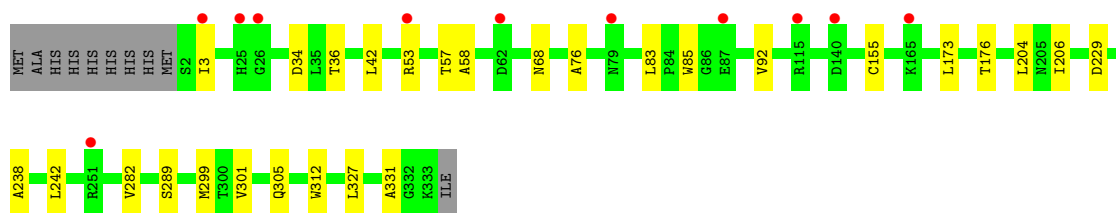
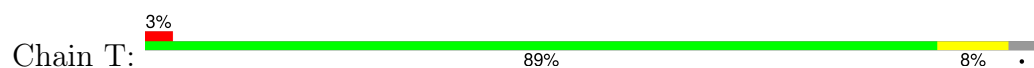
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



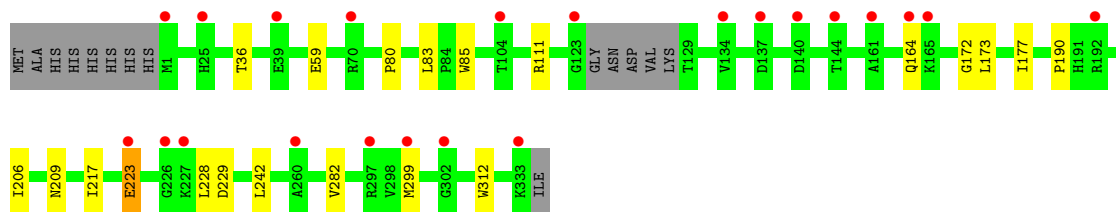
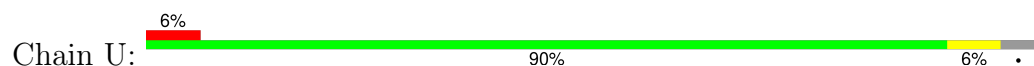
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



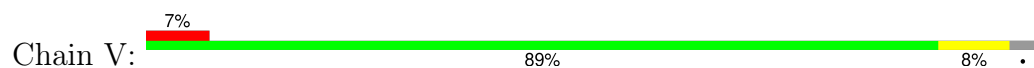
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

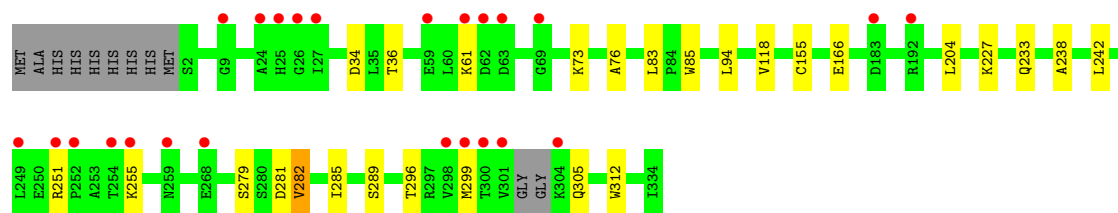


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

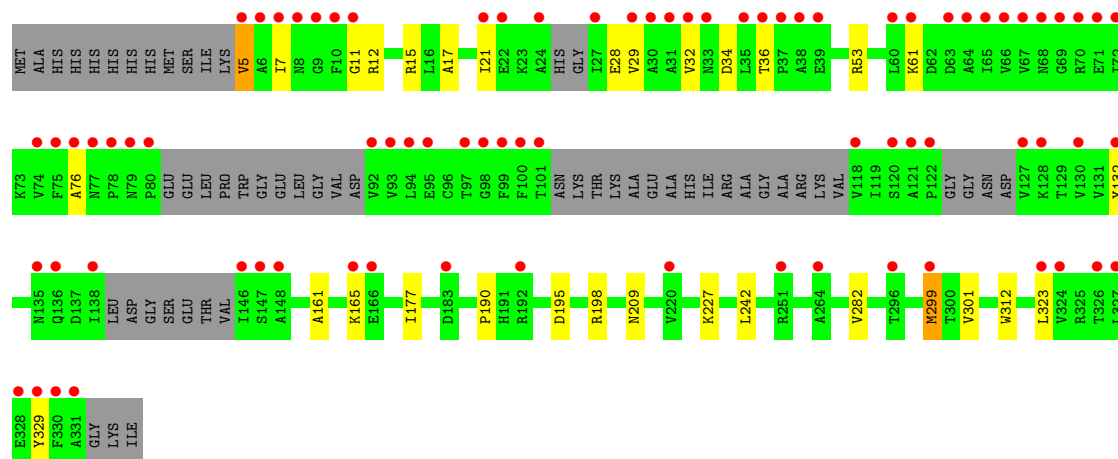
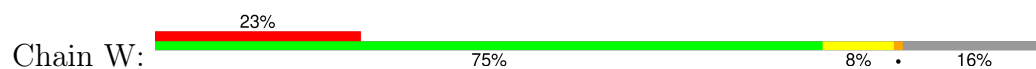


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

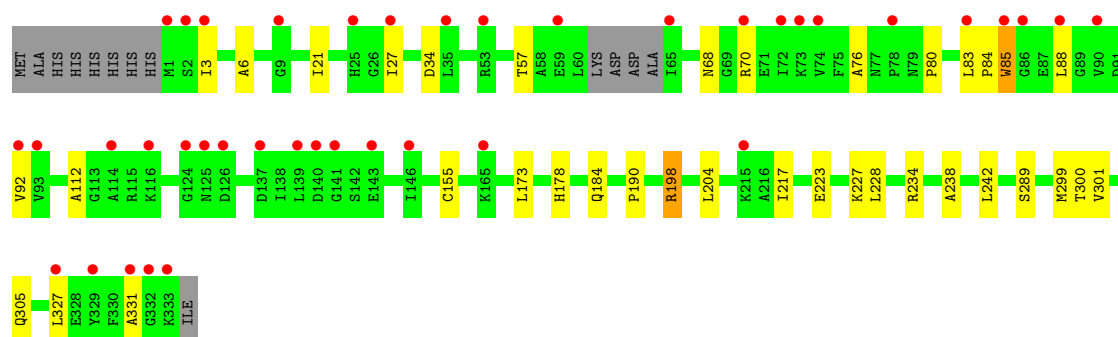
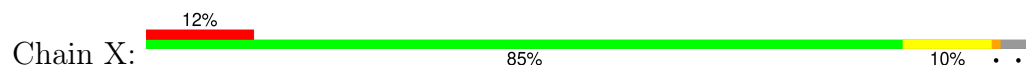




● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	105.53Å 137.84Å 157.79Å 85.95° 77.63° 86.88°	Depositor
Resolution (Å)	48.53 – 2.30 48.53 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.53-2.30) 97.4 (48.53-2.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_5438: ???)	Depositor
R, R_{free}	0.194 , 0.232 0.199 , 0.233	Depositor DCC
R_{free} test set	18765 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	60606	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, PGE

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	0.22	0/2516	0.42	0/3417
1	B	0.23	0/2515	0.42	0/3417
1	C	0.23	0/2501	0.43	0/3398
1	D	0.23	0/2527	0.43	0/3428
1	E	0.22	0/2520	0.42	0/3420
1	F	0.23	0/2528	0.44	0/3430
1	G	0.23	0/2419	0.42	0/3282
1	H	0.21	0/2525	0.42	0/3425
1	I	0.25	0/2508	0.44	0/3405
1	J	0.21	0/2526	0.40	0/3429
1	K	0.21	0/2511	0.42	0/3410
1	L	0.20	0/2507	0.41	0/3406
1	M	0.21	0/2537	0.42	0/3442
1	N	0.25	0/2534	0.45	0/3439
1	O	0.24	0/2393	0.44	0/3249
1	P	0.22	0/2400	0.40	0/3262
1	Q	0.22	0/2528	0.41	0/3431
1	R	0.23	0/2524	0.41	0/3425
1	S	0.21	0/2479	0.40	0/3366
1	T	0.22	0/2521	0.41	0/3422
1	U	0.20	0/2477	0.40	0/3365
1	V	0.21	0/2505	0.39	0/3398
1	W	0.23	0/2155	0.43	0/2926
1	X	0.21	0/2484	0.40	0/3372
All	All	0.22	0/59640	0.42	0/80964

