



wwPDB X-ray Structure Validation Summary Report

Mar 9, 2026 – 05:43 PM UTC

PDB ID : 9ZAG / pdb_00009zag
Title : Crystal structure of a glyceraldehyde-3-phosphate dehydrogenase from *Neisseria gonorrhoeae* in complex with NAD and GLYCERALDEHYDE-3-PHOSPHATE
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2025-11-19
Resolution : 1.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

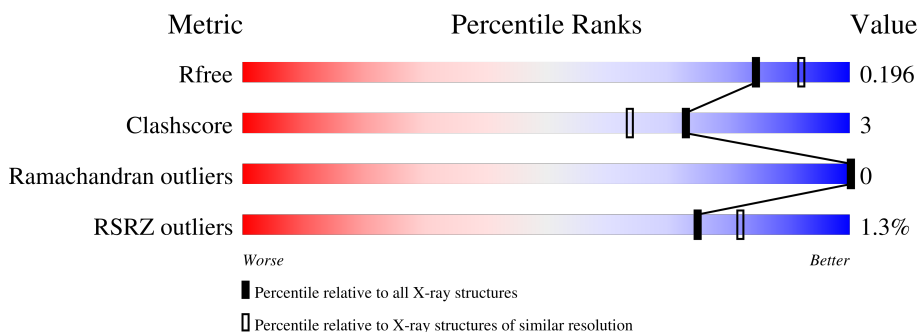
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



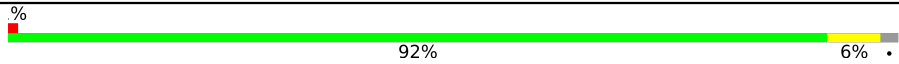
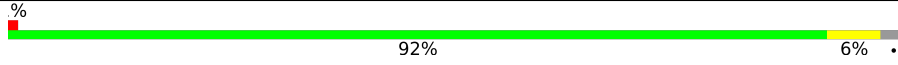
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	 2% 91% 6%
1	B	342	 % 91% 7%
1	C	342	 % 93% 5%
1	D	342	 % 91% 7%
1	E	342	 2% 90% 7%
1	F	342	 90% 7%

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Mol	Chain	Length	Quality of chain
1	G	342	
1	H	342	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21909 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
			Total	C	N	O	S			
1	A	333	2506	1572	435	488	11	0	2	0
1	B	334	2516	1581	434	489	12	0	3	0
1	C	334	2514	1576	436	491	11	0	1	0
1	D	333	2510	1574	435	491	10	0	2	0
1	E	334	2508	1573	436	489	10	0	1	0
1	F	332	2492	1562	432	488	10	0	1	0
1	G	334	2517	1578	436	492	11	0	2	0
1	H	333	2499	1568	435	486	10	0	1	0

There are 64 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

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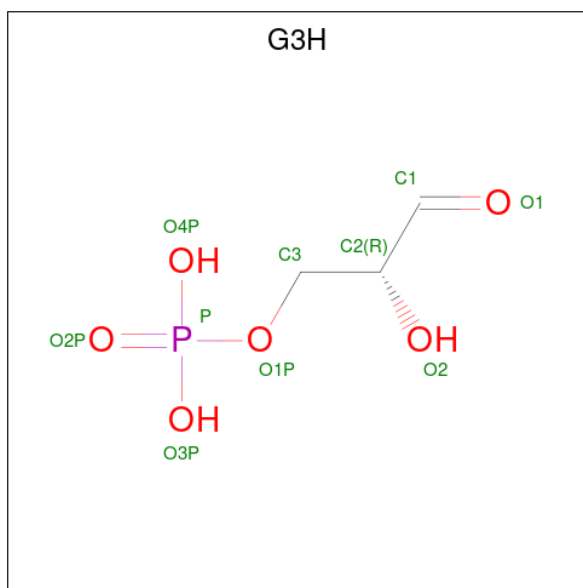
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP B4RPP8
B	-1	HIS	-	expression tag	UNP B4RPP8
B	0	HIS	-	expression tag	UNP B4RPP8
C	-7	MET	-	initiating methionine	UNP B4RPP8
C	-6	ALA	-	expression tag	UNP B4RPP8
C	-5	HIS	-	expression tag	UNP B4RPP8
C	-4	HIS	-	expression tag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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is GLYCERALDEHYDE-3-PHOSPHATE (CCD ID: G3H) (formula: C₃H₇O₆P) (labeled as "Ligand of Interest" by depositor).