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2480	0	2471	18	0
1	B	2478	0	2459	16	0
1	C	2464	0	2455	25	0
1	D	2490	0	2503	21	0
1	E	2484	0	2490	24	0
1	F	2491	0	2496	22	0
1	G	2386	0	2376	19	0
1	H	2488	0	2503	17	0
1	I	2472	0	2463	19	0
1	J	2489	0	2485	23	0
1	K	2474	0	2470	17	0
1	L	2470	0	2459	26	0
1	M	2500	0	2515	22	0
1	N	2497	0	2497	27	0
1	O	2362	0	2327	25	0
1	P	2367	0	2320	35	0
1	Q	2491	0	2495	24	0
1	R	2487	0	2492	33	0
1	S	2443	0	2430	18	0
1	T	2484	0	2485	29	0
1	U	2441	0	2420	17	0
1	V	2470	0	2475	31	0
1	W	2128	0	2097	26	0
1	X	2448	0	2446	32	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
2	I	44	0	26	0	0
2	J	44	0	26	0	0
2	K	44	0	26	0	0
2	L	44	0	26	0	0
2	M	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	44	0	26	0	0
2	O	44	0	26	1	0
2	P	44	0	26	0	0
2	Q	44	0	26	0	0
2	R	44	0	26	0	0
2	S	44	0	26	0	0
2	T	44	0	26	0	0
2	U	44	0	26	0	0
2	V	44	0	26	0	0
2	W	44	0	26	0	0
2	X	44	0	26	0	0
3	H	10	0	14	0	0
4	A	42	0	0	0	0
4	B	41	0	0	0	0
4	C	37	0	0	1	0
4	D	64	0	0	0	0
4	E	39	0	0	0	0
4	F	35	0	0	0	0
4	G	25	0	0	0	0
4	H	44	0	0	0	0
4	I	38	0	0	0	0
4	J	33	0	0	0	0
4	K	39	0	0	0	0
4	L	37	0	0	0	0
4	M	34	0	0	0	0
4	N	43	0	0	0	0
4	O	3	0	0	0	0
4	P	12	0	0	0	0
4	Q	28	0	0	0	0
4	R	19	0	0	0	0
4	S	21	0	0	1	0
4	T	45	0	0	0	0
4	U	35	0	0	0	0
4	V	22	0	0	0	0
4	W	3	0	0	0	0
4	X	17	0	0	0	0
All	All	60606	0	59267	444	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (444) 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:N:36:THR:HG21	1:P:190:PRO:HB3	1.46	0.98
1:U:36:THR:HG21	1:W:190:PRO:HB3	1.50	0.94
1:O:229:ASP:HB3	1:P:299:MET:HE1	1.56	0.84
1:I:36:THR:HG21	1:K:190:PRO:HB3	1.59	0.84
1:O:229:ASP:CB	1:P:299:MET:HE1	2.11	0.80
1:D:144:THR:HG23	1:D:145:VAL:HG23	1.63	0.78
1:U:190:PRO:HB3	1:W:36:THR:HG21	1.64	0.78
1:V:36:THR:HG21	1:X:190:PRO:HB3	1.64	0.77
1:A:36:THR:HG21	1:C:190:PRO:HB3	1.65	0.77
1:R:331:ALA:HA	1:R:334:ILE:HD12	1.65	0.77
1:C:144:THR:HG22	1:C:145:VAL:HG23	1.67	0.76
1:L:4:LYS:HE3	1:L:30:ALA:HB2	1.68	0.76
1:X:83:LEU:HD13	1:X:85:TRP:CG	2.22	0.75
1:R:190:PRO:HB3	1:T:36:THR:HG21	1.67	0.75
1:Q:281:ASP:HB3	1:T:53:ARG:HH21	1.52	0.74
1:I:299:MET:HE1	1:J:172:GLY:O	1.89	0.72
1:P:215:LYS:HG3	1:P:229:ASP:OD1	1.89	0.72
1:P:297:ARG:NH2	1:P:299:MET:HE2	2.05	0.71
1:M:255:LYS:HE3	1:M:296:THR:HB	1.72	0.71
1:I:83:LEU:HD13	1:I:85:TRP:CZ2	2.26	0.71
1:D:83:LEU:HD13	1:D:85:TRP:CZ2	2.27	0.70
1:I:190:PRO:HB3	1:K:36:THR:HG21	1.73	0.70
1:I:299:MET:HE2	1:J:229:ASP:HB3	1.73	0.70
1:V:282:VAL:HG22	1:V:285:ILE:HD13	1.74	0.69
1:Q:227:LYS:O	1:R:299:MET:HE1	1.91	0.69
1:U:36:THR:HG21	1:W:190:PRO:CB	2.23	0.69
1:S:227:LYS:O	1:T:299:MET:HE1	1.92	0.68
1:T:3:ILE:HD13	1:T:331:ALA:HB1	1.75	0.68
1:E:83:LEU:HD13	1:E:85:TRP:CZ2	2.29	0.68
1:M:299:MET:SD	1:N:173:LEU:HG	2.35	0.67
1:O:299:MET:SD	1:P:173:LEU:HG	2.35	0.66
1:F:204:LEU:HD11	1:H:238:ALA:CB	2.26	0.66
1:L:3:ILE:HD13	1:L:331:ALA:HB1	1.77	0.66
1:L:83:LEU:HD13	1:L:85:TRP:CZ2	2.31	0.65
1:S:299:MET:HE1	1:T:229:ASP:H	1.60	0.65
1:I:3:ILE:HB	1:I:27:ILE:HG22	1.79	0.65
1:W:227:LYS:O	1:X:299:MET:HE1	1.97	0.65
1:W:195:ASP:CG	1:W:198:ARG:HE	2.05	0.65
1:Q:227:LYS:C	1:R:299:MET:HE1	2.23	0.64
1:O:299:MET:HE2	1:P:171:GLU:HB2	1.81	0.63
1:R:57:THR:OG1	1:R:68:ASN:HA	1.98	0.63
1:A:238:ALA:CB	1:C:204:LEU:HD11	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:84:PRO:O	1:X:88:LEU:HD23	1.99	0.63
1:N:36:THR:HG21	1:P:190:PRO:CB	2.26	0.62
1:W:195:ASP:HB2	1:W:198:ARG:HH21	1.62	0.62
1:T:3:ILE:HD13	1:T:331:ALA:CB	2.29	0.62
1:M:83:LEU:HD13	1:M:85:TRP:CZ2	2.34	0.62
1:X:83:LEU:HD12	1:X:83:LEU:O	1.99	0.62
1:H:107:GLU:OE1	1:X:300:THR:HG22	1.99	0.62
1:J:36:THR:HG21	1:L:190:PRO:HB3	1.81	0.62
1:S:299:MET:HE1	1:T:229:ASP:N	2.14	0.62
1:X:92:VAL:HG11	1:X:327:LEU:CD1	2.30	0.62
1:X:83:LEU:HD13	1:X:85:TRP:CD2	2.35	0.61
1:B:190:PRO:HB3	1:D:36:THR:HG21	1.80	0.61
1:V:83:LEU:HD13	1:V:85:TRP:CZ2	2.35	0.61
1:Q:36:THR:HG21	1:Q:40:MET:HG2	1.81	0.61
1:Q:238:ALA:CB	1:S:204:LEU:HD11	2.30	0.61
1:R:330:PHE:CD2	1:R:334:ILE:HD11	2.36	0.60
1:X:83:LEU:HD12	1:X:83:LEU:C	2.25	0.60
1:D:3:ILE:HD13	1:D:331:ALA:HB1	1.83	0.60
1:L:59:GLU:HG2	1:L:66:VAL:HB	1.84	0.60
1:G:36:THR:CG2	1:G:40:MET:HB3	2.32	0.59
1:F:83:LEU:HD13	1:F:85:TRP:CZ2	2.37	0.59
1:H:3:ILE:HD13	1:H:331:ALA:HB1	1.83	0.59
1:U:83:LEU:HD13	1:U:85:TRP:CZ2	2.36	0.59
1:G:244:GLU:HG2	1:G:310:VAL:HG22	1.85	0.59
1:O:34:ASP:OD1	2:O:401:NAD:H1B	2.02	0.59
1:R:238:ALA:CB	1:T:204:LEU:HD11	2.32	0.59
1:F:36:THR:HG21	1:H:190:PRO:HB3	1.84	0.59
1:R:36:THR:HG21	1:R:40:MET:HG2	1.85	0.59
1:P:255:LYS:HE3	1:P:296:THR:O	2.03	0.59
1:R:3:ILE:HB	1:R:27:ILE:HG22	1.85	0.58
1:A:83:LEU:HD13	1:A:85:TRP:CZ2	2.38	0.58
1:I:299:MET:HE2	1:J:229:ASP:CB	2.33	0.58
1:M:255:LYS:HG3	1:M:296:THR:HB	1.84	0.58
1:Q:177:ILE:HD13	1:Q:242:LEU:HD11	1.85	0.58
1:E:238:ALA:CB	1:G:204:LEU:HD11	2.33	0.58
1:K:83:LEU:HD13	1:K:85:TRP:CZ2	2.39	0.57
1:Q:276:GLN:HG3	1:R:196:LEU:HD12	1.86	0.57
1:V:238:ALA:CB	1:X:204:LEU:HD11	2.35	0.57
1:M:242:LEU:HD12	1:M:242:LEU:C	2.29	0.57
1:N:204:LEU:HD11	1:P:238:ALA:CB	2.34	0.57
1:O:299:MET:HG2	1:O:306:LEU:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:85:TRP:CD1	1:P:93:VAL:HG21	2.39	0.57
1:C:81:GLU:HB3	1:N:257:GLU:HB3	1.86	0.57
1:N:297:ARG:NH1	1:N:298:VAL:O	2.37	0.57
1:I:242:LEU:HD12	1:I:242:LEU:C	2.30	0.57
1:E:229:ASP:CB	1:F:299:MET:HE2	2.35	0.56
1:G:36:THR:HG22	1:G:37:PRO:O	2.04	0.56
1:H:83:LEU:HD13	1:H:85:TRP:CZ2	2.40	0.56
1:Q:299:MET:SD	1:R:173:LEU:HG	2.45	0.56
1:W:177:ILE:HD13	1:W:242:LEU:HD11	1.87	0.56
1:R:299:MET:HE2	1:R:301:VAL:CG2	2.34	0.56
1:S:83:LEU:HD13	1:S:85:TRP:CZ2	2.41	0.56
1:G:34:ASP:O	1:G:76:ALA:HA	2.05	0.56
1:A:242:LEU:HD12	1:A:242:LEU:C	2.31	0.55
1:E:244:GLU:HG2	1:E:310:VAL:HG22	1.88	0.55
1:N:282:VAL:HG22	1:N:285:ILE:HD13	1.88	0.55
1:P:92:VAL:HG11	1:P:327:LEU:HD12	1.88	0.55
1:J:83:LEU:HD13	1:J:85:TRP:CZ2	2.41	0.55
1:K:34:ASP:O	1:K:76:ALA:HA	2.06	0.55
1:M:36:THR:HG21	1:O:190:PRO:HB3	1.89	0.55
1:X:217:ILE:HG21	1:X:228:LEU:HD12	1.89	0.55
1:N:215:LYS:HE2	1:N:229:ASP:OD1	2.06	0.55
1:J:242:LEU:C	1:J:242:LEU:HD12	2.32	0.55
1:I:299:MET:HE3	1:J:173:LEU:HG	1.89	0.55
1:F:190:PRO:HB3	1:H:36:THR:HG21	1.88	0.55
1:H:3:ILE:HB	1:H:27:ILE:HG22	1.89	0.55
1:M:115:ARG:HH22	1:M:334:ILE:HG23	1.72	0.54
1:V:242:LEU:C	1:V:242:LEU:HD12	2.32	0.54
1:X:21:ILE:HG23	1:X:27:ILE:HG23	1.89	0.54
1:O:6:ALA:HB3	1:O:93:VAL:HG22	1.90	0.54
1:R:242:LEU:HD12	1:R:242:LEU:C	2.33	0.54
1:H:242:LEU:C	1:H:242:LEU:HD12	2.33	0.54
1:T:83:LEU:HD13	1:T:85:TRP:CZ2	2.43	0.54
1:B:155:CYS:HA	1:B:289:SER:HB2	1.90	0.53
1:O:65:ILE:HG23	1:O:74:VAL:HG21	1.89	0.53
1:P:21:ILE:HG21	1:P:29:VAL:HG23	1.90	0.53
1:L:59:GLU:CG	1:L:66:VAL:HB	2.39	0.53
1:B:204:LEU:HD11	1:D:238:ALA:CB	2.39	0.53
1:C:227:LYS:HG2	1:D:301:VAL:HG11	1.89	0.53
1:E:36:THR:HG21	1:E:40:MET:HG2	1.90	0.53
1:P:21:ILE:HG23	1:P:27:ILE:HG23	1.90	0.53
1:V:166:GLU:C	1:V:251:ARG:HH21	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:3:ILE:HD13	1:X:331:ALA:HB1	1.91	0.53
1:F:242:LEU:HD12	1:F:242:LEU:C	2.34	0.53
1:S:299:MET:HE2	1:T:229:ASP:CB	2.38	0.52
1:E:299:MET:HE2	1:F:229:ASP:HB3	1.91	0.52
1:D:255:LYS:HG3	1:D:296:THR:HB	1.91	0.52
1:W:242:LEU:HD12	1:W:242:LEU:C	2.34	0.52
1:A:297:ARG:NH1	1:A:298:VAL:O	2.42	0.52
1:B:282:VAL:HG22	1:B:285:ILE:HD13	1.91	0.52
1:N:83:LEU:HD13	1:N:85:TRP:CZ2	2.44	0.52
1:O:42:LEU:HD22	1:O:60:LEU:HG	1.92	0.52
1:S:34:ASP:O	1:S:76:ALA:HA	2.10	0.52
1:X:242:LEU:C	1:X:242:LEU:HD12	2.35	0.52
1:O:242:LEU:C	1:O:242:LEU:HD12	2.35	0.52
1:B:83:LEU:HD13	1:B:85:TRP:CZ2	2.44	0.52
1:S:36:THR:CG2	1:S:41:LEU:HD21	2.39	0.52
1:O:299:MET:CE	1:P:171:GLU:HB2	2.40	0.52
1:O:229:ASP:HB3	1:P:299:MET:CE	2.33	0.52
1:P:242:LEU:HD12	1:P:242:LEU:C	2.35	0.52
1:V:255:LYS:NZ	1:V:296:THR:HB	2.25	0.52
1:C:155:CYS:HA	1:C:289:SER:HB2	1.92	0.51
1:J:34:ASP:O	1:J:76:ALA:HA	2.10	0.51
1:Q:242:LEU:C	1:Q:242:LEU:HD12	2.35	0.51
1:K:227:LYS:C	1:L:299:MET:HE1	2.35	0.51
1:M:299:MET:HE2	1:N:171:GLU:HB2	1.92	0.51
1:N:282:VAL:HG21	1:N:312:TRP:HB3	1.91	0.51
1:C:34:ASP:O	1:C:76:ALA:HA	2.11	0.51
1:K:299:MET:HE1	1:L:229:ASP:H	1.75	0.51
1:T:155:CYS:HA	1:T:289:SER:HB2	1.92	0.51
1:A:244:GLU:HG2	1:A:310:VAL:HG22	1.92	0.51
1:G:227:LYS:C	1:H:299:MET:HE1	2.36	0.51
1:F:155:CYS:HA	1:F:289:SER:HB2	1.92	0.51
1:O:229:ASP:CB	1:P:299:MET:CE	2.87	0.51
1:D:242:LEU:HD12	1:D:242:LEU:C	2.36	0.51
1:C:299:MET:HE1	1:D:228:LEU:C	2.36	0.50
1:G:299:MET:HE3	1:H:173:LEU:HG	1.94	0.50
1:R:66:VAL:HG22	1:R:71:GLU:HG2	1.92	0.50
1:U:229:ASP:CB	1:V:299:MET:HE2	2.41	0.50
1:A:299:MET:HE1	1:B:227:LYS:C	2.37	0.50
1:L:34:ASP:O	1:L:76:ALA:HA	2.11	0.50
1:N:28:GLU:OE1	1:N:70:ARG:HD2	2.12	0.50
1:G:282:VAL:HG21	1:G:312:TRP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:299:MET:CE	1:H:173:LEU:HG	2.41	0.50
1:I:36:THR:HG21	1:K:190:PRO:CB	2.37	0.50
1:K:227:LYS:HG2	1:L:301:VAL:HG11	1.93	0.50
1:G:36:THR:HG23	1:G:37:PRO:HD2	1.93	0.50
1:U:242:LEU:HD12	1:U:242:LEU:C	2.37	0.50
1:W:195:ASP:HB2	1:W:198:ARG:NH2	2.26	0.50
1:C:242:LEU:C	1:C:242:LEU:HD12	2.37	0.50
1:A:204:LEU:HD11	1:C:238:ALA:CB	2.42	0.49
1:M:227:LYS:C	1:N:299:MET:HE1	2.38	0.49
1:O:282:VAL:HG21	1:O:312:TRP:HB3	1.94	0.49
1:Q:83:LEU:HD13	1:Q:85:TRP:CZ2	2.46	0.49
1:V:255:LYS:HZ3	1:V:296:THR:HB	1.76	0.49
1:B:282:VAL:HG21	1:B:312:TRP:HB3	1.94	0.49
1:T:242:LEU:C	1:T:242:LEU:HD12	2.37	0.49
1:E:242:LEU:C	1:E:242:LEU:HD12	2.38	0.49
1:S:299:MET:HE3	1:T:173:LEU:CD2	2.43	0.49
1:B:242:LEU:C	1:B:242:LEU:HD12	2.38	0.49
1:C:81:GLU:CB	1:N:257:GLU:HB3	2.43	0.49
1:R:36:THR:CG2	1:R:40:MET:HB3	2.42	0.49
1:U:172:GLY:O	1:V:299:MET:HE1	2.12	0.49
1:V:34:ASP:O	1:V:76:ALA:HA	2.13	0.49
1:W:282:VAL:HG21	1:W:312:TRP:HB3	1.94	0.49
1:B:224:LEU:HA	1:B:227:LYS:HD2	1.93	0.49
1:N:299:MET:O	1:N:305:GLN:HA	2.13	0.49
1:V:255:LYS:HZ3	1:V:296:THR:C	2.21	0.49
1:R:299:MET:HE2	1:R:301:VAL:HG21	1.94	0.48
1:X:184:GLN:HG2	1:X:198:ARG:HG3	1.95	0.48
1:R:28:GLU:CD	1:R:70:ARG:NH2	2.71	0.48
1:J:204:LEU:HD11	1:L:238:ALA:CB	2.44	0.48
1:Q:34:ASP:O	1:Q:76:ALA:HA	2.13	0.48
1:T:34:ASP:O	1:T:76:ALA:HA	2.12	0.48
1:U:229:ASP:HB3	1:V:299:MET:HE2	1.95	0.48
1:V:255:LYS:HZ3	1:V:296:THR:CA	2.26	0.48
1:X:80:PRO:O	1:X:83:LEU:HG	2.13	0.48
1:B:238:ALA:CB	1:D:204:LEU:HD11	2.43	0.48
1:E:34:ASP:O	1:E:76:ALA:HA	2.13	0.48
1:F:299:MET:O	1:F:305:GLN:HA	2.14	0.48
1:J:25:HIS:CG	1:X:70:ARG:HE	2.32	0.48
1:R:34:ASP:O	1:R:76:ALA:HA	2.14	0.48
1:V:36:THR:HG21	1:X:190:PRO:CB	2.40	0.48
1:E:229:ASP:HB3	1:F:299:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:GLU:CD	1:G:223:GLU:H	2.21	0.48
1:A:155:CYS:HA	1:A:289:SER:HB2	1.96	0.48
1:A:333:LYS:O	1:A:334:ILE:CB	2.62	0.48
1:N:28:GLU:OE1	1:N:70:ARG:CD	2.61	0.48
1:Q:204:LEU:HD11	1:S:238:ALA:CB	2.44	0.48
1:R:299:MET:O	1:R:305:GLN:HA	2.14	0.48
1:J:190:PRO:HB3	1:L:36:THR:HG21	1.96	0.47
1:D:244:GLU:HG2	1:D:310:VAL:HG22	1.96	0.47
1:M:282:VAL:HG21	1:M:312:TRP:HB3	1.95	0.47
1:P:155:CYS:HA	1:P:289:SER:HB2	1.97	0.47
1:V:281:ASP:O	1:W:53:ARG:CZ	2.61	0.47
1:B:60:LEU:HD23	1:B:61:LYS:O	2.14	0.47
1:W:21:ILE:HG21	1:W:29:VAL:HG23	1.96	0.47
1:X:3:ILE:HD13	1:X:331:ALA:CB	2.44	0.47
1:A:21:ILE:HG21	1:A:29:VAL:HG23	1.96	0.47
1:I:228:LEU:C	1:J:299:MET:HE1	2.39	0.47
1:G:299:MET:O	1:G:305:GLN:HA	2.15	0.47
1:J:282:VAL:HG21	1:J:312:TRP:HB3	1.96	0.47
1:Q:299:MET:HE2	1:R:171:GLU:HB2	1.96	0.47
1:E:282:VAL:HG21	1:E:312:TRP:HB3	1.96	0.47
1:G:242:LEU:C	1:G:242:LEU:HD12	2.40	0.47
1:I:238:ALA:CB	1:K:204:LEU:HD11	2.44	0.47
1:K:155:CYS:HA	1:K:289:SER:HB2	1.97	0.47
1:L:198:ARG:CZ	1:L:209:ASN:OD1	2.62	0.47
1:L:242:LEU:C	1:L:242:LEU:HD12	2.39	0.47
1:N:242:LEU:HD12	1:N:242:LEU:C	2.40	0.47
1:O:65:ILE:HD12	1:O:67:VAL:HG23	1.96	0.47
1:T:299:MET:O	1:T:305:GLN:HA	2.15	0.47
1:U:282:VAL:HG21	1:U:312:TRP:HB3	1.97	0.47
1:V:255:LYS:HD2	1:V:296:THR:O	2.14	0.47
1:B:34:ASP:O	1:B:76:ALA:HA	2.14	0.47
1:C:276:GLN:HG3	1:D:196:LEU:HD12	1.95	0.47
1:D:34:ASP:O	1:D:76:ALA:HA	2.15	0.47
1:R:36:THR:HG22	1:R:40:MET:HB3	1.97	0.47
1:C:244:GLU:HG2	1:C:310:VAL:HG22	1.97	0.47
1:M:238:ALA:CB	1:O:204:LEU:HD11	2.44	0.47
1:P:297:ARG:HB3	1:P:308:LYS:HB3	1.96	0.47
1:X:34:ASP:O	1:X:76:ALA:HA	2.14	0.47
1:L:107:GLU:OE1	1:O:300:THR:HG22	2.14	0.46
1:L:161:ALA:O	1:L:165:LYS:HG2	2.15	0.46
1:A:299:MET:HE2	1:A:301:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ASP:O	1:F:76:ALA:HA	2.15	0.46
1:I:34:ASP:O	1:I:76:ALA:HA	2.15	0.46
1:O:100:PHE:HA	1:O:105:LYS:HD3	1.97	0.46
1:V:282:VAL:HG21	1:V:312:TRP:HB3	1.96	0.46
1:A:299:MET:HE2	1:A:301:VAL:CG2	2.46	0.46
1:C:329:TYR:CZ	1:C:333:LYS:HE3	2.51	0.46
1:E:299:MET:HE2	1:F:229:ASP:CB	2.46	0.46
1:J:111:ARG:CZ	1:Q:219:LEU:HD22	2.46	0.46
1:K:242:LEU:HD12	1:K:242:LEU:C	2.40	0.46
1:O:155:CYS:HA	1:O:289:SER:HB2	1.98	0.46
1:P:297:ARG:NH2	1:P:299:MET:CE	2.77	0.46
1:P:272:TYR:CE2	1:P:274:GLU:HG3	2.51	0.46
1:C:117:VAL:HB	1:C:145:VAL:HG22	1.98	0.45
1:R:92:VAL:HG11	1:R:327:LEU:CD1	2.45	0.45
1:C:57:THR:OG1	1:C:68:ASN:HA	2.16	0.45
1:L:21:ILE:HG23	1:L:27:ILE:HG23	1.99	0.45
1:M:34:ASP:O	1:M:76:ALA:HA	2.16	0.45
1:X:155:CYS:HA	1:X:289:SER:HB2	1.98	0.45
1:D:155:CYS:HA	1:D:289:SER:HB2	1.98	0.45
1:F:106:ALA:HB1	1:F:117:VAL:HG11	1.98	0.45
1:J:155:CYS:HA	1:J:289:SER:HB2	1.96	0.45
1:M:299:MET:HG2	1:M:306:LEU:O	2.16	0.45
1:I:299:MET:HE3	1:J:173:LEU:CD2	2.46	0.45
1:Q:80:PRO:HA	1:Q:83:LEU:HD12	1.99	0.45
1:Q:281:ASP:CB	1:T:53:ARG:HH21	2.25	0.45
1:M:255:LYS:HG3	1:M:296:THR:CG2	2.46	0.45
1:S:242:LEU:C	1:S:242:LEU:HD12	2.42	0.45
1:P:215:LYS:CG	1:P:229:ASP:OD1	2.62	0.45
1:D:161:ALA:O	1:D:165:LYS:HG2	2.17	0.45
1:O:282:VAL:HG22	1:O:285:ILE:HD13	1.99	0.45
1:S:299:MET:HE3	1:T:173:LEU:HD21	1.99	0.45
1:V:94:LEU:HD23	1:V:118:VAL:HB	1.99	0.45
1:H:34:ASP:O	1:H:76:ALA:HA	2.17	0.45
1:J:85:TRP:CE3	1:J:85:TRP:HA	2.52	0.45
1:M:255:LYS:HD2	1:M:296:THR:O	2.16	0.45
1:F:178:HIS:HB3	1:F:234:ARG:HD3	1.98	0.45
1:O:229:ASP:HB2	1:P:299:MET:HE1	1.96	0.45
1:A:34:ASP:O	1:A:76:ALA:HA	2.17	0.44
1:D:255:LYS:NZ	1:D:296:THR:HB	2.32	0.44
1:P:42:LEU:HD11	1:P:58:ALA:HB1	1.99	0.44
1:Q:36:THR:CG2	1:Q:40:MET:HB3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:282:VAL:HG22	1:V:285:ILE:CD1	2.43	0.44
1:W:161:ALA:O	1:W:165:LYS:HG2	2.17	0.44
1:X:57:THR:HG1	1:X:68:ASN:HA	1.81	0.44
1:Q:281:ASP:O	1:T:53:ARG:NH2	2.50	0.44
1:S:299:MET:HE2	1:T:229:ASP:HB2	1.99	0.44
1:K:299:MET:HE2	1:L:229:ASP:CB	2.48	0.44
1:W:17:ALA:O	1:W:21:ILE:HG12	2.17	0.44
1:A:282:VAL:HG21	1:A:312:TRP:HB3	2.00	0.44
1:E:204:LEU:HD11	1:G:238:ALA:CB	2.48	0.44
1:A:80:PRO:HB3	1:A:109:HIS:CE1	2.53	0.44
1:E:299:MET:O	1:E:305:GLN:HA	2.18	0.44
1:G:299:MET:HE3	1:H:173:LEU:CD2	2.48	0.44
1:G:299:MET:HE1	1:H:172:GLY:O	2.18	0.44
1:P:94:LEU:HD23	1:P:118:VAL:HB	1.99	0.44
1:T:92:VAL:HG11	1:T:327:LEU:CD1	2.48	0.44
1:W:195:ASP:OD2	1:W:198:ARG:NE	2.51	0.44
1:H:155:CYS:HA	1:H:289:SER:HB2	1.99	0.43
1:E:299:MET:HE1	1:F:172:GLY:O	2.18	0.43
1:W:299:MET:HE2	1:X:173:LEU:HG	2.00	0.43
1:O:34:ASP:HB3	1:O:41:LEU:HD11	2.00	0.43
1:P:258:ILE:O	1:P:262:MET:HG2	2.18	0.43
1:W:5:VAL:O	1:W:28:GLU:O	2.36	0.43
1:W:11:GLY:O	1:W:15:ARG:HG3	2.17	0.43
1:O:299:MET:HG3	1:O:299:MET:O	2.18	0.43
1:R:183:ASP:HB2	1:R:198:ARG:NH1	2.33	0.43
1:W:5:VAL:O	1:W:29:VAL:HA	2.19	0.43
1:E:36:THR:HG21	1:E:40:MET:CG	2.48	0.43
1:C:80:PRO:HD2	4:C:532:HOH:O	2.19	0.43
1:V:281:ASP:O	1:W:53:ARG:NE	2.51	0.43
1:G:299:MET:CE	1:H:173:LEU:CD2	2.97	0.43
1:J:281:ASP:O	1:K:53:ARG:NH2	2.52	0.43
1:T:299:MET:HE2	1:T:301:VAL:HG21	2.01	0.43
1:V:255:LYS:NZ	1:V:296:THR:N	2.66	0.43
1:E:94:LEU:HD23	1:E:118:VAL:HB	1.99	0.43
1:N:155:CYS:HA	1:N:289:SER:HB2	2.00	0.43
1:N:253:ALA:HA	1:N:257:GLU:OE2	2.18	0.43
1:P:282:VAL:HG21	1:P:312:TRP:HB3	2.01	0.43
1:G:27:ILE:HD11	1:G:327:LEU:HD21	2.01	0.43
1:L:155:CYS:HA	1:L:289:SER:HB2	2.00	0.43
1:N:215:LYS:HE2	1:N:229:ASP:CG	2.44	0.43
1:N:330:PHE:O	1:N:334:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:MET:HE1	1:B:227:LYS:O	2.19	0.43
1:E:176:THR:O	1:E:176:THR:HG23	2.19	0.43
1:Q:206:ILE:HB	1:R:279:SER:HB3	2.01	0.43
1:T:42:LEU:HD11	1:T:58:ALA:HB1	2.01	0.43
1:G:299:MET:HE3	1:G:299:MET:HB2	1.86	0.42
1:M:227:LYS:O	1:N:299:MET:HE1	2.19	0.42
1:S:198:ARG:HA	4:S:510:HOH:O	2.18	0.42
1:U:80:PRO:HA	1:U:83:LEU:HD12	2.01	0.42
1:K:227:LYS:O	1:L:299:MET:HE1	2.19	0.42
1:M:42:LEU:HD11	1:M:58:ALA:HB1	2.01	0.42
1:C:282:VAL:HG21	1:C:312:TRP:HB3	2.00	0.42
1:K:299:MET:HE3	1:L:173:LEU:CD2	2.49	0.42
1:C:4:LYS:HE3	1:C:89:GLY:O	2.19	0.42
1:E:173:LEU:CD2	1:F:299:MET:HE3	2.50	0.42
1:L:242:LEU:HD12	1:L:242:LEU:O	2.19	0.42
1:A:299:MET:O	1:A:305:GLN:HA	2.19	0.42
1:J:242:LEU:HD12	1:J:242:LEU:O	2.20	0.42
1:U:217:ILE:HG21	1:U:228:LEU:HD12	2.02	0.42
1:W:34:ASP:O	1:W:76:ALA:HA	2.19	0.42
1:F:57:THR:HG1	1:F:68:ASN:HA	1.83	0.42
1:U:299:MET:HE1	1:V:227:LYS:C	2.45	0.42
1:V:204:LEU:HD11	1:X:238:ALA:CB	2.50	0.42
1:R:36:THR:HG21	1:R:40:MET:CG	2.48	0.42
1:V:155:CYS:HA	1:V:289:SER:HB2	2.01	0.42
1:Q:36:THR:HG21	1:Q:40:MET:CG	2.48	0.42
1:W:132:TYR:HE1	1:W:329:TYR:HB2	1.84	0.42
1:W:301:VAL:HG11	1:X:227:LYS:HG2	2.01	0.42
1:I:92:VAL:HG11	1:I:327:LEU:CD1	2.49	0.42
1:O:189:ALA:O	1:O:199:ALA:HB1	2.20	0.42
1:P:6:ALA:HB2	1:P:90:VAL:HG21	2.02	0.42
1:R:266:SER:HA	1:R:270:TYR:O	2.20	0.42
1:U:173:LEU:HG	1:V:299:MET:HE3	2.02	0.42
1:X:83:LEU:HD11	1:X:112:ALA:HB3	2.01	0.42
1:N:11:GLY:O	1:N:15:ARG:HG3	2.20	0.42
1:T:57:THR:OG1	1:T:68:ASN:HA	2.20	0.42
1:T:85:TRP:CE3	1:T:85:TRP:HA	2.55	0.42
1:M:7:ILE:HB	1:M:32:VAL:HG12	2.02	0.41
1:U:164:GLN:HG2	1:U:223:GLU:HG3	2.01	0.41
1:W:7:ILE:O	1:W:32:VAL:HA	2.20	0.41
1:E:299:MET:HE3	1:F:173:LEU:CD2	2.50	0.41
1:R:204:LEU:HD11	1:T:238:ALA:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:176:THR:HG23	1:T:176:THR:O	2.20	0.41
1:V:281:ASP:O	1:W:53:ARG:NH2	2.53	0.41
1:V:299:MET:O	1:V:305:GLN:HA	2.20	0.41
1:X:6:ALA:HB1	1:X:85:TRP:CZ2	2.55	0.41
1:X:85:TRP:HA	1:X:85:TRP:CE3	2.55	0.41
1:D:255:LYS:HZ2	1:D:296:THR:HB	1.84	0.41
1:I:178:HIS:HB3	1:I:234:ARG:HD3	2.02	0.41
1:N:36:THR:CG2	1:P:190:PRO:HB3	2.34	0.41
1:B:57:THR:HG1	1:B:68:ASN:HA	1.85	0.41
1:C:85:TRP:HA	1:C:85:TRP:HE3	1.86	0.41
1:I:190:PRO:CB	1:K:36:THR:HG21	2.45	0.41
1:J:85:TRP:HA	1:J:85:TRP:HE3	1.83	0.41
1:L:282:VAL:HG13	1:L:285:ILE:CD1	2.51	0.41
1:M:255:LYS:HG3	1:M:296:THR:CB	2.49	0.41
1:P:116:LYS:CB	1:P:330:PHE:CE2	3.03	0.41
1:T:85:TRP:HA	1:T:85:TRP:HE3	1.85	0.41
1:B:176:THR:O	1:B:176:THR:HG23	2.21	0.41
1:C:246:VAL:HA	1:C:307:VAL:O	2.20	0.41
1:E:155:CYS:HA	1:E:289:SER:HB2	2.01	0.41
1:F:282:VAL:O	1:F:282:VAL:CG1	2.68	0.41
1:J:238:ALA:CB	1:L:204:LEU:HD11	2.51	0.41
1:M:242:LEU:HD12	1:M:242:LEU:O	2.21	0.41
1:D:143:GLU:CD	1:D:143:GLU:H	2.27	0.41
1:E:36:THR:CG2	1:E:40:MET:HB3	2.50	0.41
1:F:11:GLY:O	1:F:15:ARG:HG3	2.21	0.41
1:N:238:ALA:CB	1:P:204:LEU:HD11	2.51	0.41
1:R:85:TRP:HA	1:R:85:TRP:CE3	2.56	0.41
1:R:115:ARG:NH2	1:R:334:ILE:HG22	2.34	0.41
1:E:229:ASP:H	1:F:299:MET:HE1	1.84	0.41
1:Q:155:CYS:HA	1:Q:289:SER:HB2	2.02	0.41
1:V:255:LYS:NZ	1:V:296:THR:O	2.50	0.41
1:X:299:MET:O	1:X:305:GLN:HA	2.20	0.41
1:C:173:LEU:HD13	1:D:308:LYS:HB2	2.03	0.41
1:H:3:ILE:HD13	1:H:331:ALA:CB	2.48	0.41
1:I:57:THR:HG1	1:I:68:ASN:HA	1.86	0.41
1:I:128:LYS:NZ	1:I:138:ILE:O	2.54	0.41
1:M:233:GLN:HG3	1:N:177:ILE:CD1	2.51	0.41
1:R:155:CYS:HA	1:R:289:SER:HB2	2.03	0.41
1:X:178:HIS:HB3	1:X:234:ARG:HD3	2.03	0.41
1:X:299:MET:HE2	1:X:301:VAL:CG2	2.50	0.41
1:C:85:TRP:HA	1:C:85:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:THR:HA	1:F:304:LYS:O	2.21	0.41
1:J:80:PRO:HB3	1:J:109:HIS:CE1	2.56	0.41
1:J:127:VAL:HG13	1:J:145:VAL:O	2.21	0.41
1:M:128:LYS:NZ	1:M:138:ILE:O	2.53	0.41
1:Q:11:GLY:O	1:Q:15:ARG:HG3	2.21	0.41
1:S:79:ASN:HB2	1:S:82:GLU:OE1	2.21	0.41
1:S:306:LEU:HD12	1:S:306:LEU:HA	1.97	0.41
1:U:190:PRO:CB	1:W:36:THR:HG21	2.42	0.41
1:U:206:ILE:HB	1:V:279:SER:HB3	2.03	0.41
1:X:83:LEU:HD22	1:X:85:TRP:CE2	2.56	0.41
1:R:83:LEU:HD13	1:R:85:TRP:CZ2	2.55	0.41
1:C:178:HIS:HB3	1:C:234:ARG:HD3	2.03	0.40
1:L:106:ALA:HB1	1:L:117:VAL:HG11	2.04	0.40
1:L:295:GLN:O	1:L:308:LYS:HE3	2.22	0.40
1:P:314:ASP:O	1:P:318:SER:HB2	2.22	0.40
1:Q:36:THR:HG23	1:Q:37:PRO:HD2	2.03	0.40
1:Q:36:THR:HG22	1:Q:40:MET:HB3	2.02	0.40
1:S:279:SER:HB3	1:T:206:ILE:HB	2.04	0.40
1:D:128:LYS:HD2	1:D:143:GLU:HG2	2.04	0.40
1:D:255:LYS:NZ	1:D:293:ALA:O	2.50	0.40
1:E:57:THR:OG1	1:E:68:ASN:HA	2.21	0.40
1:P:36:THR:HG22	1:P:41:LEU:HD21	2.03	0.40
1:C:92:VAL:HG11	1:C:327:LEU:CD1	2.52	0.40
1:E:36:THR:HG22	1:E:40:MET:HB3	2.03	0.40
1:N:107:GLU:HA	1:N:110:ILE:HD13	2.03	0.40
1:P:36:THR:OG1	1:P:37:PRO:HD2	2.21	0.40
1:R:282:VAL:HG21	1:R:312:TRP:HB3	2.04	0.40
1:T:282:VAL:HG21	1:T:312:TRP:HB3	2.04	0.40
1:U:177:ILE:CD1	1:V:233:GLN:HG3	2.52	0.40
1:B:85:TRP:CE3	1:B:85:TRP:HA	2.57	0.40
1:K:282:VAL:HG21	1:K:312:TRP:HB3	2.03	0.40
1:R:242:LEU:HD12	1:R:242:LEU:O	2.21	0.40
1:S:180:TYR:HA	1:S:184:GLN:OE1	2.22	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	331/342 (97%)	324 (98%)	7 (2%)	0	100	100
1	B	331/342 (97%)	319 (96%)	12 (4%)	0	100	100
1	C	330/342 (96%)	321 (97%)	9 (3%)	0	100	100
1	D	330/342 (96%)	320 (97%)	10 (3%)	0	100	100
1	E	331/342 (97%)	322 (97%)	9 (3%)	0	100	100
1	F	331/342 (97%)	325 (98%)	6 (2%)	0	100	100
1	G	319/342 (93%)	310 (97%)	9 (3%)	0	100	100
1	H	330/342 (96%)	321 (97%)	9 (3%)	0	100	100
1	I	331/342 (97%)	321 (97%)	10 (3%)	0	100	100
1	J	331/342 (97%)	323 (98%)	8 (2%)	0	100	100
1	K	330/342 (96%)	319 (97%)	11 (3%)	0	100	100
1	L	330/342 (96%)	319 (97%)	11 (3%)	0	100	100
1	M	332/342 (97%)	325 (98%)	7 (2%)	0	100	100
1	N	332/342 (97%)	324 (98%)	8 (2%)	0	100	100
1	O	315/342 (92%)	307 (98%)	8 (2%)	0	100	100
1	P	316/342 (92%)	309 (98%)	7 (2%)	0	100	100
1	Q	331/342 (97%)	323 (98%)	8 (2%)	0	100	100
1	R	331/342 (97%)	321 (97%)	10 (3%)	0	100	100
1	S	326/342 (95%)	317 (97%)	9 (3%)	0	100	100
1	T	330/342 (96%)	322 (98%)	8 (2%)	0	100	100
1	U	324/342 (95%)	318 (98%)	6 (2%)	0	100	100
1	V	327/342 (96%)	317 (97%)	10 (3%)	0	100	100
1	W	275/342 (80%)	268 (98%)	7 (2%)	0	100	100
1	X	325/342 (95%)	317 (98%)	8 (2%)	0	100	100
All	All	7819/8208 (95%)	7612 (97%)	207 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	260/273 (95%)	259 (100%)	1 (0%)	89	95
1	B	259/273 (95%)	257 (99%)	2 (1%)	79	89
1	C	257/273 (94%)	254 (99%)	3 (1%)	67	81
1	D	263/273 (96%)	261 (99%)	2 (1%)	79	89
1	E	261/273 (96%)	260 (100%)	1 (0%)	89	95
1	F	263/273 (96%)	259 (98%)	4 (2%)	60	76
1	G	246/273 (90%)	244 (99%)	2 (1%)	79	89
1	H	262/273 (96%)	261 (100%)	1 (0%)	89	95
1	I	257/273 (94%)	255 (99%)	2 (1%)	79	89
1	J	262/273 (96%)	261 (100%)	1 (0%)	89	95
1	K	259/273 (95%)	258 (100%)	1 (0%)	89	95
1	L	258/273 (94%)	257 (100%)	1 (0%)	89	95
1	M	263/273 (96%)	260 (99%)	3 (1%)	70	83
1	N	263/273 (96%)	259 (98%)	4 (2%)	60	76
1	O	242/273 (89%)	232 (96%)	10 (4%)	26	39
1	P	242/273 (89%)	240 (99%)	2 (1%)	79	89
1	Q	262/273 (96%)	262 (100%)	0	100	100
1	R	262/273 (96%)	262 (100%)	0	100	100
1	S	253/273 (93%)	251 (99%)	2 (1%)	79	89
1	T	262/273 (96%)	262 (100%)	0	100	100
1	U	254/273 (93%)	250 (98%)	4 (2%)	58	74
1	V	257/273 (94%)	254 (99%)	3 (1%)	67	81
1	W	222/273 (81%)	216 (97%)	6 (3%)	40	57
1	X	256/273 (94%)	253 (99%)	3 (1%)	67	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6145/6552 (94%)	6087 (99%)	58 (1%)	75	87

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	TRP
1	B	81	GLU
1	B	282	VAL
1	C	87	GLU
1	C	144	THR
1	C	223	GLU
1	D	223	GLU
1	D	299	MET
1	E	223	GLU
1	F	2	SER
1	F	71	GLU
1	F	73	LYS
1	F	165	LYS
1	G	4	LYS
1	G	223	GLU
1	H	223	GLU
1	I	223	GLU
1	I	255	LYS
1	J	85	TRP
1	K	3	ILE
1	L	209	ASN
1	M	209	ASN
1	M	223	GLU
1	M	334	ILE
1	N	1	MET
1	N	85	TRP
1	N	95	GLU
1	N	282	VAL
1	O	3	ILE
1	O	4	LYS
1	O	65	ILE
1	O	92	VAL
1	O	115	ARG
1	O	209	ASN
1	O	223	GLU
1	O	282	VAL
1	O	308	LYS

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Mol	Chain	Res	Type
1	O	327	LEU
1	P	90	VAL
1	P	248	VAL
1	S	27	ILE
1	S	127	VAL
1	U	59	GLU
1	U	111	ARG
1	U	209	ASN
1	U	223	GLU
1	V	61	LYS
1	V	73	LYS
1	V	282	VAL
1	W	5	VAL
1	W	12	ARG
1	W	61	LYS
1	W	209	ASN
1	W	299	MET
1	W	323	LEU
1	X	85	TRP
1	X	198	ARG
1	X	223	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	GLN
1	B	209	ASN
1	C	209	ASN
1	C	259	ASN
1	E	209	ASN
1	F	20	GLN
1	F	79	ASN
1	G	20	GLN
1	G	209	ASN
1	H	209	ASN
1	L	20	GLN
1	L	55	GLN
1	M	20	GLN
1	M	55	GLN
1	N	25	HIS
1	N	209	ASN
1	Q	79	ASN

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Mol	Chain	Res	Type
1	R	55	GLN
1	S	20	GLN
1	S	225	ASN
1	T	259	ASN
1	V	209	ASN
1	W	33	ASN
1	W	55	GLN
1	X	55	GLN
1	X	209	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	P	401	-	42,48,48	1.37	4 (9%)	50,73,73	1.05	3 (6%)
2	NAD	O	401	-	42,48,48	1.41	4 (9%)	50,73,73	1.03	3 (6%)
2	NAD	M	401	-	42,48,48	1.28	4 (9%)	50,73,73	1.03	4 (8%)
2	NAD	N	401	-	42,48,48	1.37	4 (9%)	50,73,73	1.02	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	T	401	-	42,48,48	1.30	5 (11%)	50,73,73	1.08	2 (4%)
2	NAD	L	401	-	42,48,48	1.28	4 (9%)	50,73,73	1.07	3 (6%)
2	NAD	G	401	-	42,48,48	1.33	4 (9%)	50,73,73	1.04	3 (6%)
2	NAD	V	401	-	42,48,48	1.21	4 (9%)	50,73,73	1.06	2 (4%)
2	NAD	K	401	-	42,48,48	1.28	4 (9%)	50,73,73	1.01	2 (4%)
3	PGE	H	402	-	9,9,9	0.27	0	8,8,8	0.50	0
2	NAD	X	401	-	42,48,48	1.30	4 (9%)	50,73,73	1.05	4 (8%)
2	NAD	J	401	-	42,48,48	1.41	4 (9%)	50,73,73	1.00	2 (4%)
2	NAD	F	401	-	42,48,48	1.25	4 (9%)	50,73,73	0.96	2 (4%)
2	NAD	Q	401	-	42,48,48	1.40	5 (11%)	50,73,73	1.01	3 (6%)
2	NAD	C	401	-	42,48,48	1.24	5 (11%)	50,73,73	1.04	3 (6%)
2	NAD	I	401	-	42,48,48	1.14	3 (7%)	50,73,73	1.06	5 (10%)
2	NAD	U	401	-	42,48,48	1.29	4 (9%)	50,73,73	1.00	3 (6%)
2	NAD	S	401	-	42,48,48	1.43	3 (7%)	50,73,73	1.08	3 (6%)
2	NAD	R	401	-	42,48,48	1.29	3 (7%)	50,73,73	1.03	3 (6%)
2	NAD	W	401	-	42,48,48	1.34	4 (9%)	50,73,73	1.04	3 (6%)
2	NAD	D	401	-	42,48,48	1.22	4 (9%)	50,73,73	1.13	6 (12%)
2	NAD	A	401	-	42,48,48	1.36	4 (9%)	50,73,73	0.96	3 (6%)
2	NAD	H	401	-	42,48,48	1.39	4 (9%)	50,73,73	1.14	3 (6%)
2	NAD	B	401	-	42,48,48	1.38	4 (9%)	50,73,73	0.98	3 (6%)
2	NAD	E	401	-	42,48,48	1.25	4 (9%)	50,73,73	1.02	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	P	401	-	-	6/26/62/62	0/5/5/5
2	NAD	O	401	-	-	17/26/62/62	0/5/5/5
2	NAD	M	401	-	-	4/26/62/62	0/5/5/5
2	NAD	N	401	-	-	6/26/62/62	0/5/5/5
2	NAD	T	401	-	-	7/26/62/62	0/5/5/5
2	NAD	L	401	-	-	5/26/62/62	0/5/5/5
2	NAD	G	401	-	-	5/26/62/62	0/5/5/5
2	NAD	V	401	-	-	3/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	K	401	-	-	5/26/62/62	0/5/5/5
3	PGE	H	402	-	-	2/7/7/7	-
2	NAD	X	401	-	-	5/26/62/62	0/5/5/5
2	NAD	J	401	-	-	8/26/62/62	0/5/5/5
2	NAD	F	401	-	-	6/26/62/62	0/5/5/5
2	NAD	Q	401	-	-	5/26/62/62	0/5/5/5
2	NAD	C	401	-	-	5/26/62/62	0/5/5/5
2	NAD	I	401	-	-	5/26/62/62	0/5/5/5
2	NAD	U	401	-	-	5/26/62/62	0/5/5/5
2	NAD	S	401	-	-	10/26/62/62	0/5/5/5
2	NAD	R	401	-	-	5/26/62/62	0/5/5/5
2	NAD	W	401	-	-	12/26/62/62	0/5/5/5
2	NAD	D	401	-	-	7/26/62/62	0/5/5/5
2	NAD	A	401	-	-	6/26/62/62	0/5/5/5
2	NAD	H	401	-	-	6/26/62/62	0/5/5/5
2	NAD	B	401	-	-	7/26/62/62	0/5/5/5
2	NAD	E	401	-	-	6/26/62/62	0/5/5/5