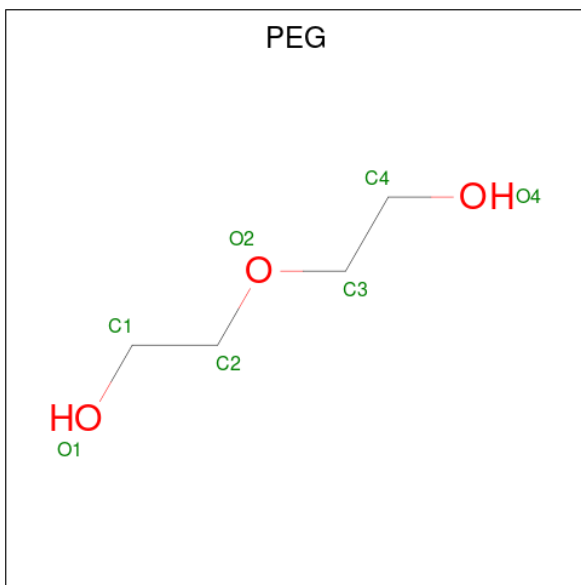
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	1	Total	C	O	P	0	0
			10	3	6	1		
2	C	1	Total	C	O	P	0	0
			10	3	6	1		
2	D	1	Total	C	O	P	0	0
			10	3	6	1		
2	E	1	Total	C	O	P	0	0
			10	3	6	1		
2	F	1	Total	C	O	P	0	0
			10	3	6	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	O	P	0	0
			10	3	6	1		
2	H	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



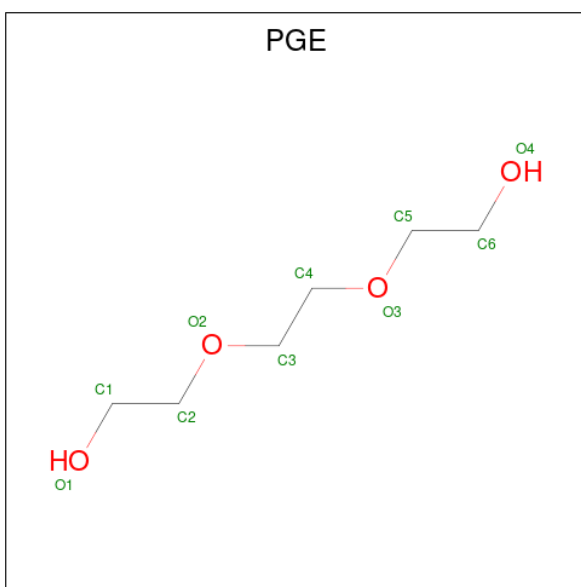
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	Na	0	0
			1	1		
5	F	1	Total	Na	0	0
			1	1		
5	G	1	Total	Na	0	0
			1	1		
5	H	1	Total	Na	0	0
			1	1		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).