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401	NAD	PA-O3	6.32	1.66	1.59
2	O	401	NAD	PA-O3	6.06	1.66	1.59
2	S	401	NAD	PA-O3	5.83	1.65	1.59
2	H	401	NAD	PA-O3	5.80	1.65	1.59
2	W	401	NAD	PA-O3	5.68	1.65	1.59
2	Q	401	NAD	PA-O3	5.64	1.65	1.59
2	B	401	NAD	PA-O3	5.62	1.65	1.59
2	G	401	NAD	PA-O3	5.61	1.65	1.59
2	P	401	NAD	PA-O3	5.54	1.65	1.59
2	X	401	NAD	PA-O3	5.37	1.65	1.59
2	R	401	NAD	PA-O3	5.36	1.65	1.59
2	A	401	NAD	PA-O3	5.33	1.65	1.59
2	N	401	NAD	PA-O3	5.32	1.65	1.59
2	U	401	NAD	PA-O3	5.25	1.65	1.59
2	K	401	NAD	PA-O3	5.11	1.65	1.59
2	M	401	NAD	PA-O3	5.05	1.65	1.59
2	E	401	NAD	PA-O3	4.99	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	401	NAD	PA-O3	4.99	1.64	1.59
2	L	401	NAD	PA-O3	4.95	1.64	1.59
2	F	401	NAD	PA-O3	4.71	1.64	1.59
2	V	401	NAD	PA-O3	4.57	1.64	1.59
2	D	401	NAD	PA-O3	4.52	1.64	1.59
2	S	401	NAD	PN-O3	4.41	1.64	1.59
2	C	401	NAD	PA-O3	4.39	1.64	1.59
2	I	401	NAD	PA-O3	4.32	1.64	1.59
2	N	401	NAD	PN-O3	4.31	1.64	1.59
2	B	401	NAD	PN-O3	4.22	1.64	1.59
2	O	401	NAD	PN-O3	4.16	1.64	1.59
2	P	401	NAD	PN-O3	3.96	1.63	1.59
2	C	401	NAD	PN-O3	3.68	1.63	1.59
2	Q	401	NAD	PN-O3	3.62	1.63	1.59
2	L	401	NAD	PN-O3	3.54	1.63	1.59
2	X	401	NAD	PN-O3	3.51	1.63	1.59
2	A	401	NAD	PN-O3	3.49	1.63	1.59
2	F	401	NAD	PN-O3	3.48	1.63	1.59
2	G	401	NAD	PN-O3	3.48	1.63	1.59
2	W	401	NAD	PN-O3	3.43	1.63	1.59
2	J	401	NAD	PN-O3	3.38	1.63	1.59
2	H	401	NAD	PN-O3	3.34	1.63	1.59
2	M	401	NAD	PN-O3	3.30	1.63	1.59
2	U	401	NAD	PN-O3	3.29	1.63	1.59
2	R	401	NAD	PN-O3	3.26	1.63	1.59
2	T	401	NAD	PN-O3	3.25	1.63	1.59
2	K	401	NAD	PN-O3	3.20	1.63	1.59
2	D	401	NAD	PN-O3	3.12	1.62	1.59
2	V	401	NAD	PN-O3	2.99	1.62	1.59
2	U	401	NAD	C8A-N7A	-2.79	1.29	1.34
2	Q	401	NAD	C8A-N7A	-2.70	1.29	1.34
2	T	401	NAD	O4D-C1D	-2.66	1.37	1.40
2	A	401	NAD	C8A-N7A	-2.62	1.29	1.34
2	E	401	NAD	PN-O3	2.59	1.62	1.59
2	F	401	NAD	C8A-N7A	-2.55	1.30	1.34
2	C	401	NAD	C8A-N7A	-2.50	1.30	1.34
2	S	401	NAD	C8A-N7A	-2.47	1.30	1.34
2	V	401	NAD	C8A-N7A	-2.47	1.30	1.34
2	N	401	NAD	C8A-N7A	-2.46	1.30	1.34
2	P	401	NAD	C8A-N7A	-2.45	1.30	1.34
2	X	401	NAD	C8A-N7A	-2.43	1.30	1.34
2	D	401	NAD	C8A-N7A	-2.42	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	401	NAD	C8A-N7A	-2.42	1.30	1.34
2	H	401	NAD	C8A-N7A	-2.40	1.30	1.34
2	E	401	NAD	C8A-N7A	-2.40	1.30	1.34
2	M	401	NAD	C1B-N9A	-2.39	1.44	1.49
2	K	401	NAD	C8A-N7A	-2.39	1.30	1.34
2	N	401	NAD	C1B-N9A	-2.39	1.44	1.49
2	L	401	NAD	C8A-N7A	-2.39	1.30	1.34
2	R	401	NAD	C8A-N7A	-2.39	1.30	1.34
2	T	401	NAD	C1B-N9A	-2.38	1.44	1.49
2	M	401	NAD	C8A-N7A	-2.38	1.30	1.34
2	E	401	NAD	C1B-N9A	-2.38	1.44	1.49
2	T	401	NAD	C8A-N7A	-2.37	1.30	1.34
2	O	401	NAD	C8A-N7A	-2.36	1.30	1.34
2	Q	401	NAD	C1B-N9A	-2.35	1.44	1.49
2	B	401	NAD	C8A-N7A	-2.33	1.30	1.34
2	I	401	NAD	C8A-N7A	-2.32	1.30	1.34
2	P	401	NAD	C1B-N9A	-2.32	1.44	1.49
2	G	401	NAD	C8A-N7A	-2.31	1.30	1.34
2	J	401	NAD	C1B-N9A	-2.31	1.44	1.49
2	Q	401	NAD	O4D-C1D	-2.25	1.37	1.40
2	C	401	NAD	C1B-N9A	-2.25	1.44	1.49
2	L	401	NAD	C1B-N9A	-2.25	1.44	1.49
2	F	401	NAD	C1B-N9A	-2.24	1.44	1.49
2	D	401	NAD	C1B-N9A	-2.23	1.44	1.49
2	A	401	NAD	C1B-N9A	-2.22	1.44	1.49
2	J	401	NAD	C8A-N7A	-2.21	1.30	1.34
2	I	401	NAD	C1B-N9A	-2.19	1.44	1.49
2	U	401	NAD	C1B-N9A	-2.19	1.44	1.49
2	X	401	NAD	C1B-N9A	-2.15	1.44	1.49
2	G	401	NAD	C1B-N9A	-2.12	1.44	1.49
2	B	401	NAD	C1B-N9A	-2.11	1.44	1.49
2	W	401	NAD	C1B-N9A	-2.10	1.44	1.49
2	V	401	NAD	C1B-N9A	-2.09	1.44	1.49
2	O	401	NAD	C1B-N9A	-2.09	1.44	1.49
2	K	401	NAD	C1B-N9A	-2.06	1.44	1.49
2	H	401	NAD	C1B-N9A	-2.06	1.44	1.49
2	C	401	NAD	O4D-C1D	-2.04	1.38	1.40

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	401	NAD	O3-PA-O1A	-3.24	100.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	NAD	O2A-PA-O1A	3.03	126.56	112.44
2	H	401	NAD	O7N-C7N-N7N	2.93	126.85	122.62
2	T	401	NAD	O2A-PA-O1A	2.86	125.77	112.44
2	V	401	NAD	O2A-PA-O1A	2.80	125.45	112.44
2	M	401	NAD	O2A-PA-O1A	2.76	125.30	112.44
2	P	401	NAD	O3-PA-O1A	-2.66	102.71	110.70
2	W	401	NAD	O3-PA-O1A	-2.62	102.82	110.70
2	J	401	NAD	O2A-PA-O1A	2.61	124.56	112.44
2	X	401	NAD	O2A-PA-O1A	2.59	124.50	112.44
2	B	401	NAD	C3N-C7N-N7N	-2.47	114.69	117.74
2	Q	401	NAD	O7N-C7N-N7N	2.46	126.17	122.62
2	H	401	NAD	C3N-C7N-N7N	-2.46	114.71	117.74
2	P	401	NAD	O2A-PA-O1A	2.42	123.71	112.44
2	E	401	NAD	O2A-PA-O1A	2.41	123.67	112.44
2	H	401	NAD	O2A-PA-O1A	2.38	123.50	112.44
2	L	401	NAD	O2A-PA-O1A	2.38	123.50	112.44
2	O	401	NAD	O2A-PA-O1A	2.37	123.46	112.44
2	M	401	NAD	C6N-N1N-C1D	-2.35	115.11	119.73
2	D	401	NAD	O2A-PA-O1A	2.34	123.31	112.44
2	D	401	NAD	C6N-N1N-C1D	-2.33	115.15	119.73
2	A	401	NAD	O2A-PA-O1A	2.32	123.24	112.44
2	V	401	NAD	C6N-N1N-C1D	-2.32	115.18	119.73
2	S	401	NAD	O3-PA-O1A	-2.30	103.77	110.70
2	G	401	NAD	O2N-PN-O3	2.30	113.50	107.27
2	S	401	NAD	C6N-N1N-C1D	-2.30	115.21	119.73
2	E	401	NAD	C6N-N1N-C1D	-2.30	115.22	119.73
2	J	401	NAD	C6N-N1N-C1D	-2.29	115.23	119.73
2	O	401	NAD	C6N-N1N-C1D	-2.29	115.23	119.73
2	S	401	NAD	O2A-PA-O1A	2.29	123.09	112.44
2	L	401	NAD	C6N-N1N-C1D	-2.26	115.29	119.73
2	F	401	NAD	O2A-PA-O1A	2.25	122.93	112.44
2	N	401	NAD	O7N-C7N-N7N	2.25	125.86	122.62
2	R	401	NAD	C6N-N1N-C1D	-2.24	115.33	119.73
2	W	401	NAD	O7N-C7N-N7N	2.22	125.83	122.62
2	C	401	NAD	C6N-N1N-C1D	-2.22	115.37	119.73
2	E	401	NAD	O2N-PN-O3	2.21	113.25	107.27
2	N	401	NAD	O2A-PA-O1A	2.19	122.66	112.44
2	C	401	NAD	O2A-PA-O1A	2.19	122.64	112.44
2	F	401	NAD	C6N-N1N-C1D	-2.19	115.43	119.73
2	U	401	NAD	O3-PA-O1A	-2.19	104.12	110.70
2	R	401	NAD	O7N-C7N-N7N	2.18	125.76	122.62
2	K	401	NAD	O2A-PA-O1A	2.17	122.55	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	NAD	O2N-PN-O3	2.17	113.13	107.27
2	G	401	NAD	O2A-PA-O1A	2.17	122.52	112.44
2	R	401	NAD	O2A-PA-O1A	2.16	122.48	112.44
2	X	401	NAD	O2N-PN-O3	2.16	113.10	107.27
2	T	401	NAD	C6N-N1N-C1D	-2.15	115.50	119.73
2	Q	401	NAD	O2A-PA-O1A	2.15	122.46	112.44
2	U	401	NAD	O2A-PA-O1A	2.15	122.45	112.44
2	M	401	NAD	O2N-PN-O3	2.15	113.08	107.27
2	U	401	NAD	C6N-N1N-C1D	-2.14	115.52	119.73
2	D	401	NAD	O4B-C1B-N9A	-2.13	105.92	108.75
2	D	401	NAD	C3N-C7N-N7N	-2.13	115.12	117.74
2	Q	401	NAD	C6N-N1N-C1D	-2.13	115.56	119.73
2	P	401	NAD	C6N-N1N-C1D	-2.11	115.58	119.73
2	I	401	NAD	C5A-C6A-N6A	2.11	123.52	120.31
2	I	401	NAD	C6N-N1N-C1D	-2.10	115.60	119.73
2	D	401	NAD	C2N-N1N-C1D	2.10	123.77	119.13
2	O	401	NAD	O2N-PN-O3	2.10	112.95	107.27
2	C	401	NAD	O3-PA-O1A	-2.10	104.40	110.70
2	G	401	NAD	O3-PA-O1A	-2.08	104.44	110.70
2	E	401	NAD	C2N-N1N-C1D	2.08	123.72	119.13
2	M	401	NAD	O3-PA-O1A	-2.08	104.45	110.70
2	B	401	NAD	C6N-N1N-C1D	-2.08	115.65	119.73
2	A	401	NAD	C6N-N1N-C1D	-2.08	115.65	119.73
2	X	401	NAD	O3-PA-O1A	-2.06	104.50	110.70
2	B	401	NAD	O2A-PA-O1A	2.04	121.95	112.44
2	K	401	NAD	O7N-C7N-C3N	-2.04	117.10	119.60
2	W	401	NAD	O2A-PA-O1A	2.03	121.87	112.44
2	I	401	NAD	O3-PA-O1A	-2.03	104.61	110.70
2	N	401	NAD	C6N-N1N-C1D	-2.01	115.78	119.73
2	X	401	NAD	C6N-N1N-C1D	-2.01	115.78	119.73
2	D	401	NAD	O2N-PN-O1N	2.01	121.78	112.44
2	A	401	NAD	C3N-C7N-N7N	-2.01	115.27	117.74

There are no chirality outliers.

All (158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	B	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	E	401	NAD	O4D-C1D-N1N-C2N
2	E	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	C5B-O5B-PA-O2A
2	F	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	C2D-C1D-N1N-C2N
2	F	401	NAD	C2D-C1D-N1N-C6N
2	G	401	NAD	O4D-C1D-N1N-C2N
2	G	401	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	C2D-C1D-N1N-C2N
2	G	401	NAD	C2D-C1D-N1N-C6N
2	H	401	NAD	O4D-C1D-N1N-C2N
2	H	401	NAD	O4D-C1D-N1N-C6N
2	H	401	NAD	C2D-C1D-N1N-C6N
2	I	401	NAD	O4D-C1D-N1N-C2N
2	I	401	NAD	O4D-C1D-N1N-C6N
2	J	401	NAD	C5B-O5B-PA-O2A
2	J	401	NAD	O4D-C1D-N1N-C2N
2	J	401	NAD	O4D-C1D-N1N-C6N
2	J	401	NAD	C2D-C1D-N1N-C2N
2	J	401	NAD	C2D-C1D-N1N-C6N
2	K	401	NAD	O4D-C1D-N1N-C2N
2	K	401	NAD	O4D-C1D-N1N-C6N
2	K	401	NAD	C2D-C1D-N1N-C6N
2	L	401	NAD	O4D-C1D-N1N-C2N
2	L	401	NAD	O4D-C1D-N1N-C6N
2	L	401	NAD	C2D-C1D-N1N-C2N
2	L	401	NAD	C2D-C1D-N1N-C6N
2	M	401	NAD	O4D-C1D-N1N-C2N
2	M	401	NAD	O4D-C1D-N1N-C6N
2	N	401	NAD	O4D-C1D-N1N-C2N
2	N	401	NAD	O4D-C1D-N1N-C6N
2	N	401	NAD	C2D-C1D-N1N-C2N
2	N	401	NAD	C2D-C1D-N1N-C6N
2	O	401	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	O	401	NAD	O4B-C4B-C5B-O5B
2	O	401	NAD	C3B-C4B-C5B-O5B
2	O	401	NAD	C5D-O5D-PN-O3
2	O	401	NAD	C5D-O5D-PN-O2N
2	O	401	NAD	O4D-C1D-N1N-C2N
2	O	401	NAD	O4D-C1D-N1N-C6N
2	P	401	NAD	O4D-C1D-N1N-C2N
2	P	401	NAD	O4D-C1D-N1N-C6N
2	P	401	NAD	C2D-C1D-N1N-C6N
2	Q	401	NAD	O4D-C1D-N1N-C2N
2	Q	401	NAD	O4D-C1D-N1N-C6N
2	Q	401	NAD	C2D-C1D-N1N-C6N
2	R	401	NAD	O4D-C1D-N1N-C2N
2	R	401	NAD	O4D-C1D-N1N-C6N
2	R	401	NAD	C2D-C1D-N1N-C2N
2	R	401	NAD	C2D-C1D-N1N-C6N
2	S	401	NAD	O4D-C1D-N1N-C2N
2	S	401	NAD	O4D-C1D-N1N-C6N
2	S	401	NAD	C2D-C1D-N1N-C6N
2	T	401	NAD	C5B-O5B-PA-O2A
2	T	401	NAD	O4D-C1D-N1N-C2N
2	T	401	NAD	O4D-C1D-N1N-C6N
2	T	401	NAD	C2D-C1D-N1N-C2N
2	T	401	NAD	C2D-C1D-N1N-C6N
2	U	401	NAD	O4D-C1D-N1N-C2N
2	U	401	NAD	O4D-C1D-N1N-C6N
2	U	401	NAD	C2D-C1D-N1N-C6N
2	V	401	NAD	O4D-C1D-N1N-C2N
2	V	401	NAD	O4D-C1D-N1N-C6N
2	W	401	NAD	C5D-O5D-PN-O3
2	W	401	NAD	O4D-C1D-N1N-C2N
2	W	401	NAD	O4D-C1D-N1N-C6N
2	W	401	NAD	C2D-C1D-N1N-C2N
2	W	401	NAD	C2D-C1D-N1N-C6N
2	X	401	NAD	O4D-C1D-N1N-C2N
2	X	401	NAD	O4D-C1D-N1N-C6N
3	H	402	PGE	O2-C3-C4-O3
2	W	401	NAD	O4D-C4D-C5D-O5D
2	W	401	NAD	C3D-C4D-C5D-O5D
2	O	401	NAD	C2N-C3N-C7N-O7N
2	O	401	NAD	C4N-C3N-C7N-O7N
2	H	401	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	I	401	NAD	O4B-C4B-C5B-O5B
2	T	401	NAD	O4B-C4B-C5B-O5B
2	O	401	NAD	C4N-C3N-C7N-N7N
2	J	401	NAD	O4B-C4B-C5B-O5B
2	P	401	NAD	O4B-C4B-C5B-O5B
2	O	401	NAD	C2N-C3N-C7N-N7N
2	H	401	NAD	C3B-C4B-C5B-O5B
2	S	401	NAD	O4B-C4B-C5B-O5B
2	T	401	NAD	C3B-C4B-C5B-O5B
2	I	401	NAD	C3B-C4B-C5B-O5B
2	W	401	NAD	O4B-C4B-C5B-O5B
2	J	401	NAD	C3B-C4B-C5B-O5B
2	B	401	NAD	C5B-O5B-PA-O2A
2	D	401	NAD	C5B-O5B-PA-O2A
2	O	401	NAD	C5B-O5B-PA-O1A
2	O	401	NAD	C5D-O5D-PN-O1N
2	S	401	NAD	C5B-O5B-PA-O2A
2	W	401	NAD	C5D-O5D-PN-O1N
3	H	402	PGE	O1-C1-C2-O2
2	E	401	NAD	O4B-C4B-C5B-O5B
2	L	401	NAD	O4B-C4B-C5B-O5B
2	O	401	NAD	PA-O3-PN-O2N
2	W	401	NAD	PA-O3-PN-O2N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C6N
2	E	401	NAD	C2D-C1D-N1N-C2N
2	E	401	NAD	C2D-C1D-N1N-C6N
2	H	401	NAD	C2D-C1D-N1N-C2N
2	I	401	NAD	C2D-C1D-N1N-C6N
2	K	401	NAD	C2D-C1D-N1N-C2N
2	M	401	NAD	C2D-C1D-N1N-C2N
2	M	401	NAD	C2D-C1D-N1N-C6N
2	O	401	NAD	C2D-C1D-N1N-C6N
2	P	401	NAD	C2D-C1D-N1N-C2N
2	Q	401	NAD	C2D-C1D-N1N-C2N
2	S	401	NAD	C2D-C1D-N1N-C2N
2	U	401	NAD	C2D-C1D-N1N-C2N
2	X	401	NAD	C2D-C1D-N1N-C2N
2	X	401	NAD	C2D-C1D-N1N-C6N
2	A	401	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	F	401	NAD	O4B-C4B-C5B-O5B
2	P	401	NAD	C3B-C4B-C5B-O5B
2	U	401	NAD	O4B-C4B-C5B-O5B
2	S	401	NAD	PA-O3-PN-O1N
2	R	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	O4B-C4B-C5B-O5B
2	V	401	NAD	O4B-C4B-C5B-O5B
2	S	401	NAD	C4N-C3N-C7N-N7N
2	K	401	NAD	O4B-C4B-C5B-O5B
2	Q	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	PA-O3-PN-O1N
2	B	401	NAD	PA-O3-PN-O1N
2	D	401	NAD	PA-O3-PN-O1N
2	O	401	NAD	PA-O3-PN-O1N
2	W	401	NAD	PA-O3-PN-O1N
2	S	401	NAD	C4N-C3N-C7N-O7N
2	B	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	O4B-C4B-C5B-O5B
2	G	401	NAD	O4B-C4B-C5B-O5B
2	N	401	NAD	O4B-C4B-C5B-O5B
2	W	401	NAD	C3B-C4B-C5B-O5B
2	X	401	NAD	O4B-C4B-C5B-O5B
2	S	401	NAD	C3B-C4B-C5B-O5B
2	O	401	NAD	C4B-C5B-O5B-PA
2	E	401	NAD	C3B-C4B-C5B-O5B
2	J	401	NAD	PA-O3-PN-O1N
2	N	401	NAD	PA-O3-PN-O1N

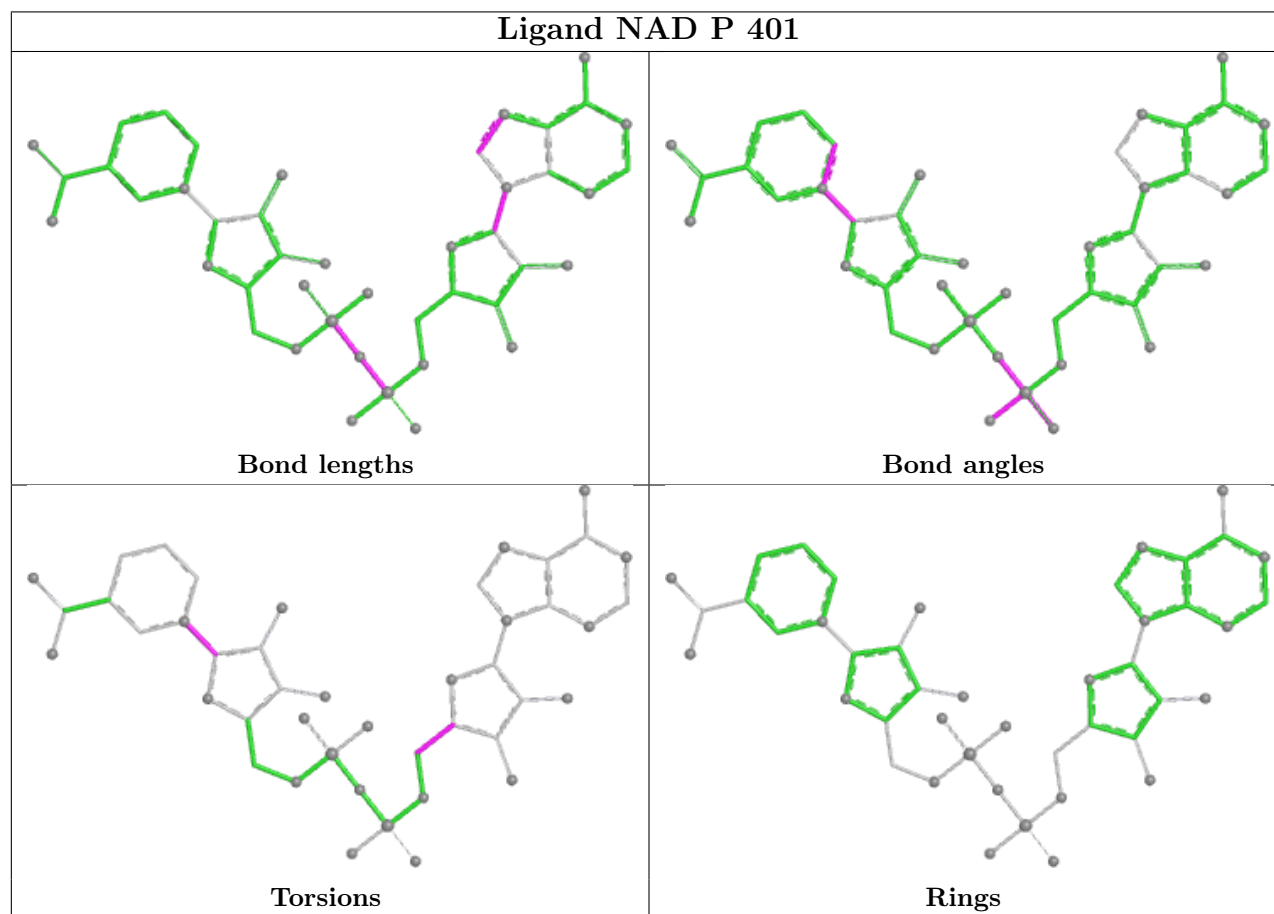
There are no ring outliers.

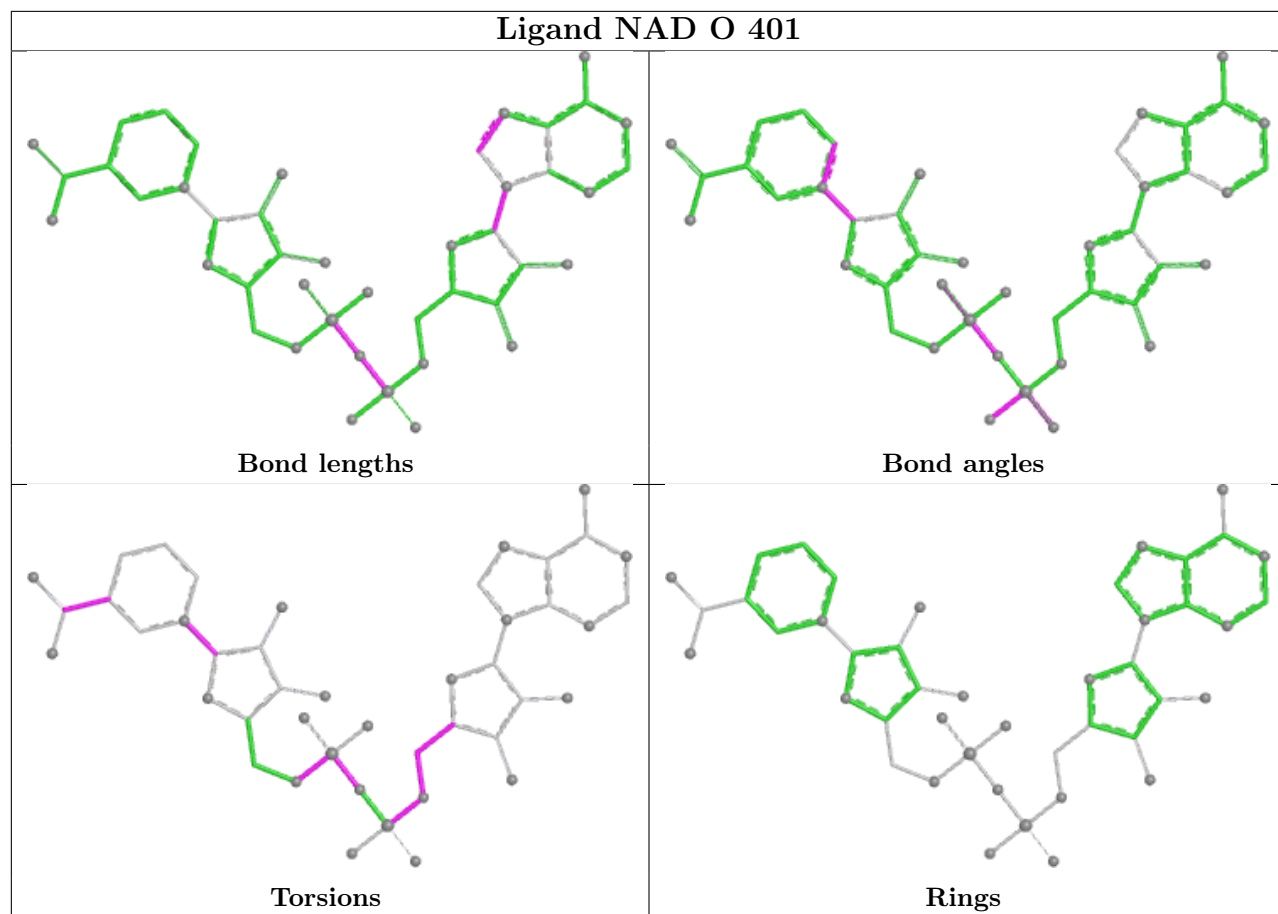
1 monomer is involved in 1 short contact:

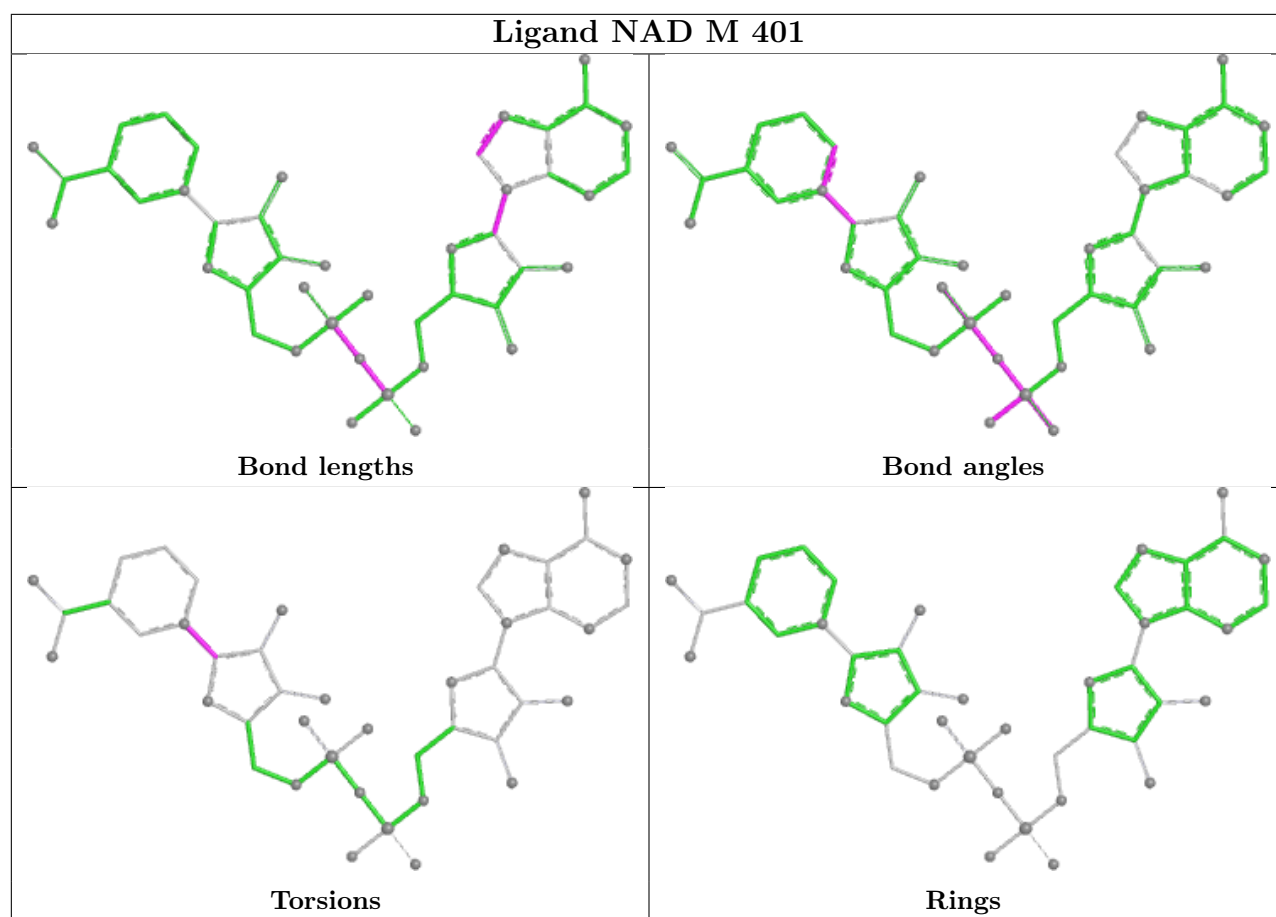
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	401	NAD	1	0

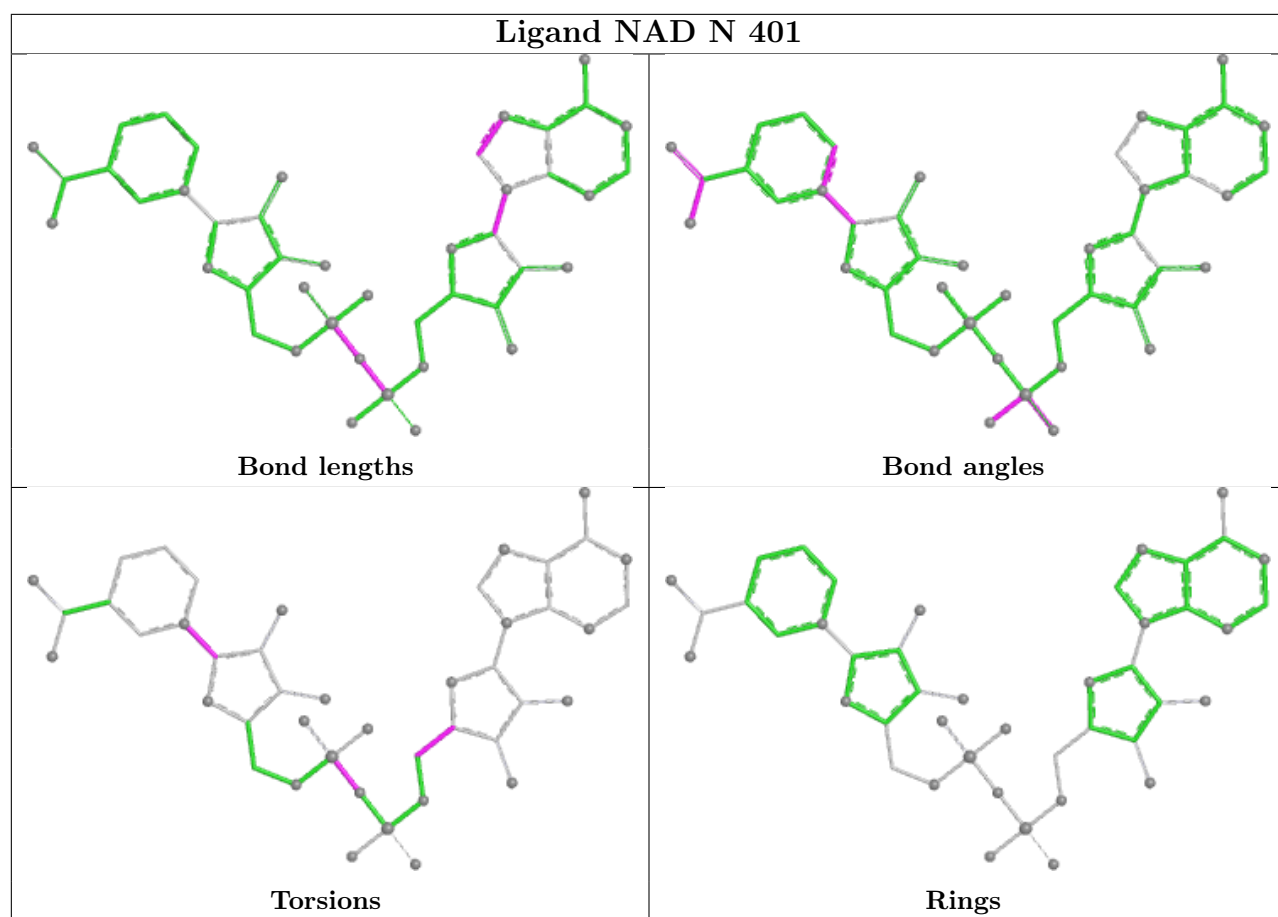
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

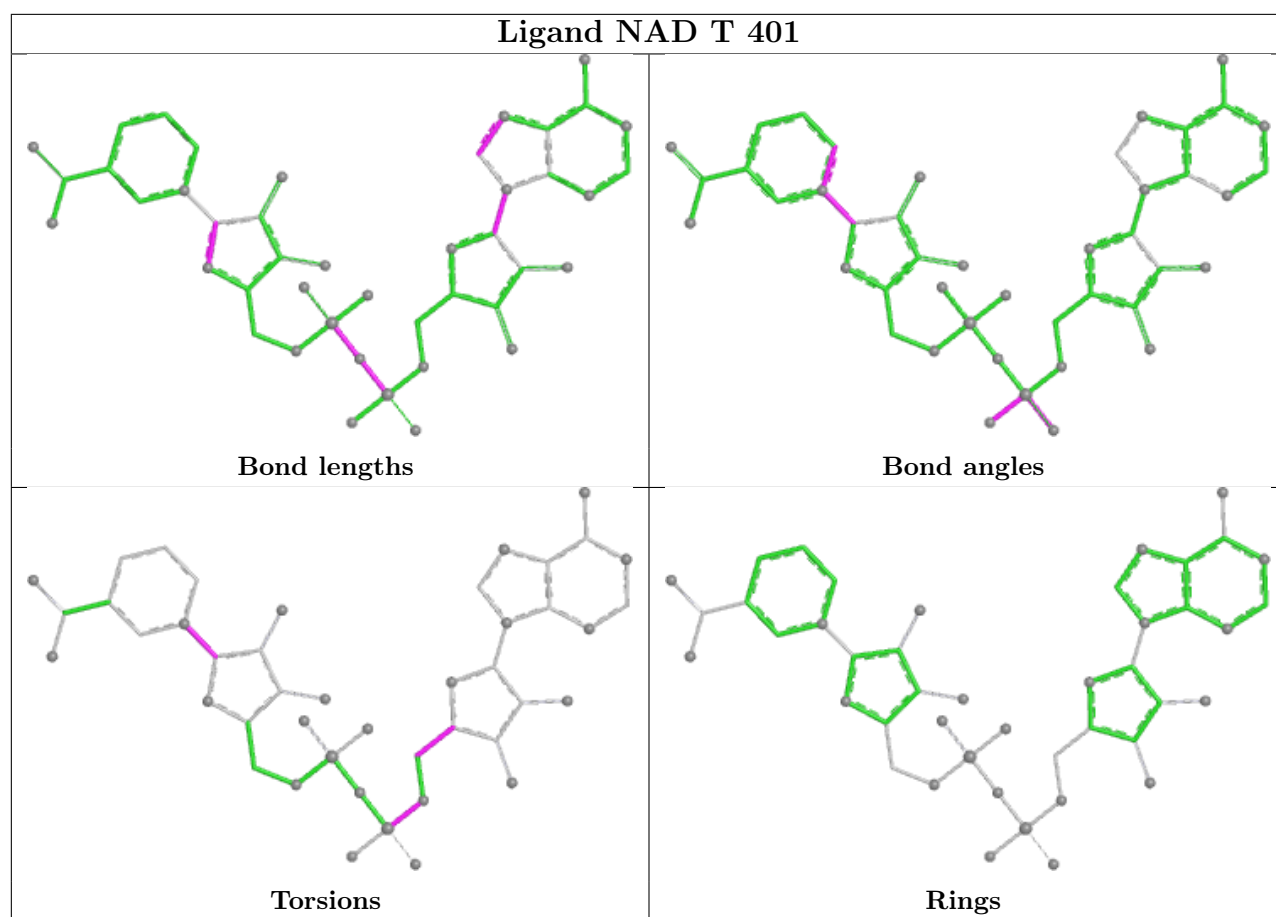
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

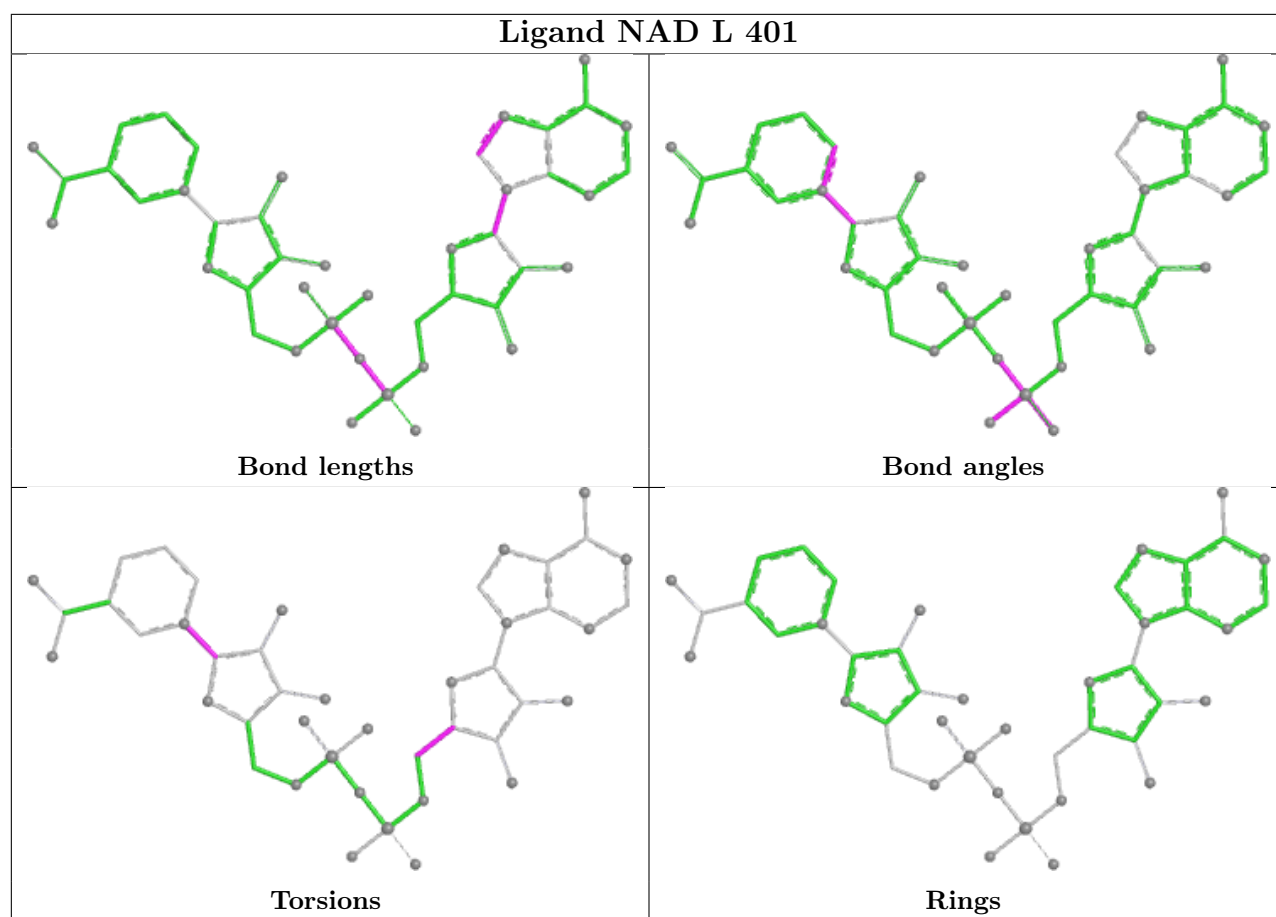


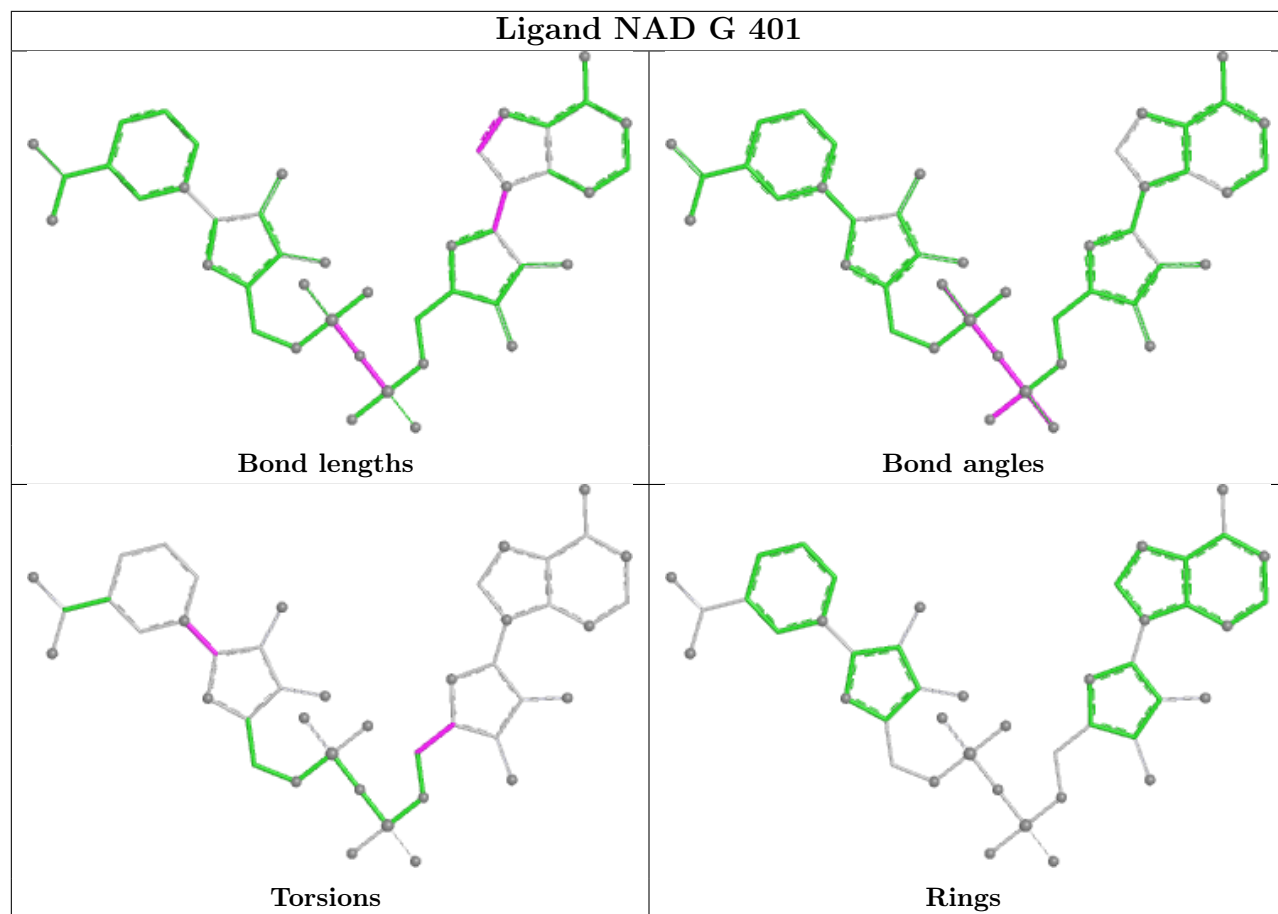


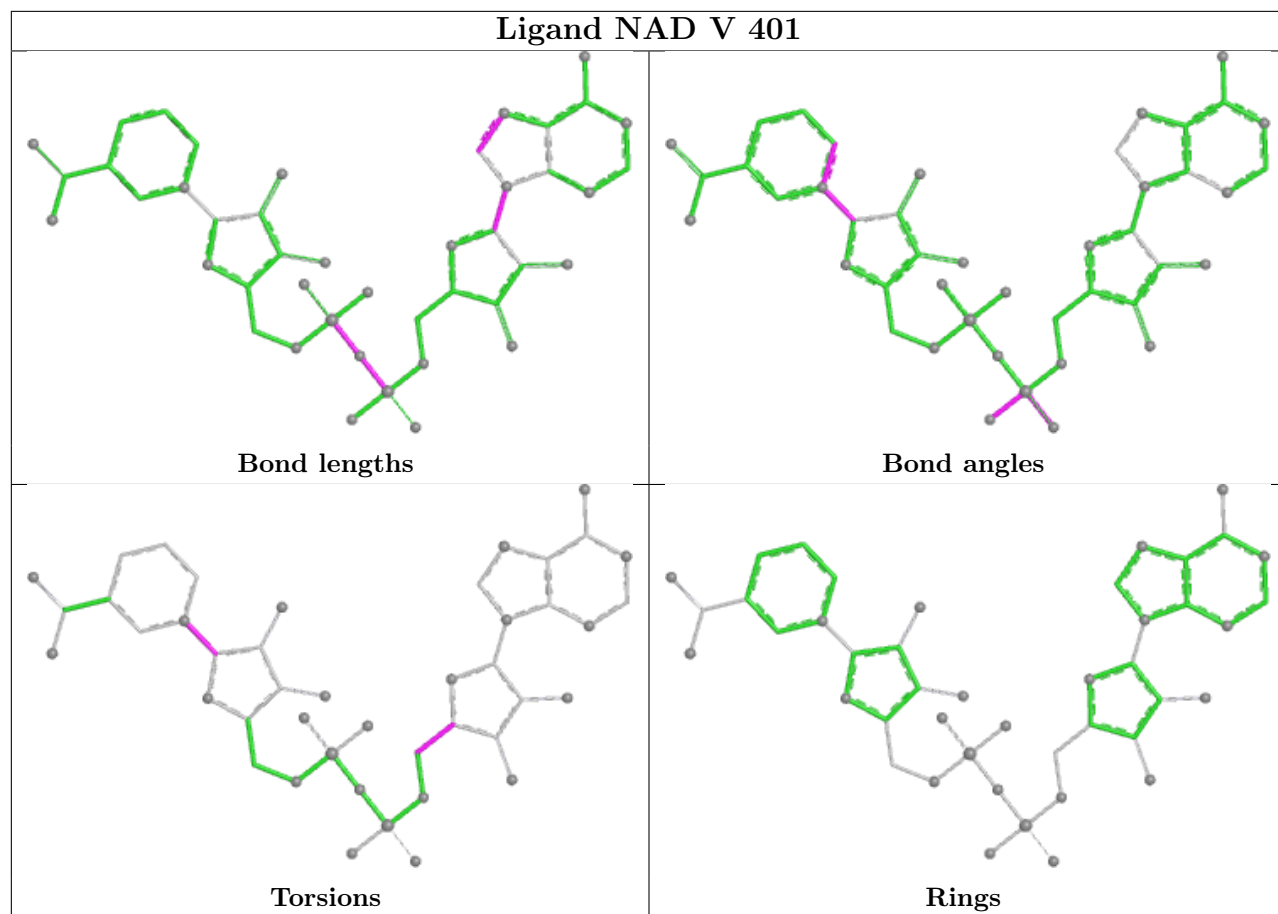


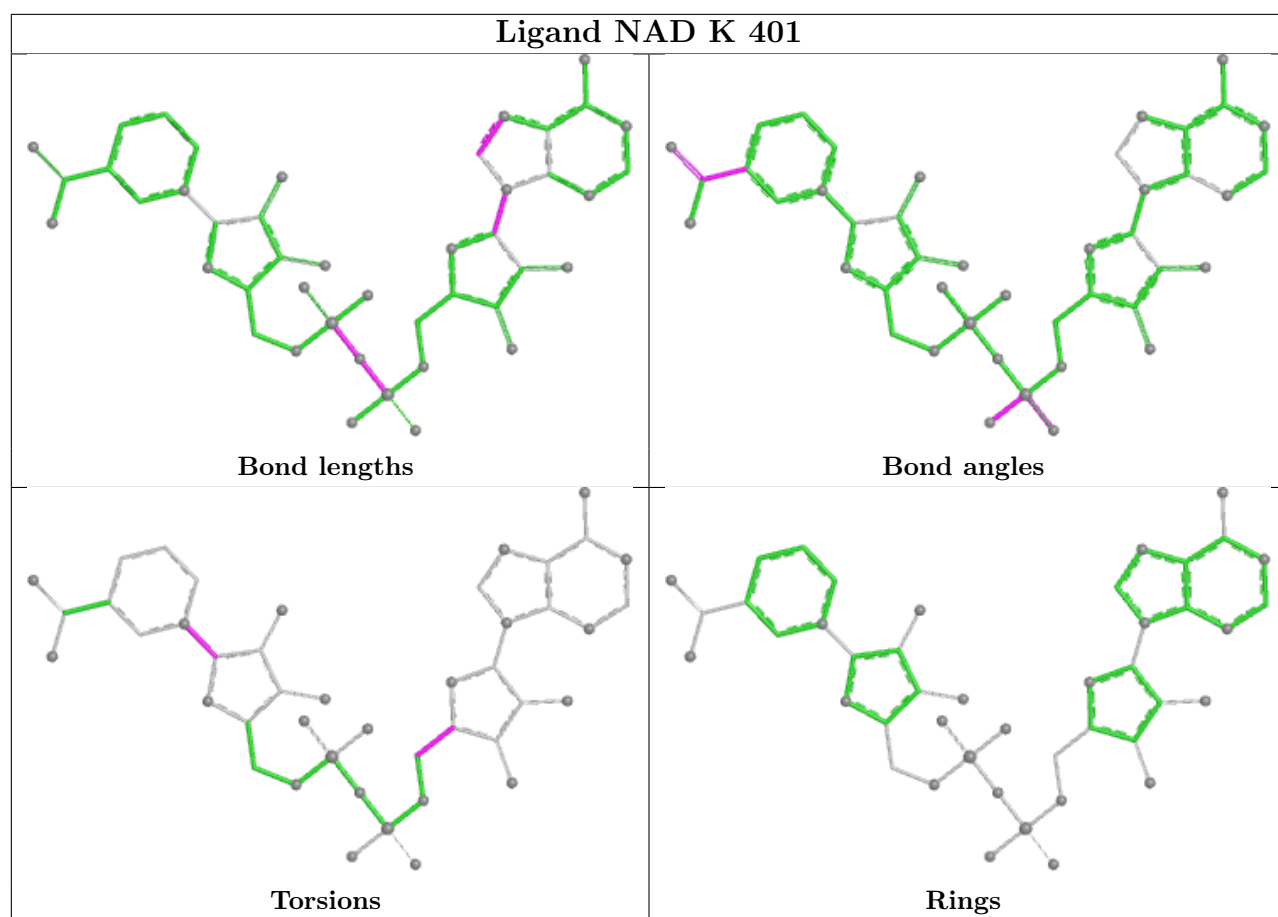


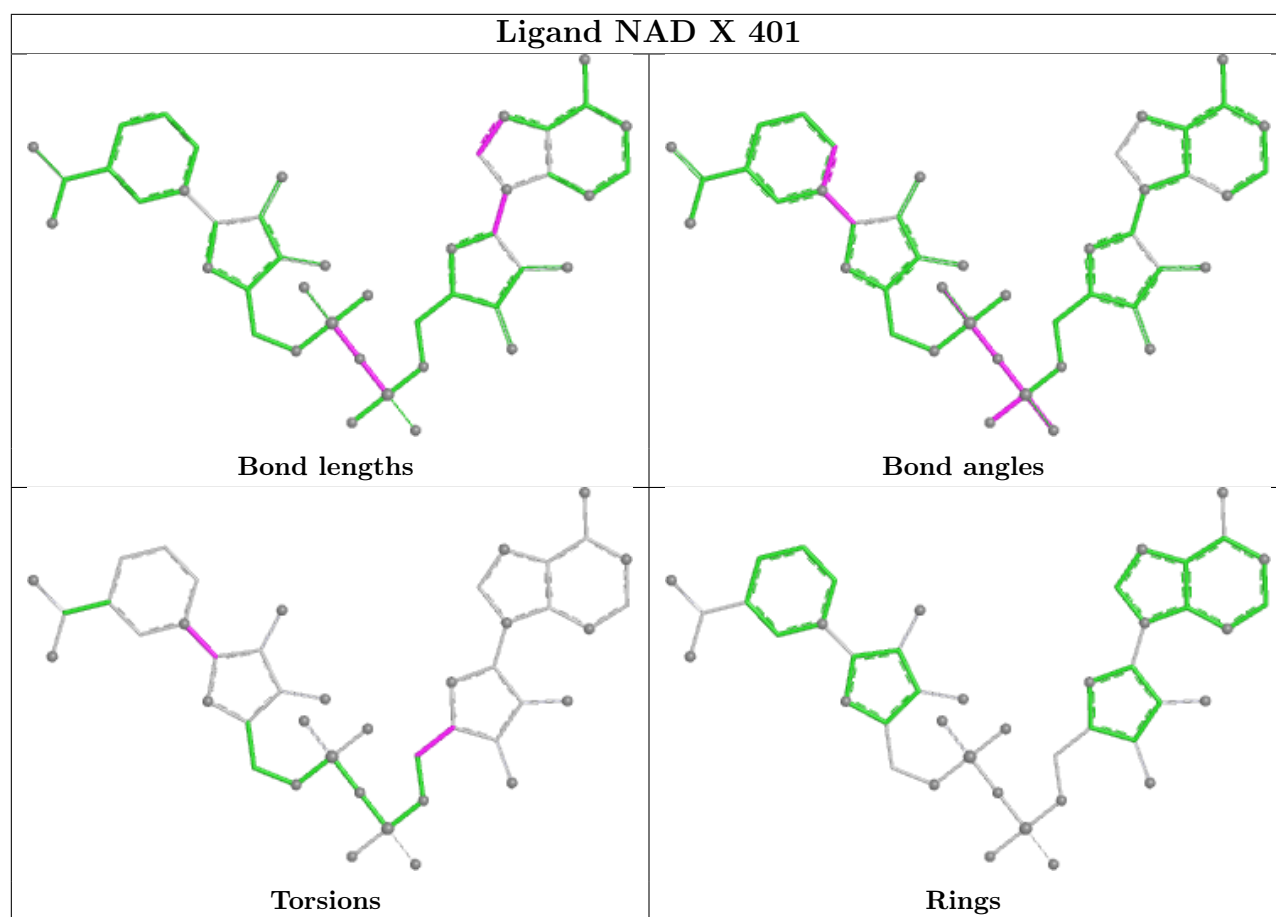


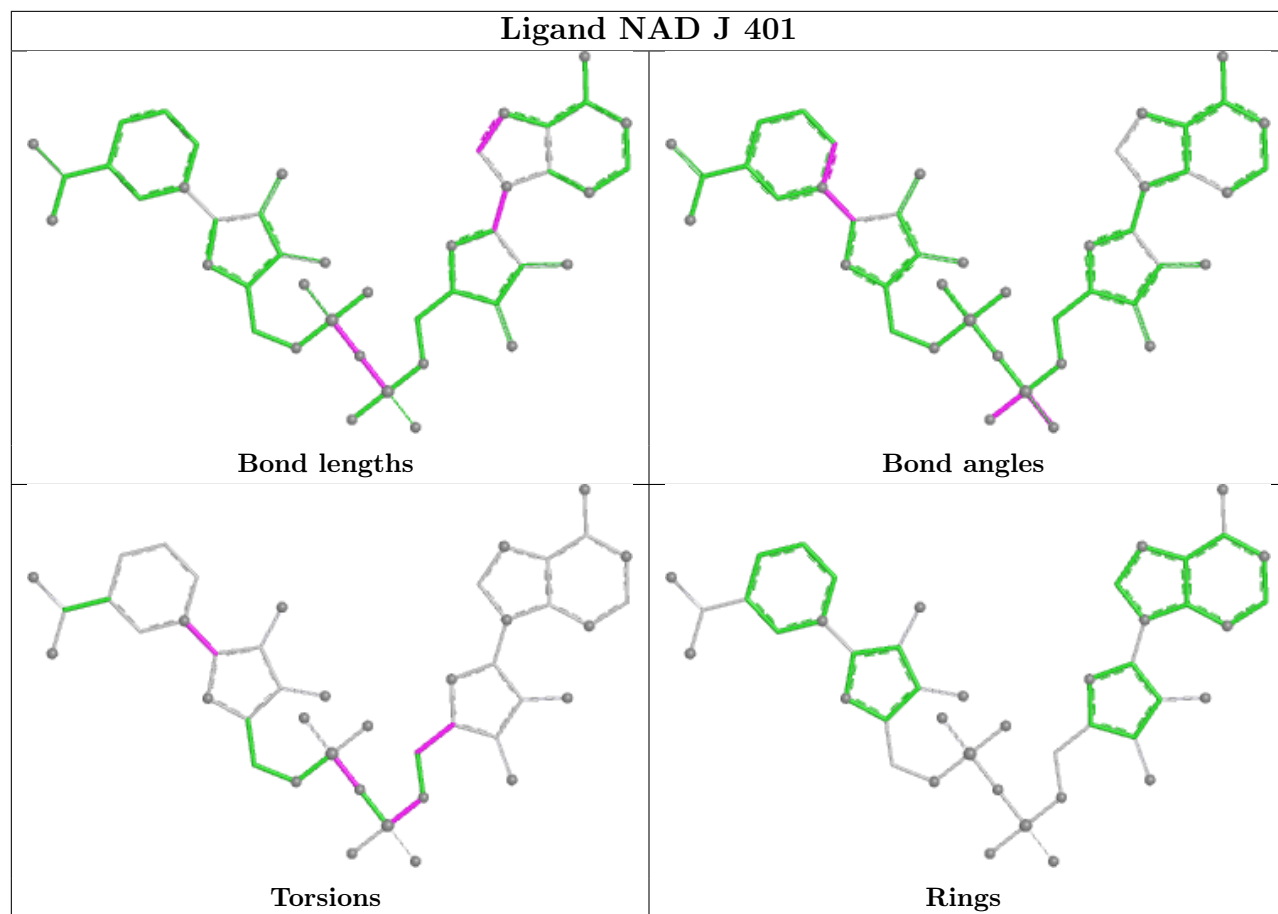


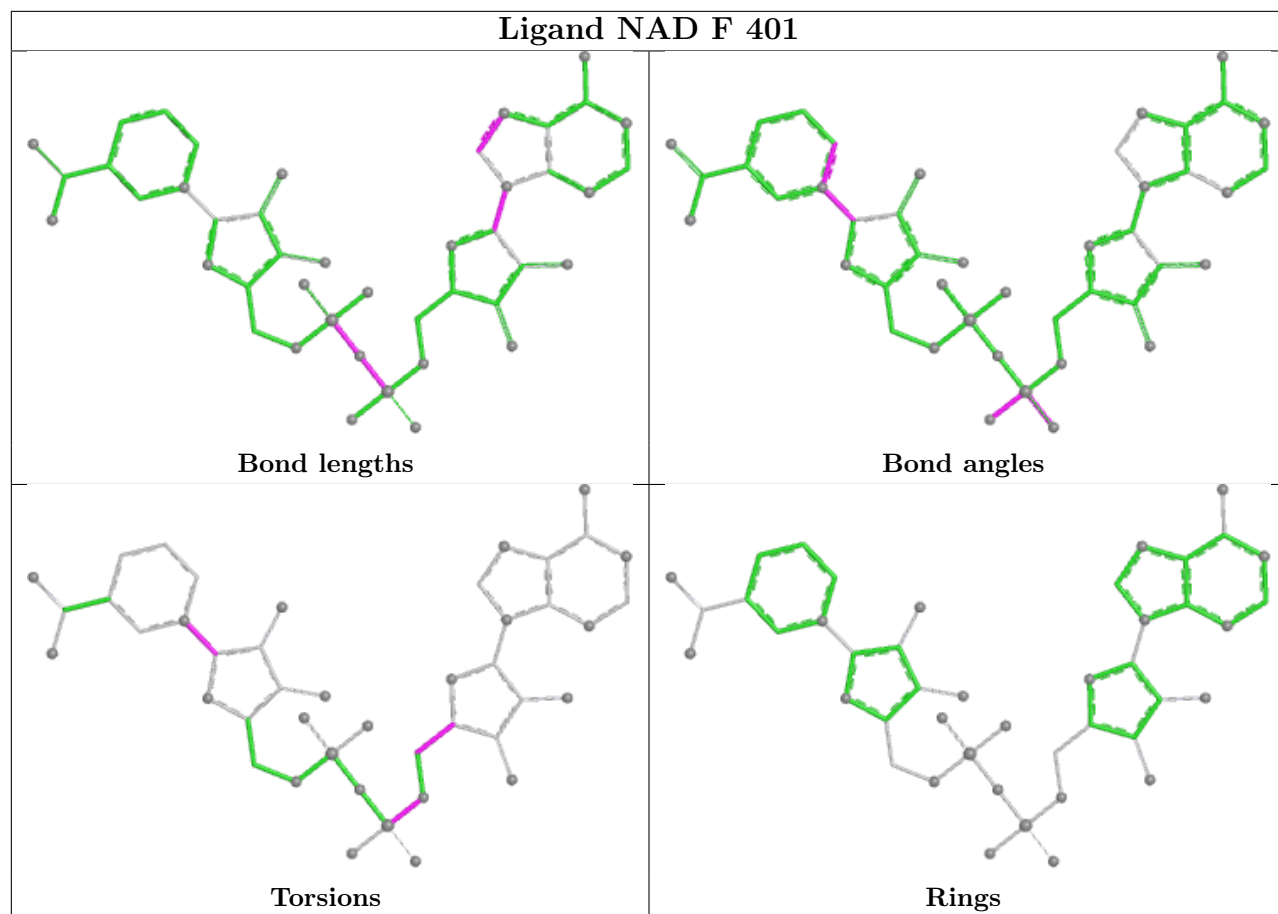


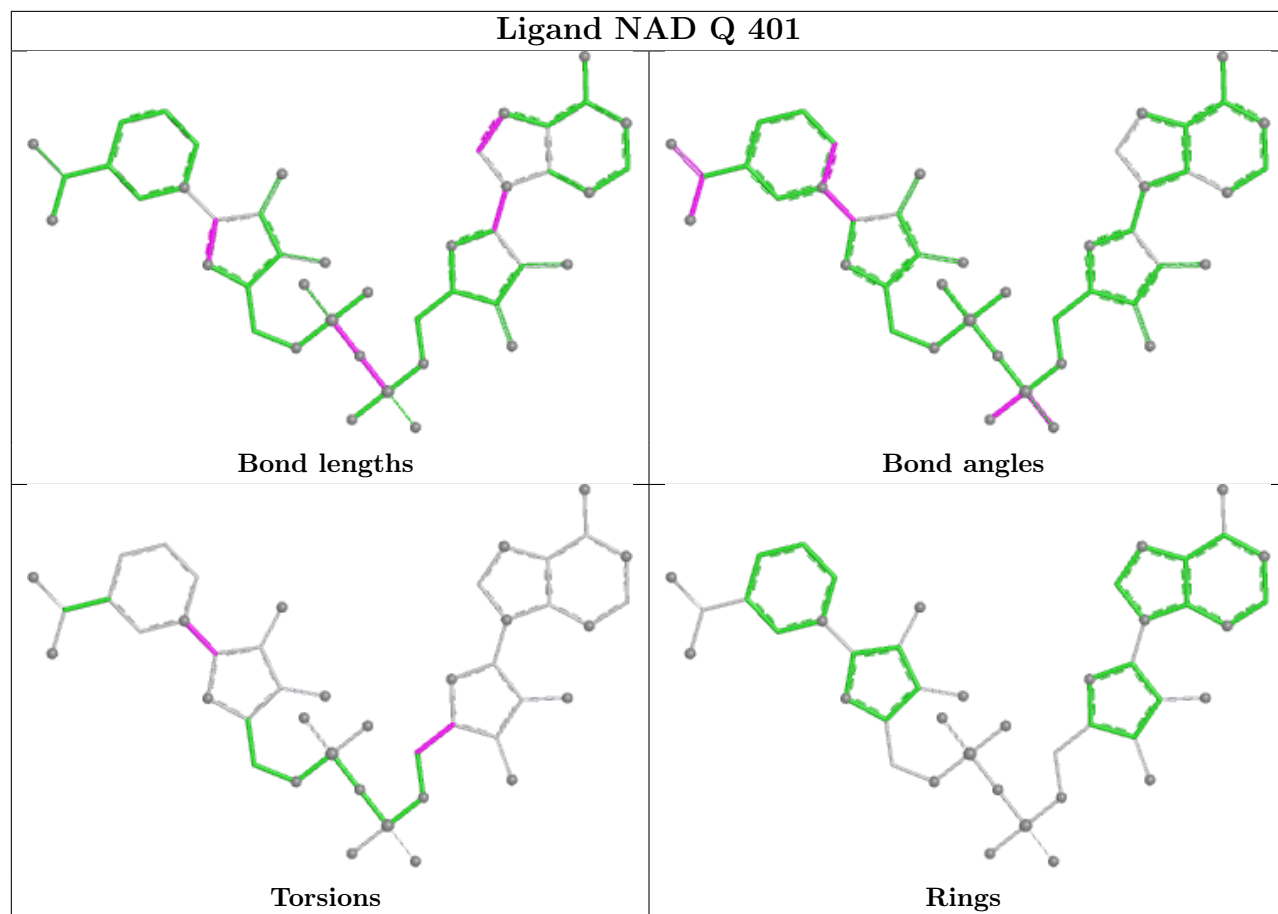


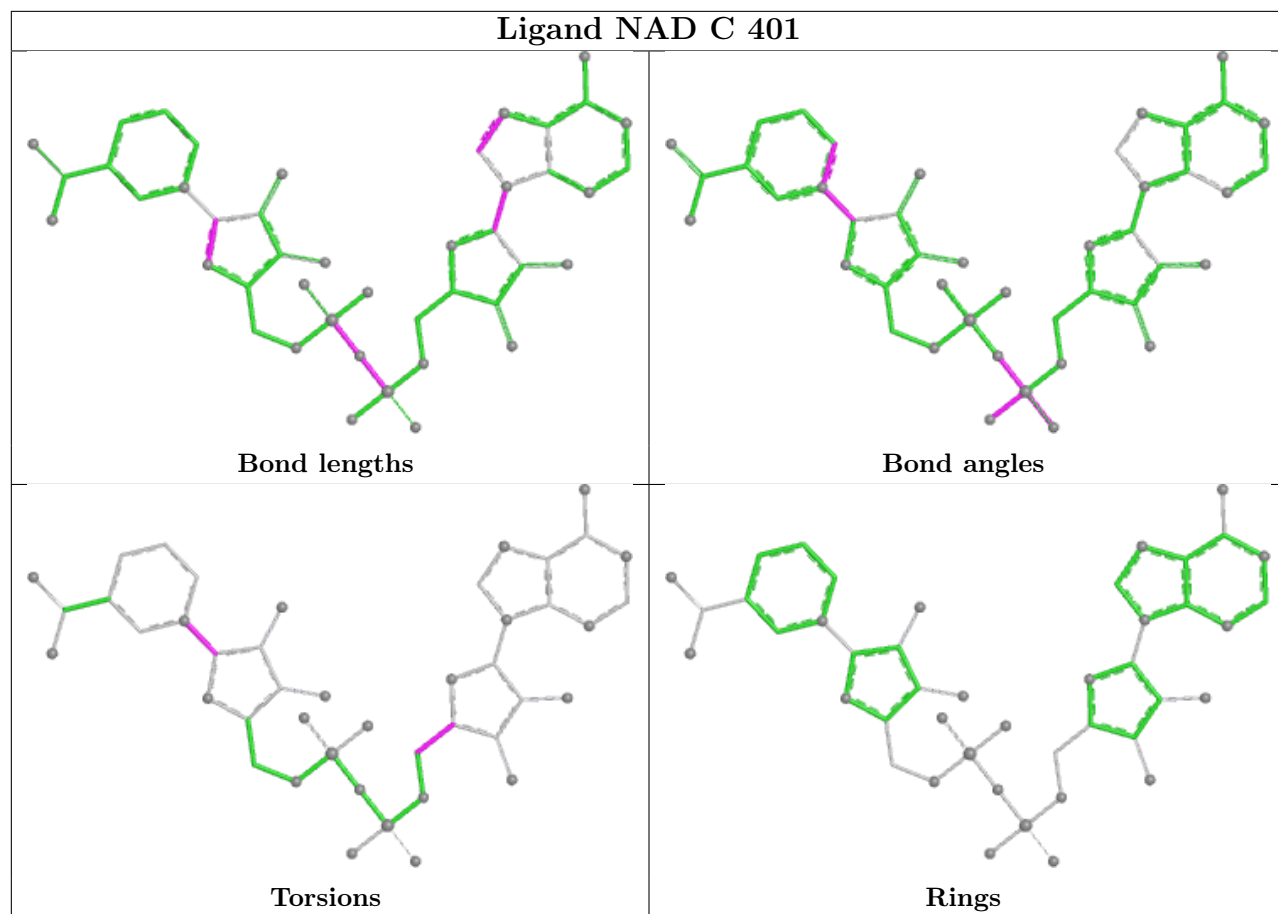


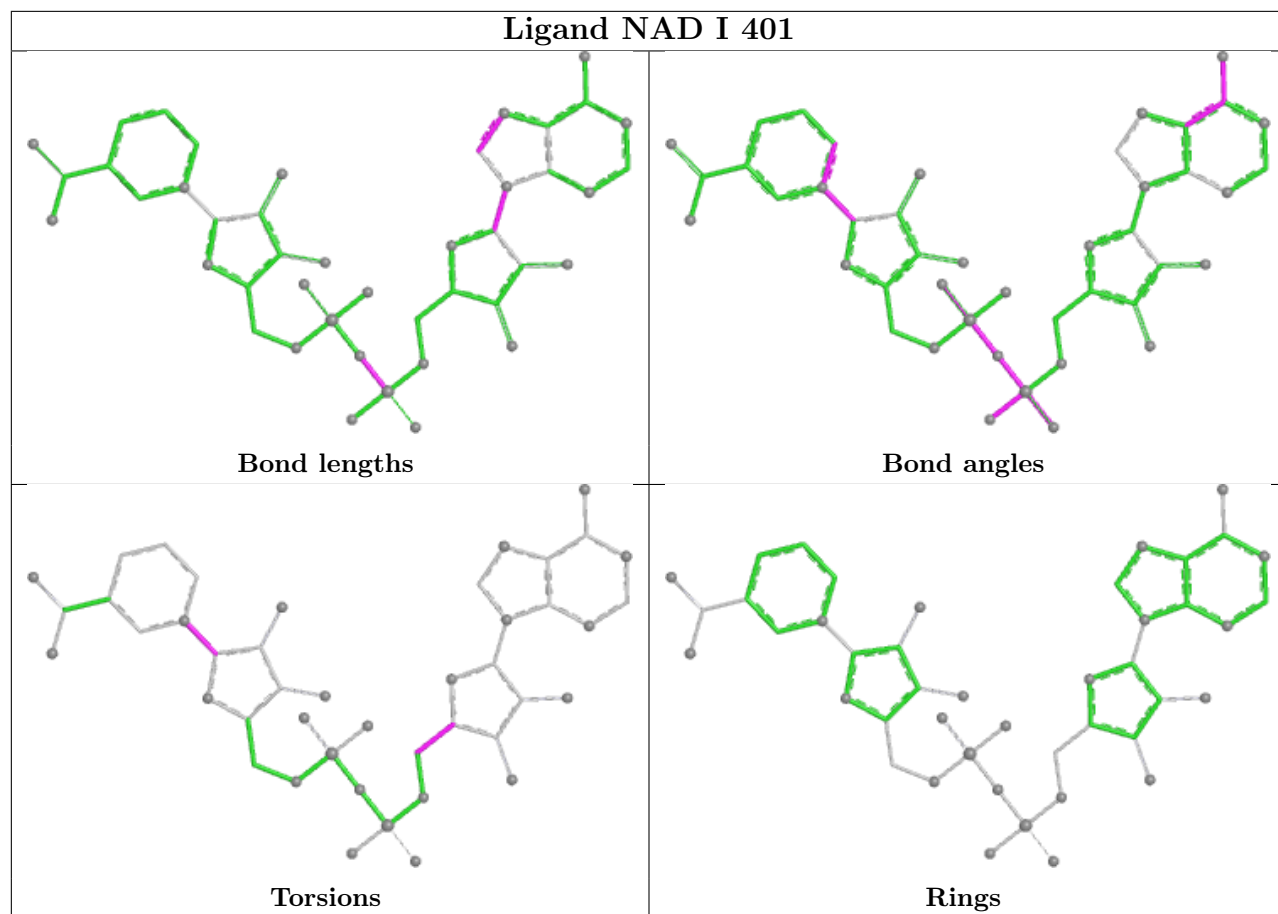


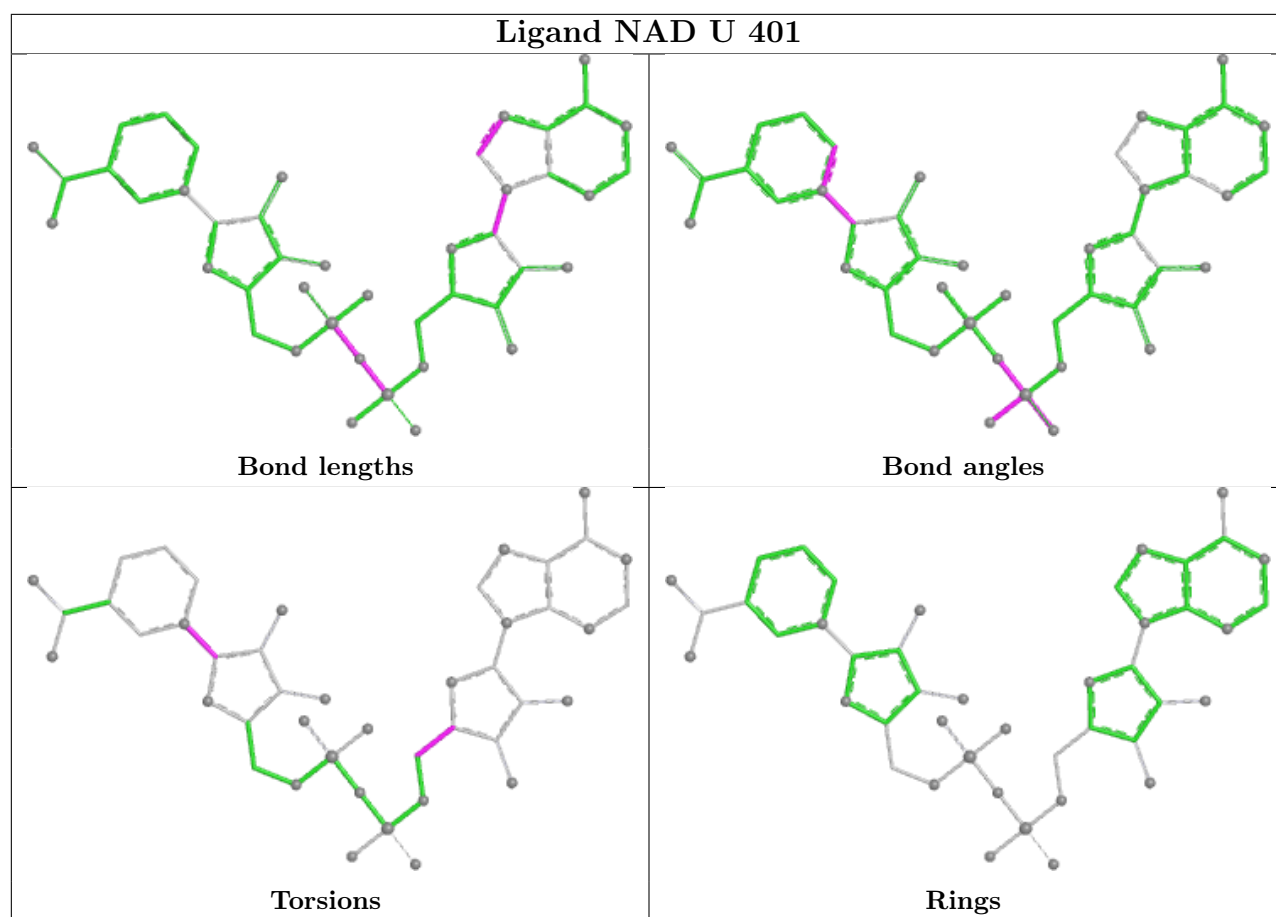


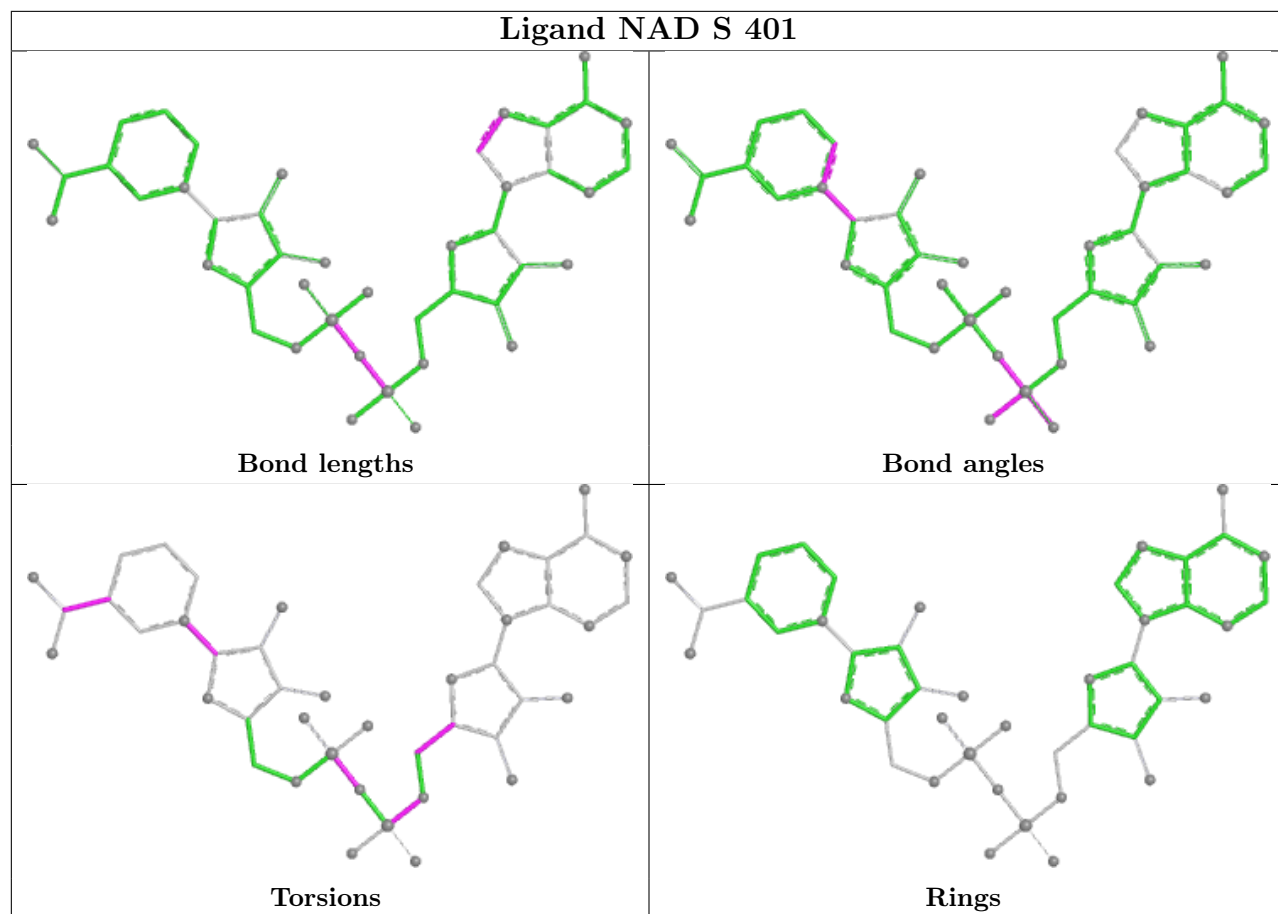


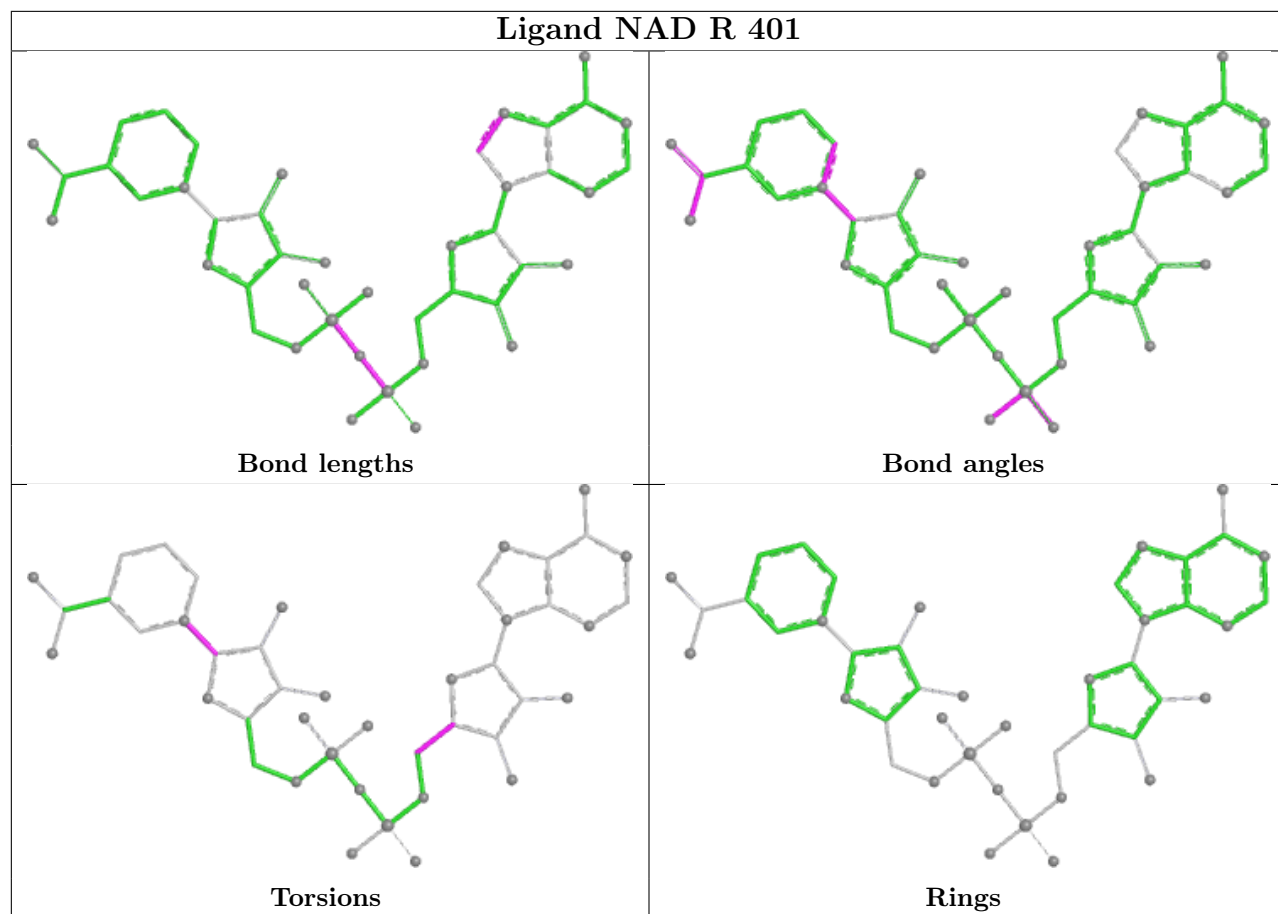


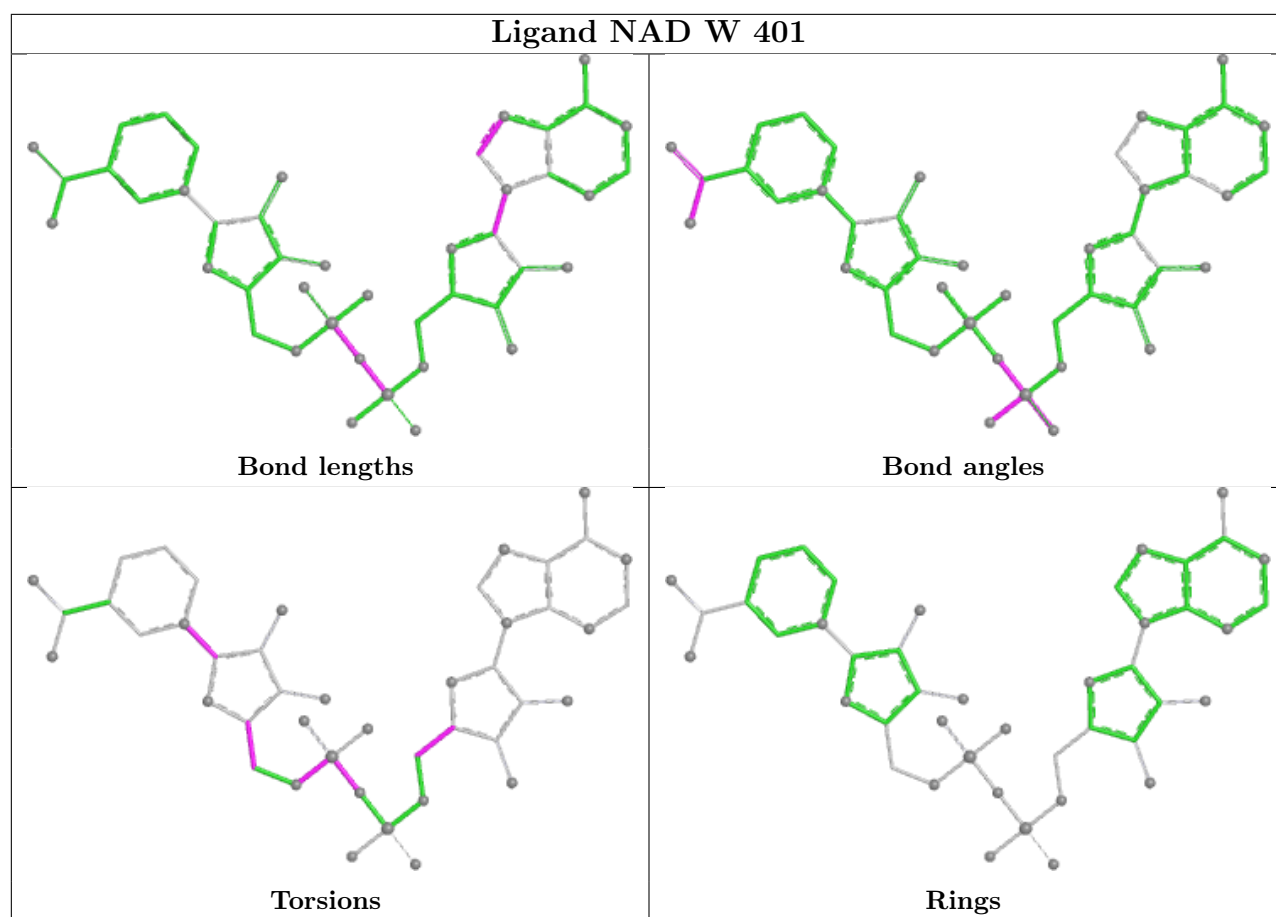


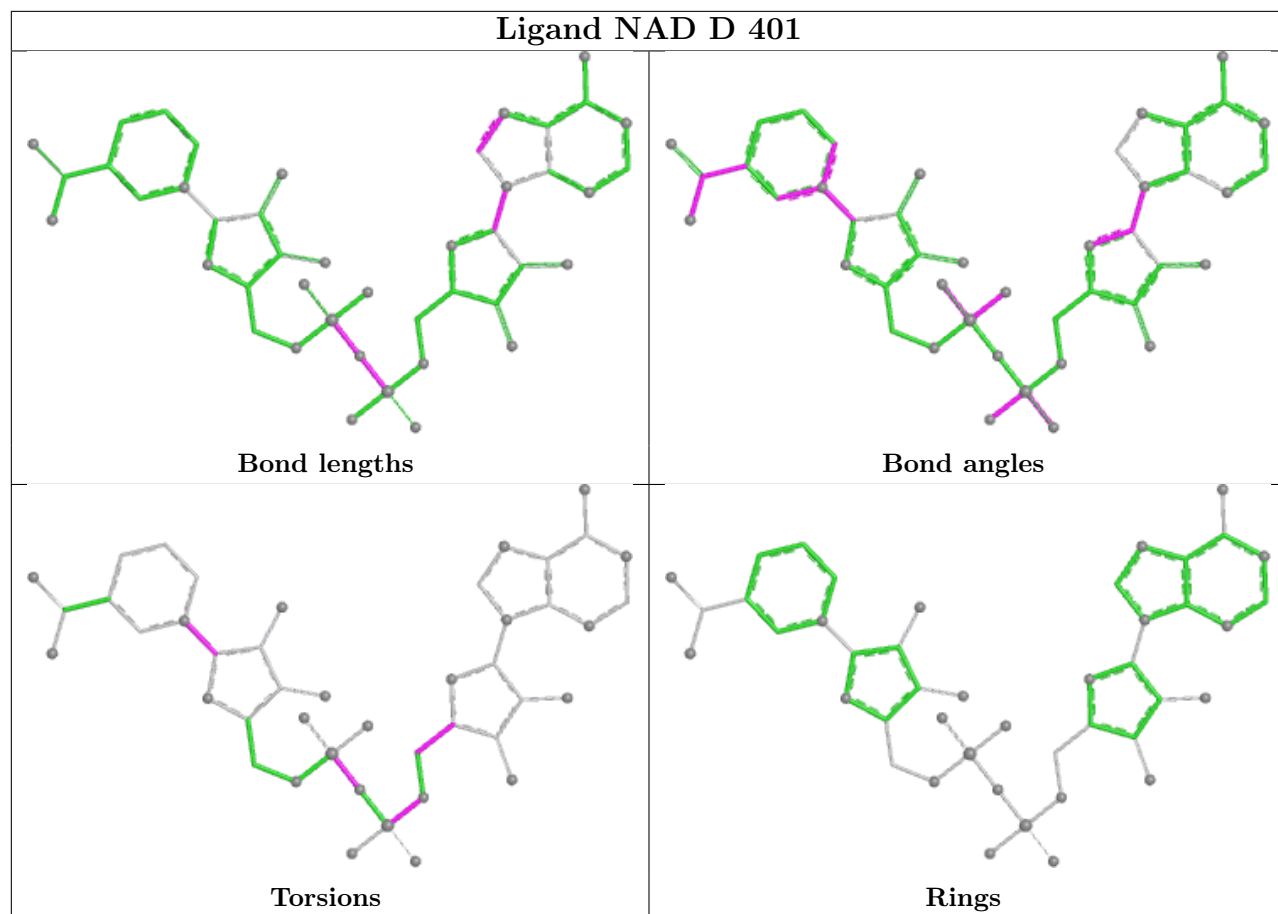


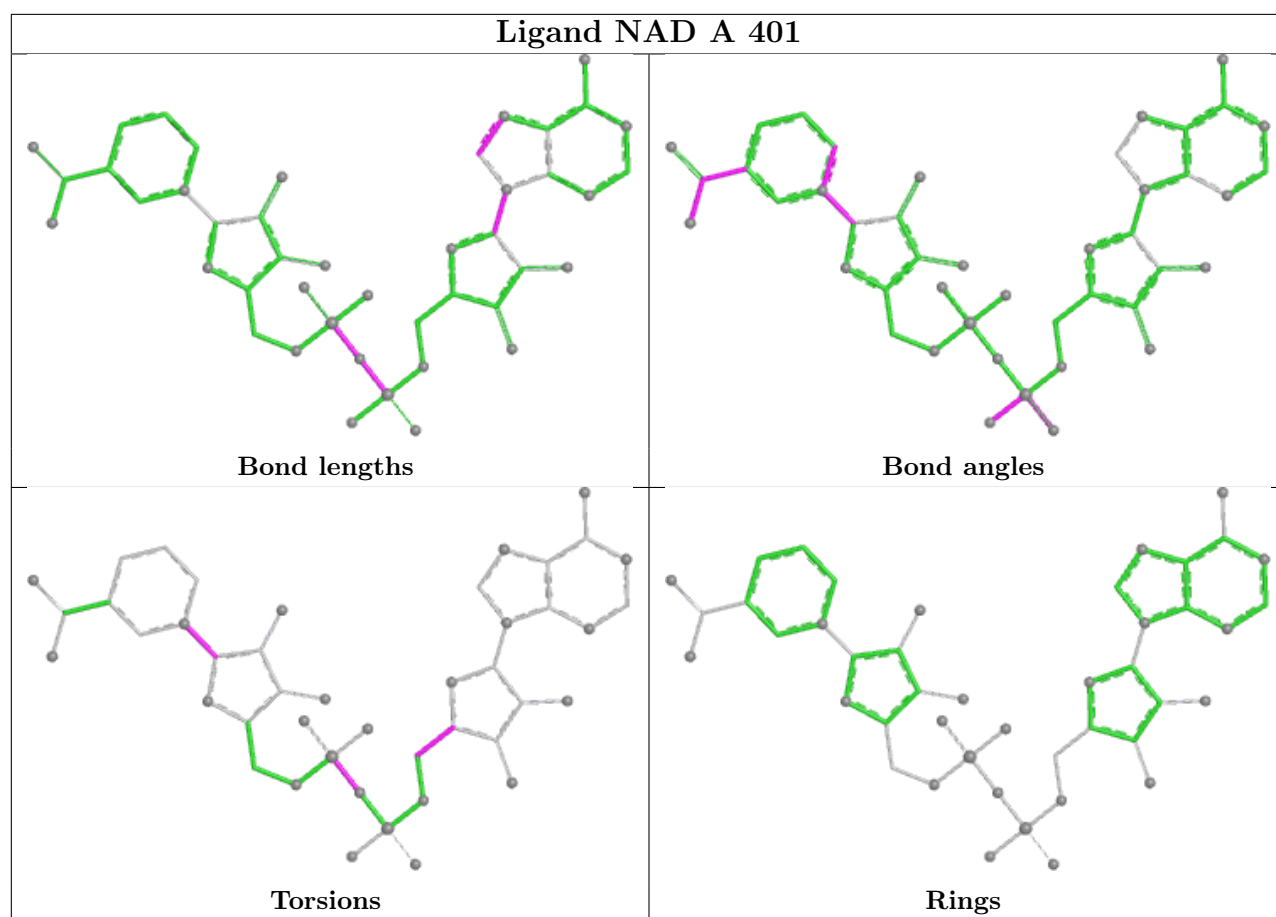


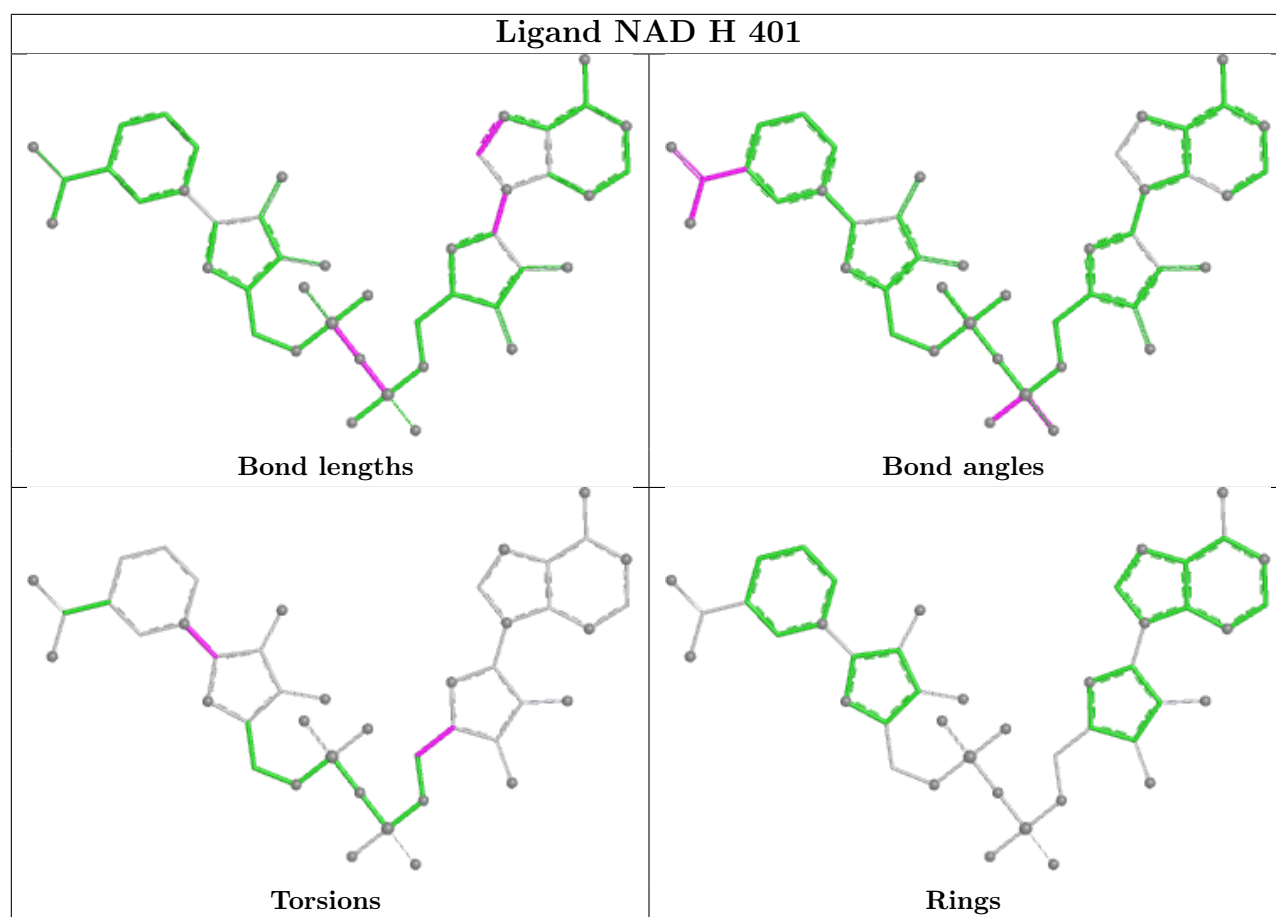


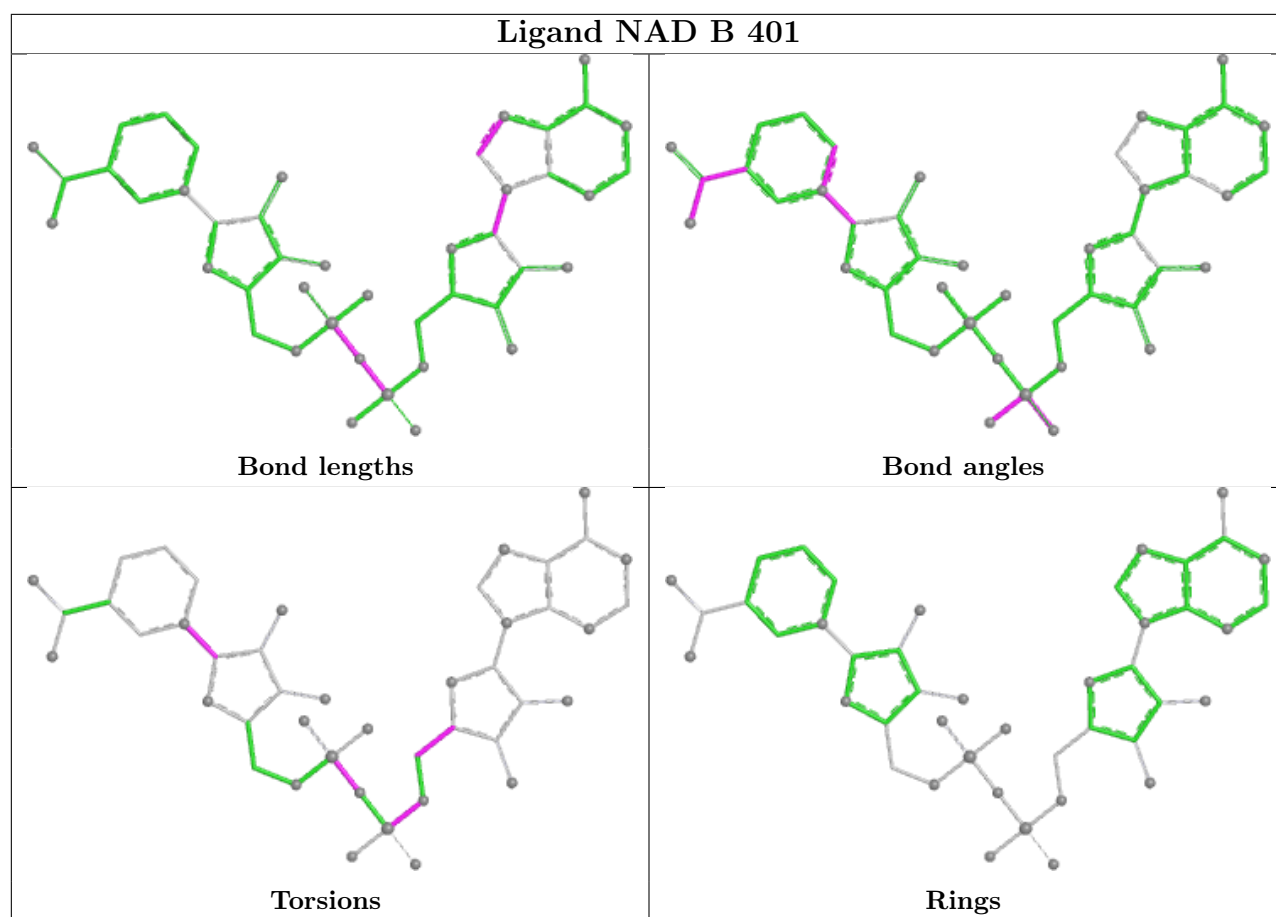


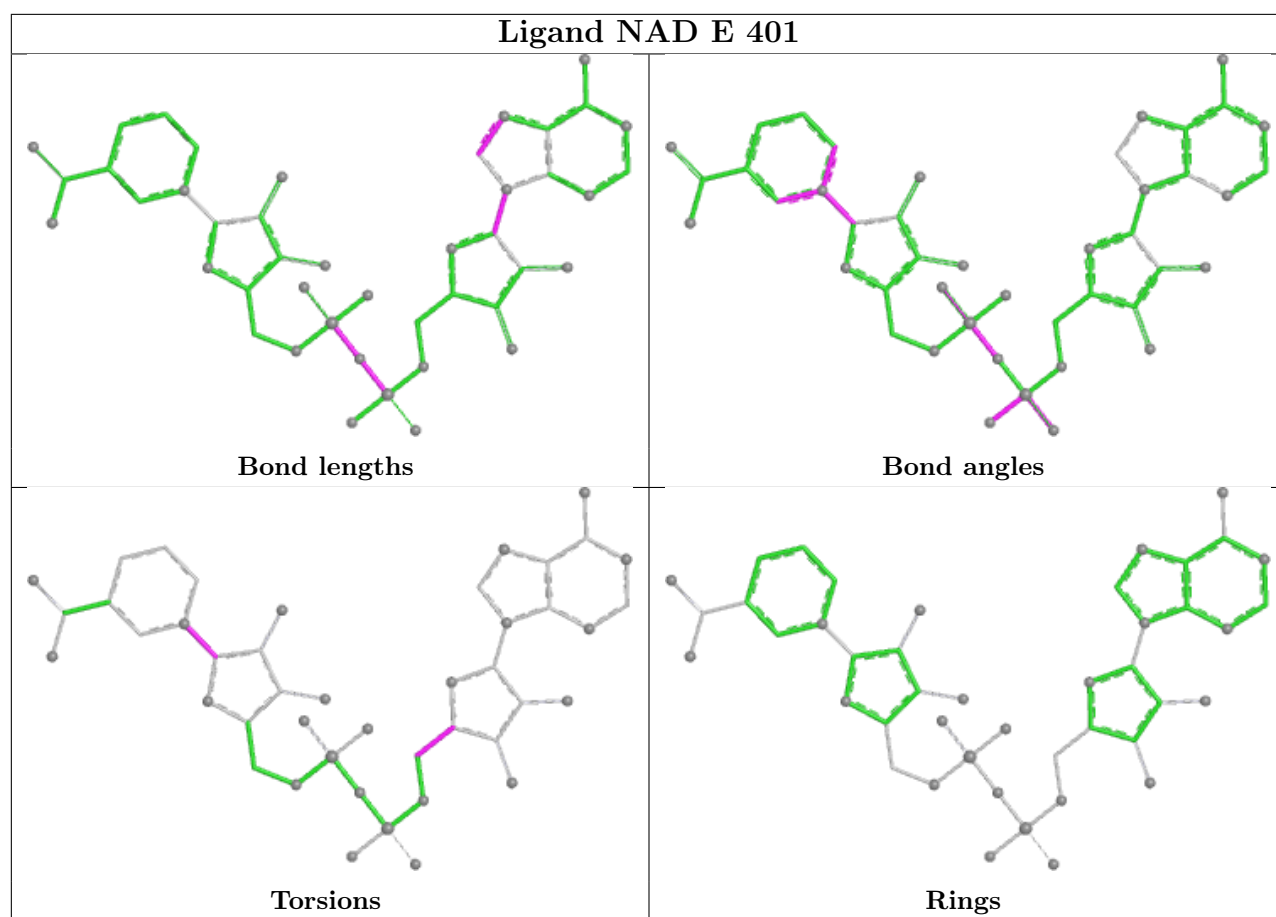












5.7 Other polymers [i](#)

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	333/342 (97%)	-0.01	7 (2%) 63 64	21, 34, 54, 98	0
1	B	333/342 (97%)	0.14	11 (3%) 49 51	22, 36, 60, 95	0
1	C	332/342 (97%)	0.02	8 (2%) 59 61	21, 34, 52, 105	0
1	D	332/342 (97%)	-0.08	9 (2%) 56 57	20, 31, 51, 121	0
1	E	333/342 (97%)	0.21	13 (3%) 44 45	24, 36, 61, 81	0
1	F	333/342 (97%)	0.02	7 (2%) 63 64	23, 33, 51, 87	0
1	G	323/342 (94%)	0.43	23 (7%) 23 25	22, 40, 77, 114	0
1	H	332/342 (97%)	0.13	12 (3%) 46 48	24, 35, 60, 73	0
1	I	333/342 (97%)	0.24	15 (4%) 39 40	24, 37, 65, 82	0
1	J	333/342 (97%)	0.28	9 (2%) 56 57	26, 39, 62, 114	0
1	K	332/342 (97%)	0.27	18 (5%) 32 34	21, 36, 72, 98	0
1	L	332/342 (97%)	0.30	15 (4%) 39 40	25, 39, 64, 97	0
1	M	334/342 (97%)	0.40	23 (6%) 24 26	25, 39, 75, 98	0
1	N	334/342 (97%)	-0.01	6 (1%) 67 68	21, 31, 51, 79	0
1	O	321/342 (93%)	1.21	80 (24%) 2 2	26, 56, 109, 140	0
1	P	324/342 (94%)	1.19	77 (23%) 2 3	22, 55, 85, 119	0
1	Q	333/342 (97%)	0.18	8 (2%) 59 61	24, 36, 60, 102	0
1	R	333/342 (97%)	0.41	20 (6%) 29 31	25, 40, 74, 104	0
1	S	330/342 (96%)	0.45	22 (6%) 25 27	25, 41, 70, 99	0
1	T	332/342 (97%)	0.16	11 (3%) 49 51	24, 36, 61, 92	0
1	U	328/342 (95%)	0.54	22 (6%) 25 27	27, 45, 73, 98	0
1	V	331/342 (96%)	0.56	24 (7%) 22 24	26, 45, 73, 93	0
1	W	287/342 (83%)	1.36	80 (27%) 2 2	25, 58, 102, 135	0
1	X	329/342 (96%)	0.63	40 (12%) 10 11	25, 44, 92, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	7897/8208 (96%)	0.37	560 (7%)	23	25	20, 38, 76, 140	0

All (560) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	109	HIS	7.3
1	W	21	ILE	7.1
1	W	93	VAL	6.8
1	W	5	VAL	6.5
1	W	331	ALA	5.9
1	W	74	VAL	5.7
1	P	85	TRP	5.7
1	W	127	VAL	5.6
1	R	125	ASN	5.6
1	P	61	LYS	5.3
1	B	125	ASN	5.3
1	W	118	VAL	5.2
1	P	3	ILE	5.2
1	O	145	VAL	5.1
1	V	252	PRO	5.1
1	W	94	LEU	5.1
1	V	251	ARG	5.1
1	W	148	ALA	4.9
1	P	84	PRO	4.7
1	O	117	VAL	4.7
1	O	112	ALA	4.7
1	O	333	LYS	4.6
1	X	141	GLY	4.6
1	W	7	ILE	4.6
1	M	25	HIS	4.5
1	V	63	ASP	4.5
1	W	29	VAL	4.4
1	W	146	ILE	4.4
1	P	88	LEU	4.4
1	H	3	ILE	4.4
1	M	62	ASP	4.3
1	W	24	ALA	4.3
1	P	145	VAL	4.3
1	G	183	ASP	4.3
1	W	77	ASN	4.3
1	P	91	ASP	4.2
1	P	144	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	O	99	PHE	4.2
1	L	3	ILE	4.2
1	O	63	ASP	4.2
1	W	75	PHE	4.2
1	O	108	ALA	4.2
1	W	76	ALA	4.2
1	D	3	ILE	4.2
1	D	25	HIS	4.1
1	W	27	ILE	4.1
1	R	25	HIS	4.1
1	E	183	ASP	4.1
1	O	33	ASN	4.1
1	O	101	THR	4.1
1	P	167	PHE	4.1
1	W	100	PHE	4.1
1	M	334	ILE	4.1
1	O	35	LEU	4.0
1	M	70	ARG	4.0
1	O	27	ILE	4.0
1	O	332	GLY	4.0
1	O	106	ALA	4.0
1	O	3	ILE	4.0
1	W	64	ALA	4.0
1	P	90	VAL	3.9
1	I	252	PRO	3.9
1	O	130	VAL	3.9
1	G	62	ASP	3.9
1	O	100	PHE	3.9
1	K	138	ILE	3.9
1	W	78	PRO	3.9
1	W	138	ILE	3.9
1	W	9	GLY	3.9
1	R	334	ILE	3.8
1	W	32	VAL	3.8
1	P	299	MET	3.8
1	W	38	ALA	3.8
1	E	62	ASP	3.8
1	K	3	ILE	3.8
1	W	63	ASP	3.8
1	O	124	GLY	3.8
1	M	1	MET	3.8
1	P	108	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	R	126	ASP	3.8
1	O	89	GLY	3.8
1	W	36	THR	3.8
1	J	2	SER	3.7
1	W	192	ARG	3.7
1	L	62	ASP	3.7
1	X	83	LEU	3.7
1	P	115	ARG	3.7
1	W	8	ASN	3.7
1	O	29	VAL	3.7
1	O	266	SER	3.7
1	W	79	ASN	3.7
1	P	333	LYS	3.6
1	B	26	GLY	3.6
1	P	86	GLY	3.6
1	X	3	ILE	3.6
1	O	231	SER	3.6
1	Q	62	ASP	3.6
1	W	72	ILE	3.6
1	W	147	SER	3.6
1	O	299	MET	3.6
1	O	76	ALA	3.6
1	V	255	LYS	3.6
1	V	27	ILE	3.6
1	W	101	THR	3.6
1	P	93	VAL	3.6
1	W	92	VAL	3.6
1	X	85	TRP	3.6
1	P	117	VAL	3.5
1	V	301	VAL	3.5
1	O	78	PRO	3.5
1	W	33	ASN	3.5
1	X	332	GLY	3.5
1	D	63	ASP	3.5
1	S	63	ASP	3.5
1	O	109	HIS	3.5
1	V	254	THR	3.5
1	X	1	MET	3.5
1	P	114	ALA	3.5
1	C	62	ASP	3.5
1	M	63	ASP	3.5
1	K	25	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	P	138	ILE	3.5
1	O	77	ASN	3.5
1	W	30	ALA	3.5
1	P	112	ALA	3.4
1	P	107	GLU	3.4
1	O	75	PHE	3.4
1	C	61	LYS	3.4
1	O	110	ILE	3.4
1	O	119	ILE	3.4
1	I	299	MET	3.4
1	P	92	VAL	3.4
1	H	263	LYS	3.4
1	U	227	LYS	3.4
1	X	333	LYS	3.4
1	I	63	ASP	3.4
1	L	2	SER	3.3
1	O	60	LEU	3.3
1	W	35	LEU	3.3
1	O	114	ALA	3.3
1	W	6	ALA	3.3
1	K	183	ASP	3.3
1	S	126	ASP	3.3
1	A	334	ILE	3.3
1	P	4	LYS	3.3
1	O	90	VAL	3.3
1	O	92	VAL	3.3
1	O	183	ASP	3.3
1	W	97	THR	3.3
1	O	118	VAL	3.3
1	S	35	LEU	3.3
1	S	88	LEU	3.3
1	D	62	ASP	3.2
1	T	25	HIS	3.2
1	W	330	PHE	3.2
1	V	298	VAL	3.2
1	R	124	GLY	3.2
1	W	69	GLY	3.2
1	X	53	ARG	3.2
1	B	25	HIS	3.2
1	V	59	GLU	3.2
1	G	125	ASN	3.2
1	O	126	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	X	70	ARG	3.2
1	H	25	HIS	3.2
1	V	61	LYS	3.2
1	P	80	PRO	3.2
1	O	327	LEU	3.2
1	P	247	SER	3.2
1	I	25	HIS	3.2
1	K	61	LYS	3.2
1	B	2	SER	3.2
1	W	66	VAL	3.1
1	W	130	VAL	3.1
1	W	128	LYS	3.1
1	P	165	LYS	3.1
1	U	161	ALA	3.1
1	O	94	LEU	3.1
1	I	1	MET	3.1
1	W	31	ALA	3.1
1	G	138	ILE	3.1
1	N	334	ILE	3.1
1	P	105	LYS	3.1
1	C	308	LYS	3.1
1	P	297	ARG	3.1
1	W	60	LEU	3.0
1	W	99	PHE	3.0
1	O	192	ARG	3.0
1	X	2	SER	3.0
1	O	81	GLU	3.0
1	R	81	GLU	3.0
1	V	62	ASP	3.0
1	W	61	LYS	3.0
1	O	80	PRO	3.0
1	C	25	HIS	3.0
1	I	303	GLY	3.0
1	D	2	SER	3.0
1	T	87	GLU	3.0
1	P	307	VAL	3.0
1	G	36	THR	3.0
1	H	27	ILE	3.0
1	D	26	GLY	3.0
1	O	9	GLY	3.0
1	W	323	LEU	3.0
1	O	115	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	X	90	VAL	3.0
1	P	140	ASP	3.0
1	W	326	THR	2.9
1	R	27	ILE	2.9
1	G	85	TRP	2.9
1	S	125	ASN	2.9
1	O	142	SER	2.9
1	V	304	LYS	2.9
1	L	25	HIS	2.9
1	X	114	ALA	2.9
1	C	71	GLU	2.9
1	M	59	GLU	2.9
1	X	65	ILE	2.9
1	M	299	MET	2.9
1	P	104	THR	2.9
1	S	110	ILE	2.9
1	U	70	ARG	2.9
1	K	63	ASP	2.9
1	X	137	ASP	2.9
1	P	252	PRO	2.9
1	X	215	LYS	2.9
1	H	53	ARG	2.9
1	X	88	LEU	2.9
1	B	183	ASP	2.8
1	L	140	ASP	2.8
1	P	137	ASP	2.8
1	R	183	ASP	2.8
1	P	260	ALA	2.8
1	R	64	ALA	2.8
1	O	116	LYS	2.8
1	U	165	LYS	2.8
1	I	251	ARG	2.8
1	O	141	GLY	2.8
1	O	147	SER	2.8
1	J	25	HIS	2.8
1	F	63	ASP	2.8
1	P	298	VAL	2.8
1	W	80	PRO	2.8
1	W	324	VAL	2.8
1	W	251	ARG	2.8
1	S	144	THR	2.8
1	U	104	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	27	ILE	2.8
1	A	2	SER	2.8
1	P	116	LYS	2.8
1	O	127	VAL	2.8
1	W	70	ARG	2.8
1	P	64	ALA	2.8
1	G	88	LEU	2.8
1	O	88	LEU	2.8
1	O	146	ILE	2.8
1	W	183	ASP	2.8
1	O	70	ARG	2.8
1	U	297	ARG	2.8
1	I	24	ALA	2.8
1	O	113	GLY	2.8
1	Q	25	HIS	2.8
1	U	25	HIS	2.8
1	O	140	ASP	2.7
1	G	145	VAL	2.7
1	W	98	GLY	2.7
1	J	61	LYS	2.7
1	P	110	ILE	2.7
1	L	297	ARG	2.7
1	U	299	MET	2.7
1	O	62	ASP	2.7
1	T	62	ASP	2.7
1	O	139	LEU	2.7
1	W	165	LYS	2.7
1	F	125	ASN	2.7
1	A	81	GLU	2.7
1	K	27	ILE	2.7
1	L	328	GLU	2.7
1	X	27	ILE	2.7
1	G	25	HIS	2.7
1	O	331	ALA	2.7
1	S	116	LYS	2.7
1	R	88	LEU	2.7
1	I	192	ARG	2.7
1	B	27	ILE	2.7
1	S	27	ILE	2.7
1	K	2	SER	2.7
1	L	63	ASP	2.7
1	R	63	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	25	HIS	2.7
1	U	226	GLY	2.6
1	M	192	ARG	2.6
1	O	125	ASN	2.6
1	P	87	GLU	2.6
1	Q	299	MET	2.6
1	W	39	GLU	2.6
1	P	142	SER	2.6
1	E	137	ASP	2.6
1	P	5	VAL	2.6
1	U	260	ALA	2.6
1	P	113	GLY	2.6
1	O	61	LYS	2.6
1	P	263	LYS	2.6
1	S	25	HIS	2.6
1	R	32	VAL	2.6
1	K	64	ALA	2.6
1	X	124	GLY	2.6
1	W	68	ASN	2.6
1	E	27	ILE	2.6
1	P	27	ILE	2.6
1	P	78	PRO	2.6
1	P	25	HIS	2.6
1	S	183	ASP	2.6
1	P	111	ARG	2.6
1	G	9	GLY	2.6
1	X	93	VAL	2.6
1	X	139	LEU	2.6
1	T	79	ASN	2.6
1	B	334	ILE	2.6
1	U	333	LYS	2.6
1	H	62	ASP	2.6
1	E	53	ARG	2.6
1	M	26	GLY	2.5
1	W	329	TYR	2.5
1	V	25	HIS	2.5
1	W	122	PRO	2.5
1	I	183	ASP	2.5
1	T	140	ASP	2.5
1	G	124	GLY	2.5
1	P	89	GLY	2.5
1	P	124	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	W	11	GLY	2.5
1	U	144	THR	2.5
1	G	27	ILE	2.5
1	P	258	ILE	2.5
1	S	111	ARG	2.5
1	O	91	ASP	2.5
1	X	327	LEU	2.5
1	R	104	THR	2.5
1	V	300	THR	2.5
1	X	125	ASN	2.5
1	A	70	ARG	2.5
1	L	251	ARG	2.5
1	J	27	ILE	2.5
1	M	27	ILE	2.5
1	G	63	ASP	2.5
1	J	62	ASP	2.5
1	K	62	ASP	2.5
1	X	126	ASP	2.5
1	W	71	GLU	2.5
1	J	124	GLY	2.5
1	X	92	VAL	2.5
1	P	139	LEU	2.5
1	S	60	LEU	2.5
1	M	43	HIS	2.5
1	W	132	TYR	2.4
1	B	63	ASP	2.4
1	L	39	GLU	2.4
1	U	1	MET	2.4
1	V	183	ASP	2.4
1	R	332	GLY	2.4
1	T	165	LYS	2.4
1	X	86	GLY	2.4
1	X	116	LYS	2.4
1	G	90	VAL	2.4
1	J	127	VAL	2.4
1	O	64	ALA	2.4
1	P	261	ALA	2.4
1	X	331	ALA	2.4
1	L	59	GLU	2.4
1	M	65	ILE	2.4
1	N	137	ASP	2.4
1	U	137	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	333	LYS	2.4
1	A	303	GLY	2.4
1	V	26	GLY	2.4
1	M	64	ALA	2.4
1	R	70	ARG	2.4
1	K	79	ASN	2.4
1	W	120	SER	2.4
1	B	61	LYS	2.4
1	O	4	LYS	2.4
1	O	34	ASP	2.4
1	P	183	ASP	2.4
1	X	140	ASP	2.4
1	G	86	GLY	2.4
1	R	303	GLY	2.4
1	R	251	ARG	2.4
1	G	24	ALA	2.4
1	G	144	THR	2.4
1	N	59	GLU	2.4
1	W	22	GLU	2.4
1	H	183	ASP	2.4
1	D	192	ARG	2.4
1	M	69	GLY	2.4
1	E	108	ALA	2.4
1	K	88	LEU	2.4
1	P	24	ALA	2.4
1	P	94	LEU	2.4
1	H	299	MET	2.3
1	K	28	GLU	2.3
1	O	198	ARG	2.3
1	M	79	ASN	2.3
1	V	249	LEU	2.3
1	V	259	ASN	2.3
1	W	327	LEU	2.3
1	W	328	GLU	2.3
1	X	143	GLU	2.3
1	H	63	ASP	2.3
1	J	63	ASP	2.3
1	S	2	SER	2.3
1	S	3	ILE	2.3
1	O	56	GLY	2.3
1	S	26	GLY	2.3
1	V	69	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	61	LYS	2.3
1	P	30	ALA	2.3
1	P	59	GLU	2.3
1	P	79	ASN	2.3
1	Q	1	MET	2.3
1	S	114	ALA	2.3
1	X	73	LYS	2.3
1	O	144	THR	2.3
1	R	127	VAL	2.3
1	W	10	PHE	2.3
1	H	192	ARG	2.3
1	W	65	ILE	2.3
1	O	329	TYR	2.3
1	K	76	ALA	2.3
1	O	31	ALA	2.3
1	O	58	ALA	2.3
1	P	265	ALA	2.3
1	R	144	THR	2.3
1	W	220	VAL	2.3
1	Q	192	ARG	2.3
1	Q	183	ASP	2.3
1	W	136	GLN	2.3
1	F	299	MET	2.2
1	W	95	GLU	2.2
1	J	24	ALA	2.2
1	O	97	THR	2.2
1	X	78	PRO	2.2
1	C	183	ASP	2.2
1	X	72	ILE	2.2
1	X	146	ILE	2.2
1	O	103	LYS	2.2
1	P	304	LYS	2.2
1	T	26	GLY	2.2
1	U	302	GLY	2.2
1	V	9	GLY	2.2
1	C	125	ASN	2.2
1	P	77	ASN	2.2
1	X	329	TYR	2.2
1	P	53	ARG	2.2
1	P	170	VAL	2.2
1	M	75	PHE	2.2
1	M	2	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	123	GLY	2.2
1	E	1	MET	2.2
1	P	306	LEU	2.2
1	V	192	ARG	2.2
1	K	24	ALA	2.2
1	V	24	ALA	2.2
1	P	100	PHE	2.2
1	F	183	ASP	2.2
1	N	251	ARG	2.2
1	T	115	ARG	2.2
1	Q	219	LEU	2.2
1	W	135	ASN	2.2
1	G	114	ALA	2.2
1	U	164	GLN	2.2
1	U	134	VAL	2.2
1	O	165	LYS	2.2
1	P	229	ASP	2.2
1	I	27	ILE	2.1
1	K	87	GLU	2.1
1	M	39	GLU	2.1
1	S	82	GLU	2.1
1	V	268	GLU	2.1
1	M	111	ARG	2.1
1	T	251	ARG	2.1
1	D	24	ALA	2.1
1	P	57	THR	2.1
1	P	301	VAL	2.1
1	V	299	MET	2.1
1	A	62	ASP	2.1
1	L	183	ASP	2.1
1	W	166	GLU	2.1
1	I	2	SER	2.1
1	K	231	SER	2.1
1	O	120	SER	2.1
1	P	141	GLY	2.1
1	O	323	LEU	2.1
1	E	61	LYS	2.1
1	M	304	LYS	2.1
1	G	112	ALA	2.1
1	O	214	ALA	2.1
1	W	264	ALA	2.1
1	W	296	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	5	VAL	2.1
1	P	262	MET	2.1
1	B	328	GLU	2.1
1	U	39	GLU	2.1
1	U	223	GLU	2.1
1	A	297	ARG	2.1
1	H	140	ASP	2.1
1	E	212	GLY	2.1
1	E	297	ARG	2.1
1	G	69	GLY	2.1
1	S	53	ARG	2.1
1	T	53	ARG	2.1
1	F	193	LYS	2.1
1	K	215	LYS	2.1
1	P	128	LYS	2.1
1	X	35	LEU	2.1
1	G	76	ALA	2.1
1	O	104	THR	2.1
1	I	71	GLU	2.1
1	N	297	ARG	2.1
1	B	62	ASP	2.1
1	C	126	ASP	2.1
1	H	126	ASP	2.1
1	U	140	ASP	2.1
1	P	332	GLY	2.1
1	P	146	ILE	2.1
1	X	25	HIS	2.1
1	Q	333	LYS	2.1
1	I	79	ASN	2.1
1	O	41	LEU	2.1
1	S	83	LEU	2.1
1	W	299	MET	2.1
1	E	71	GLU	2.0
1	L	87	GLU	2.0
1	P	166	GLU	2.0
1	R	87	GLU	2.0
1	U	192	ARG	2.0
1	S	90	VAL	2.0
1	X	74	VAL	2.0
1	G	137	ASP	2.0
1	N	183	ASP	2.0
1	U	123	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	2	SER	2.0
1	I	255	LYS	2.0
1	P	255	LYS	2.0
1	X	165	LYS	2.0
1	E	299	MET	2.0
1	G	6	ALA	2.0
1	M	24	ALA	2.0
1	O	111	ARG	2.0
1	O	251	ARG	2.0
1	P	6	ALA	2.0
1	S	87	GLU	2.0
1	W	121	ALA	2.0
1	X	59	GLU	2.0
1	W	67	VAL	2.0
1	F	62	ASP	2.0
1	X	9	GLY	2.0
1	D	27	ILE	2.0
1	T	3	ILE	2.0
1	W	37	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	O	401	44/44	0.77	0.16	46,71,91,95	0
2	NAD	W	401	44/44	0.84	0.15	50,72,89,92	0
3	PGE	H	402	10/10	0.88	0.13	47,53,59,66	0
2	NAD	X	401	44/44	0.92	0.10	32,45,53,55	0

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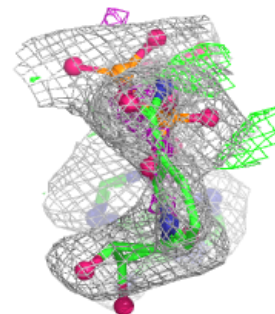
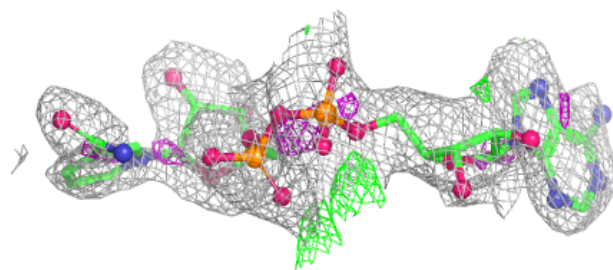
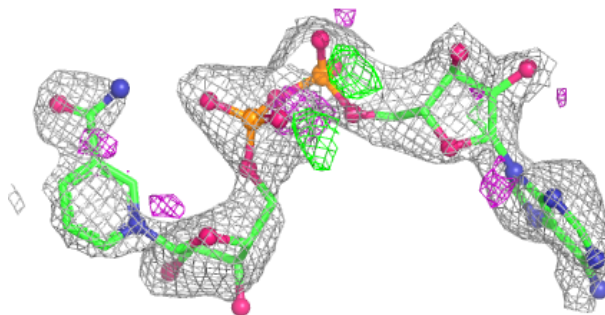
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	G	401	44/44	0.93	0.09	32,41,49,56	0
2	NAD	P	401	44/44	0.94	0.09	31,43,53,56	0
2	NAD	F	401	44/44	0.95	0.07	24,30,33,58	0
2	NAD	K	401	44/44	0.96	0.07	26,35,41,42	0
2	NAD	Q	401	44/44	0.96	0.07	30,36,39,41	0
2	NAD	R	401	44/44	0.96	0.07	30,38,43,50	0
2	NAD	S	401	44/44	0.96	0.08	32,41,51,53	0
2	NAD	T	401	44/44	0.96	0.07	21,29,36,38	0
2	NAD	U	401	44/44	0.96	0.07	21,36,41,43	0
2	NAD	L	401	44/44	0.96	0.07	27,35,39,40	0
2	NAD	M	401	44/44	0.96	0.07	26,37,45,52	0
2	NAD	E	401	44/44	0.96	0.07	23,33,39,40	0
2	NAD	A	401	44/44	0.97	0.06	22,29,33,35	0
2	NAD	B	401	44/44	0.97	0.06	23,32,35,40	0
2	NAD	C	401	44/44	0.97	0.06	24,28,34,37	0
2	NAD	V	401	44/44	0.97	0.06	24,33,39,41	0
2	NAD	I	401	44/44	0.97	0.06	22,29,34,35	0
2	NAD	J	401	44/44	0.97	0.06	21,31,36,37	0
2	NAD	D	401	44/44	0.97	0.06	20,26,32,33	0
2	NAD	N	401	44/44	0.98	0.05	21,27,31,33	0
2	NAD	H	401	44/44	0.98	0.06	22,30,34,35	0

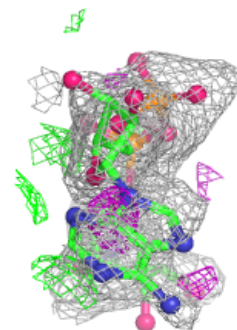
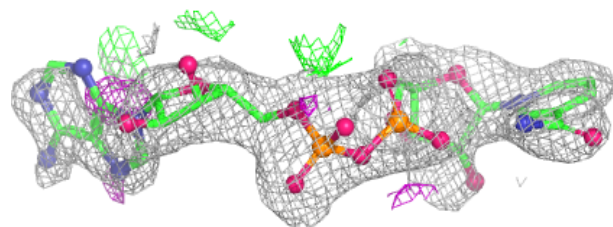
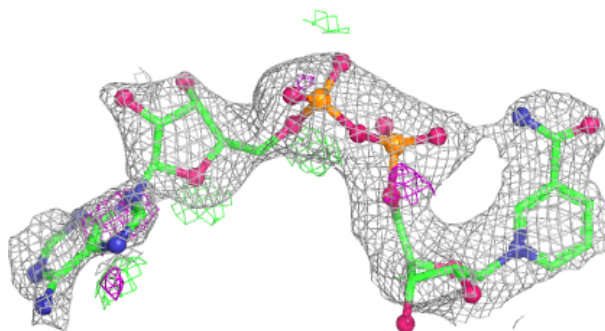
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD O 401:

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

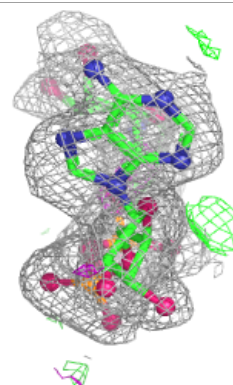
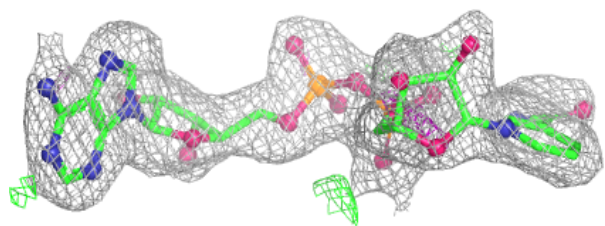
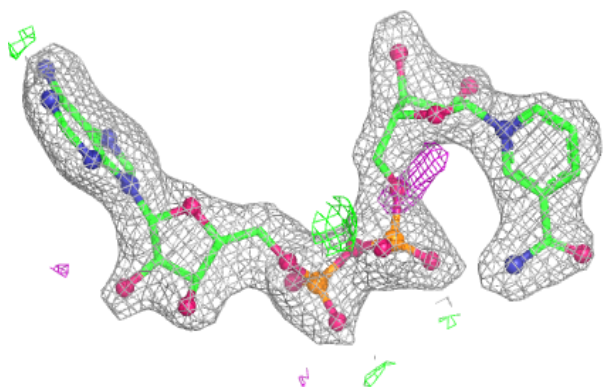
**Electron density around NAD W 401:**

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

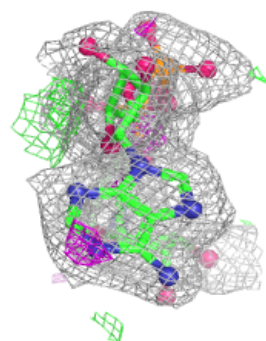
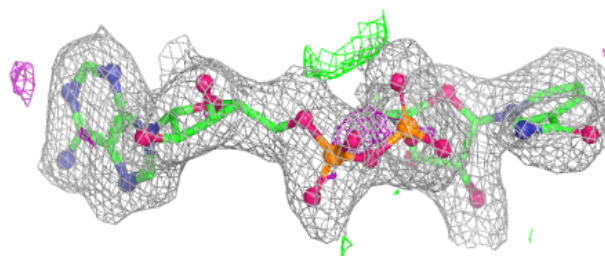
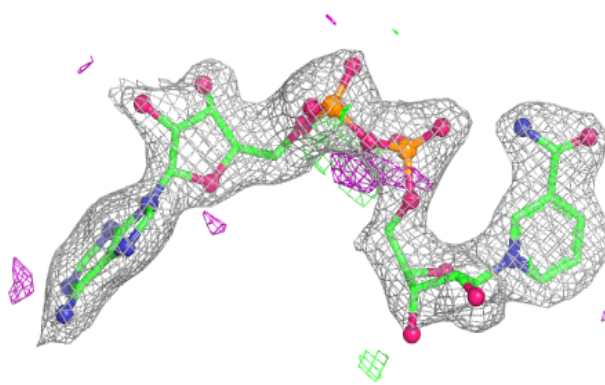


Electron density around NAD X 401:

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

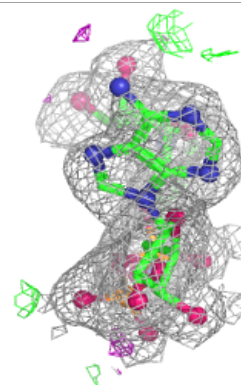
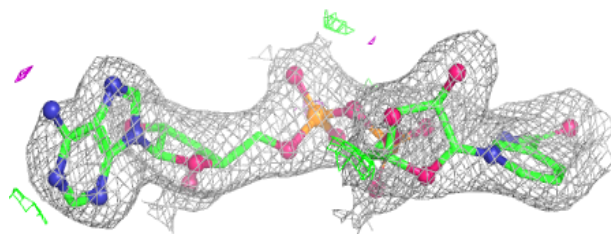
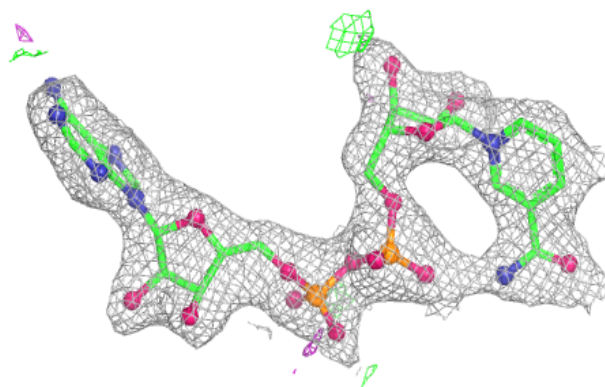
**Electron density around NAD G 401:**

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

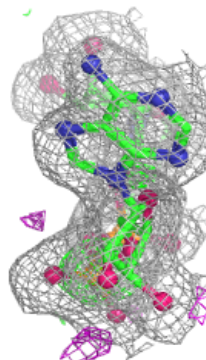
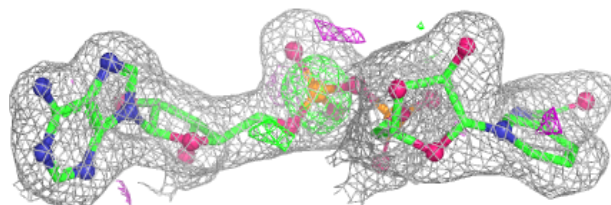
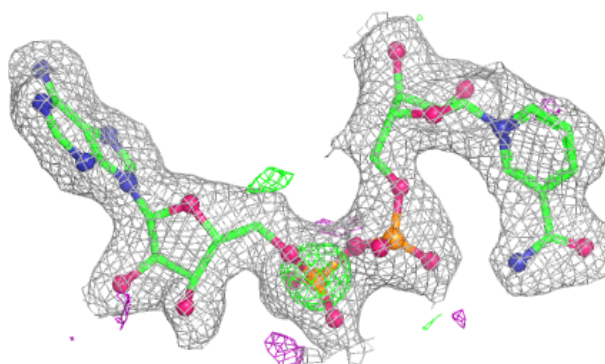


Electron density around NAD P 401:

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

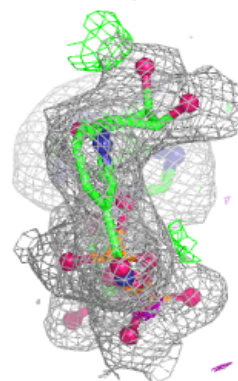
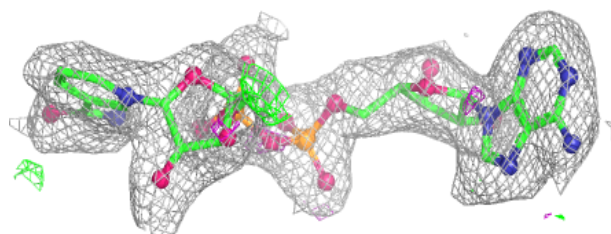
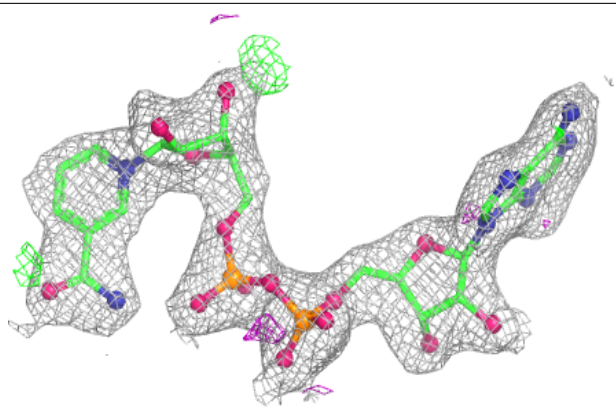
**Electron density around NAD F 401:**

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

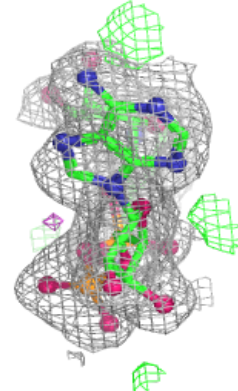
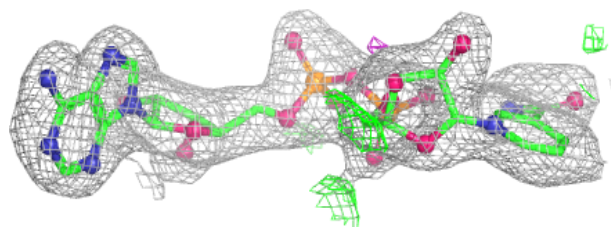
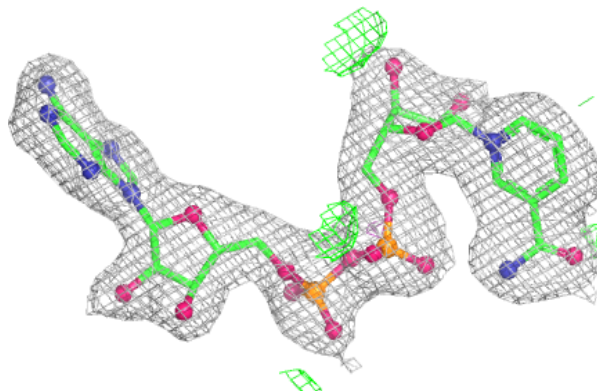


Electron density around NAD K 401:

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

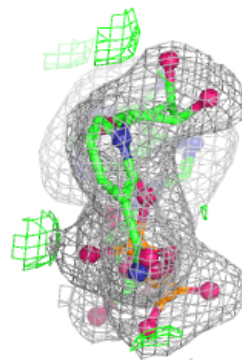
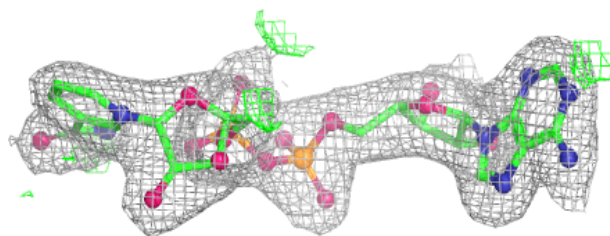
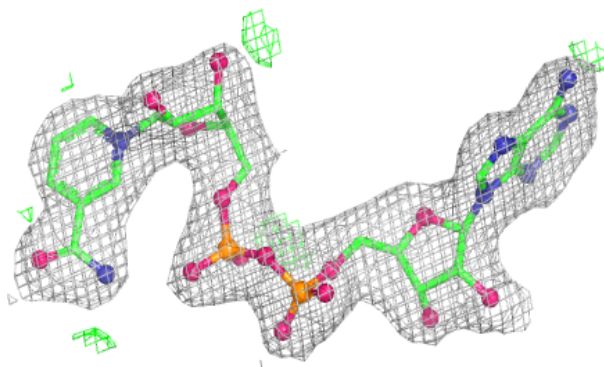
**Electron density around NAD Q 401:**

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

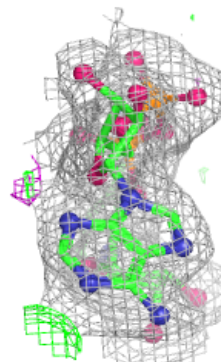
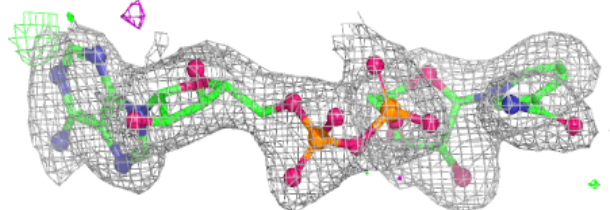
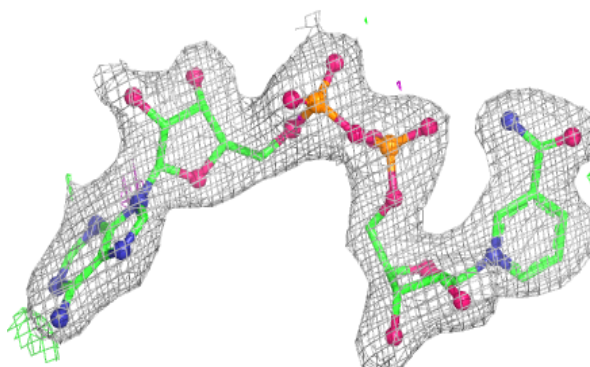


Electron density around NAD R 401:

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

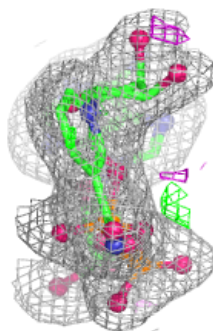
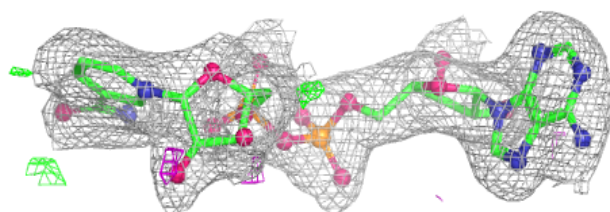
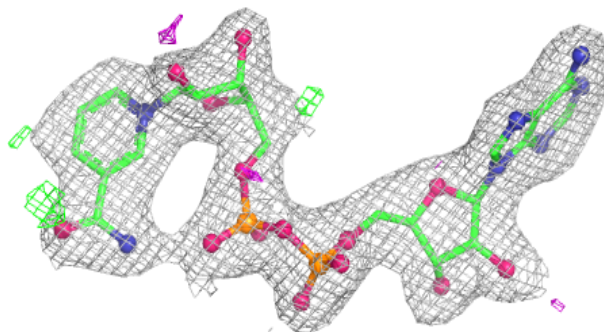
**Electron density around NAD S 401:**

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

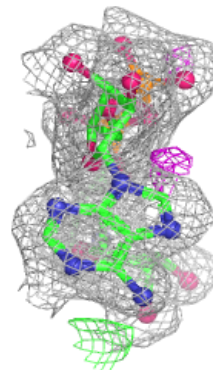
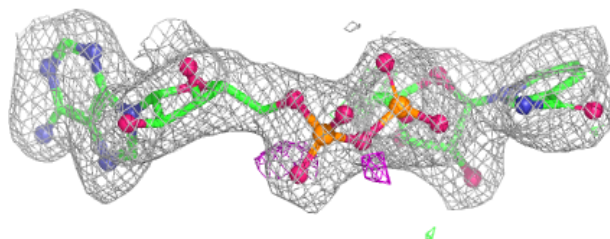
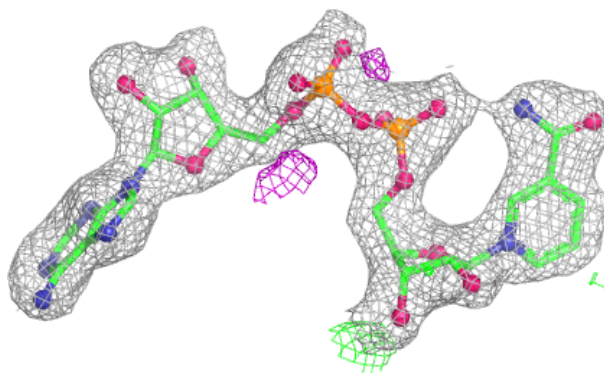


Electron density around NAD T 401:

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

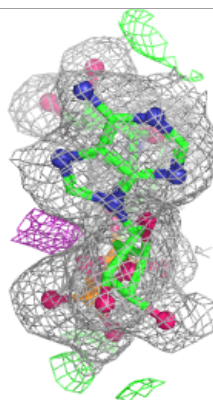
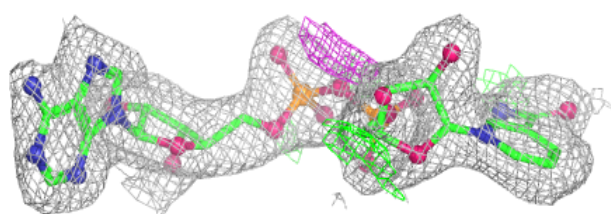
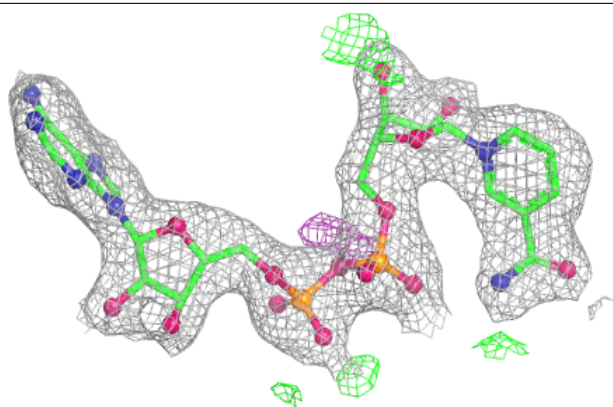
**Electron density around NAD U 401:**

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

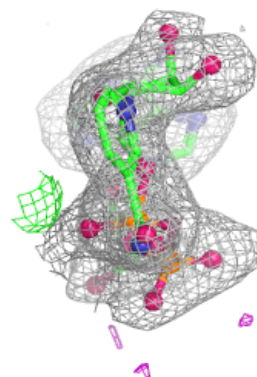
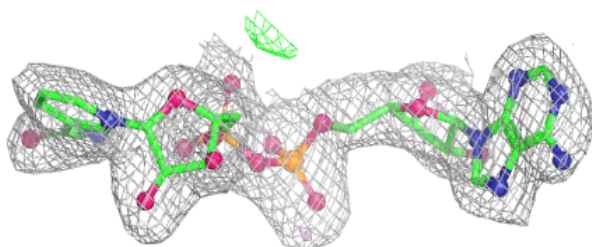
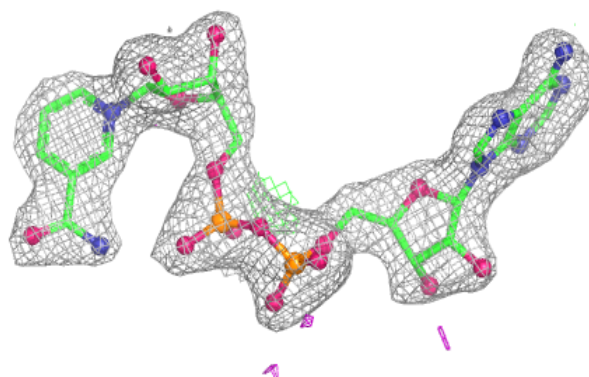


Electron density around NAD L 401:

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

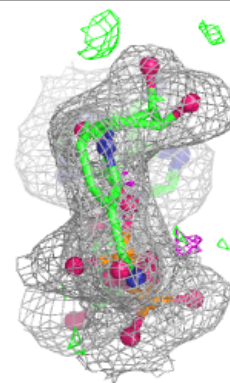
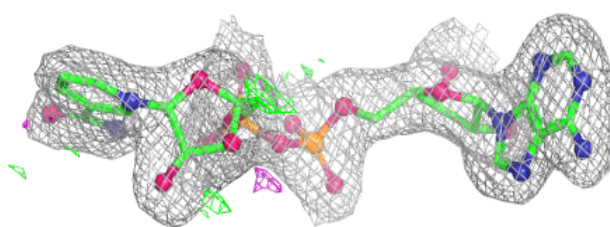
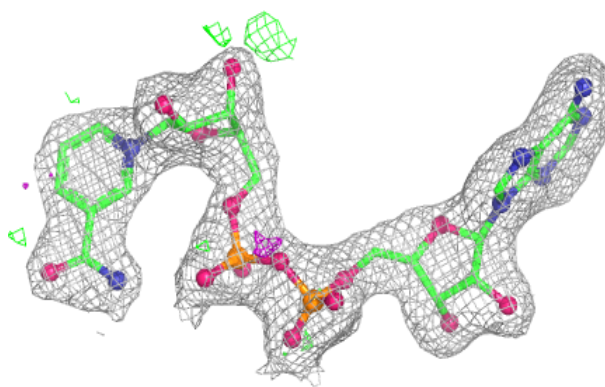
**Electron density around NAD M 401:**

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

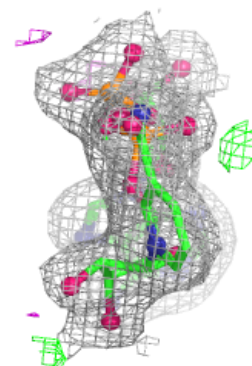
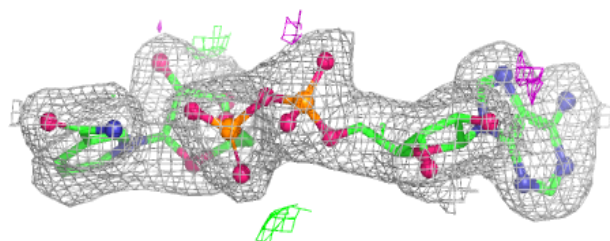
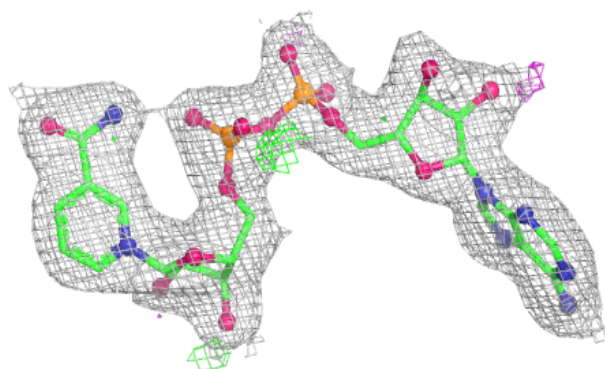


Electron density around NAD E 401:

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

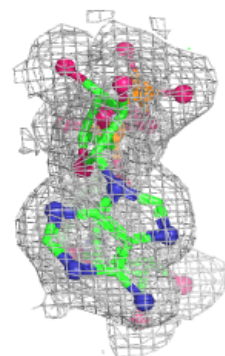
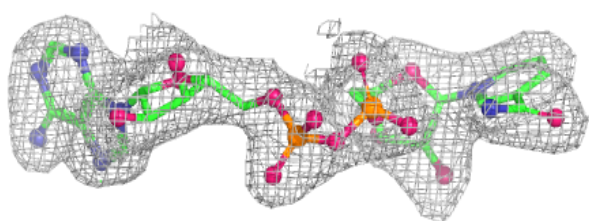
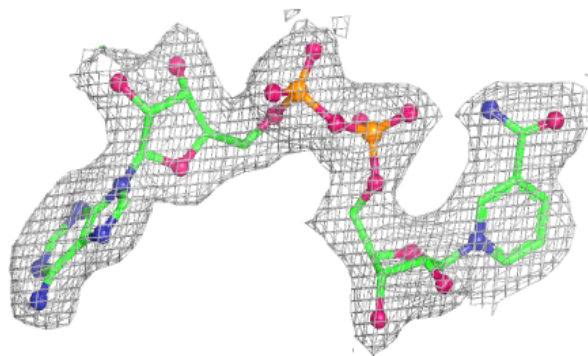
**Electron density around NAD A 401:**

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

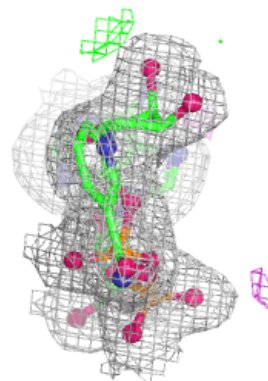
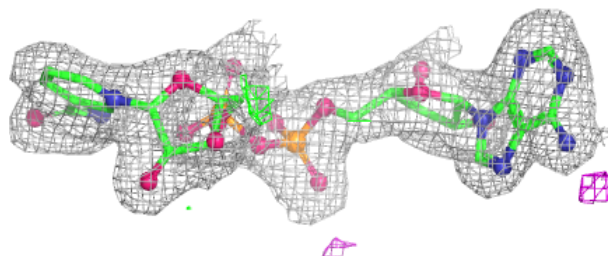
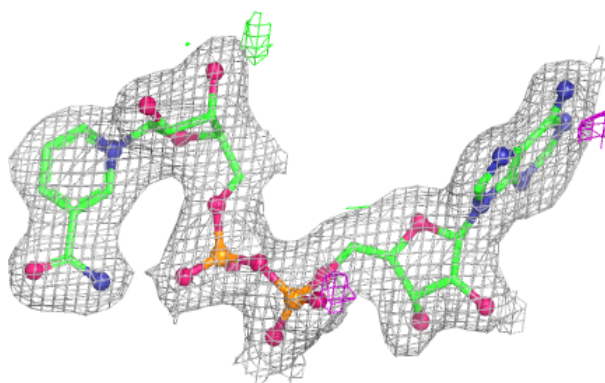


Electron density around NAD B 401:

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

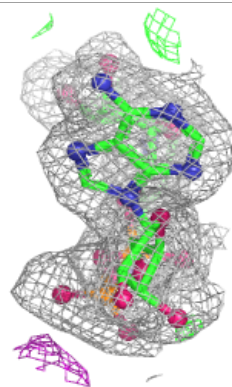
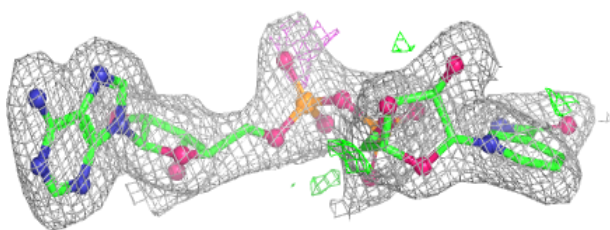
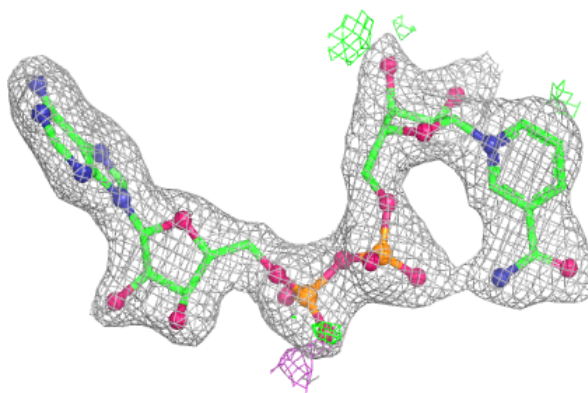
**Electron density around NAD C 401:**

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

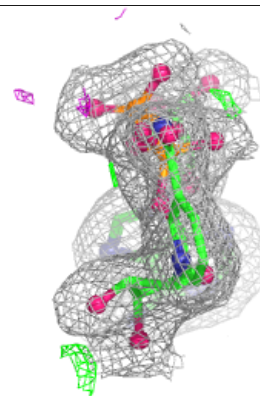
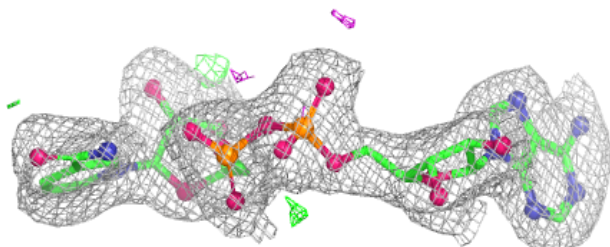
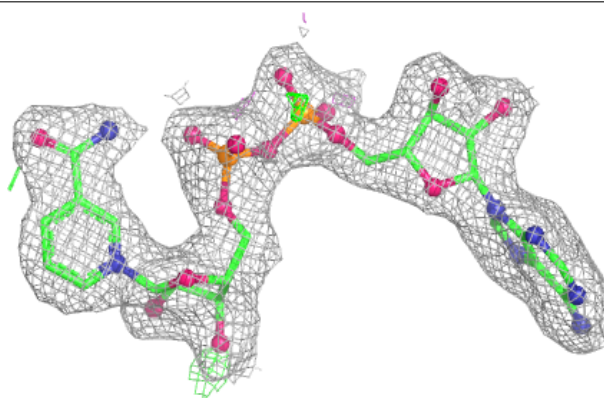


Electron density around NAD V 401:

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

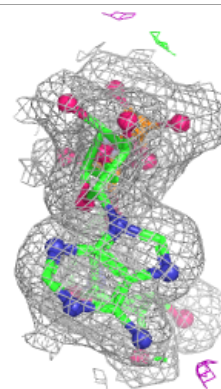
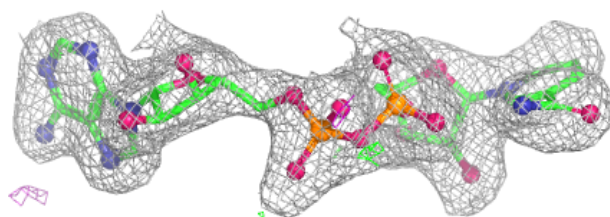
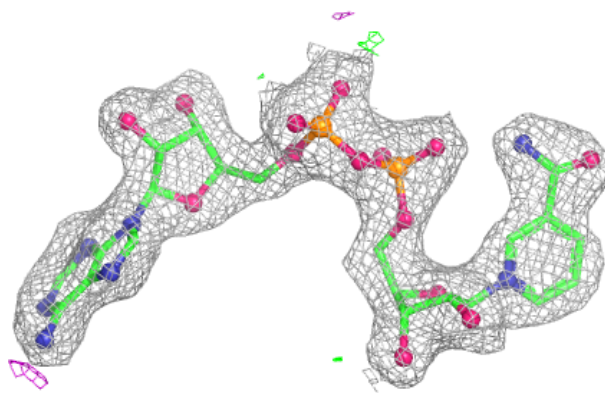
**Electron density around NAD I 401:**

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

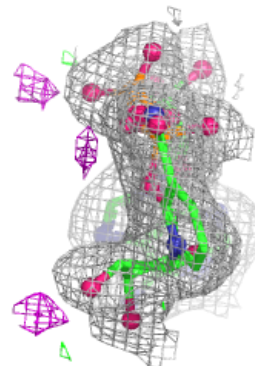
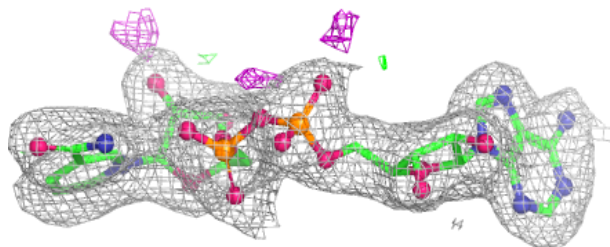
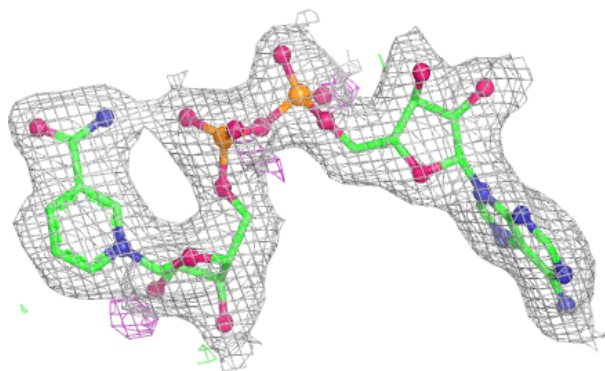


Electron density around NAD J 401:

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

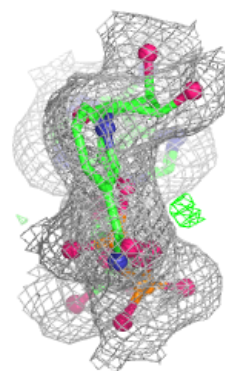
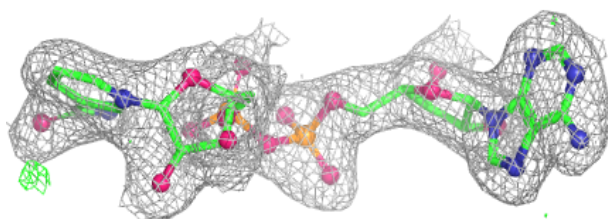
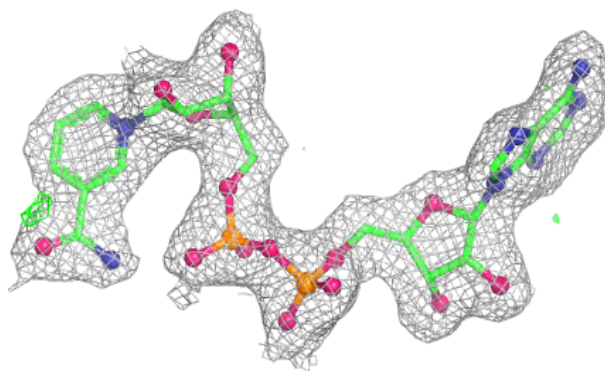
**Electron density around NAD D 401:**

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

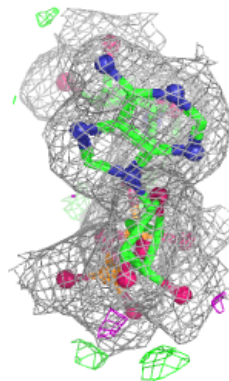
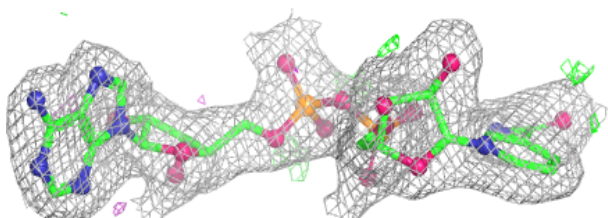
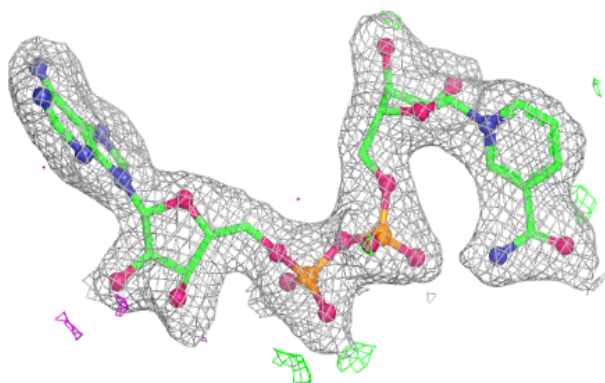


Electron density around NAD N 401:

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

**Electron density around NAD H 401:**

$2mF_o-DF_c$ (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.