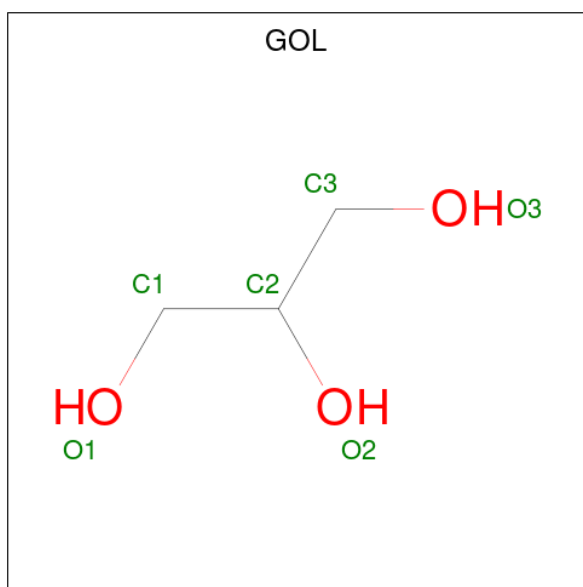


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

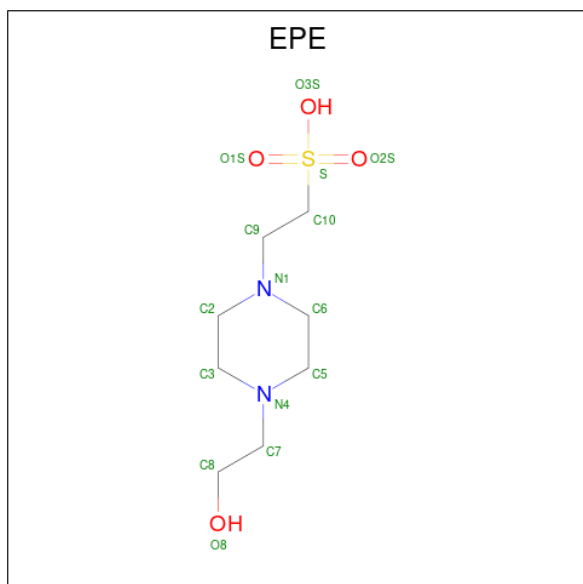
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	H	1	15	8	2	4	1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	177	Total 177	O 177	0	0
10	B	169	Total 169	O 169	0	0
10	C	160	Total 160	O 160	0	0
10	D	176	Total 176	O 176	0	0
10	E	143	Total 143	O 143	0	0
10	F	156	Total 156	O 156	0	0
10	G	155	Total 155	O 155	0	0
10	H	162	Total 162	O 162	0	0

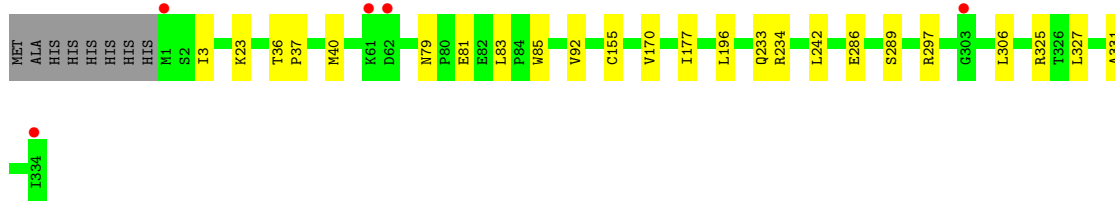
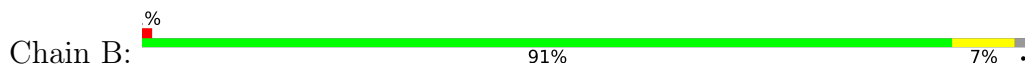
3 Residue-property plots [i](#)

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



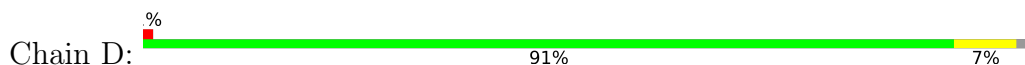
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

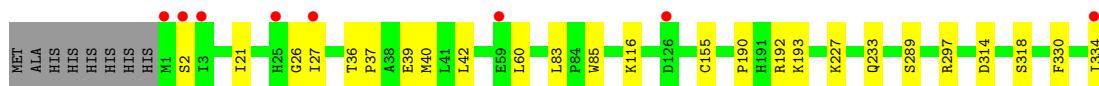


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

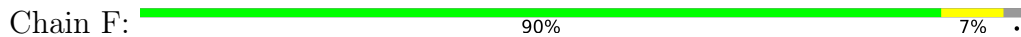


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

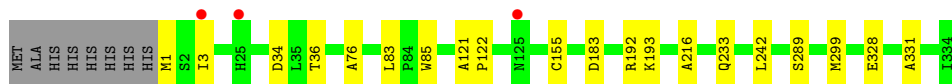
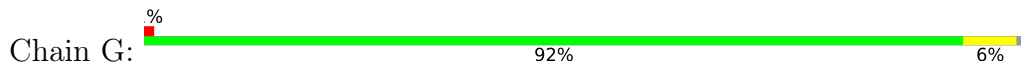




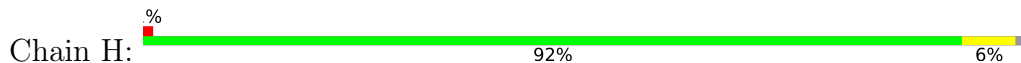
● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.65Å 105.54Å 167.70Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	48.89 – 1.91 48.89 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.89-1.91) 99.9 (48.89-1.91)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.91Å)	Xtrriage
Refinement program	PHENIX (dev_5438: ???)	Depositor
R, R_{free}	0.155 , 0.187 0.166 , 0.196	Depositor DCC
R_{free} test set	9116 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtrriage
Anisotropy	0.126	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21909	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1239e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, G3H, NAD, PGE, PEG, NA, CL, EPE

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	0.40	0/2549	0.62	0/3457
1	B	0.38	0/2561	0.61	0/3471
1	C	0.37	0/2554	0.58	0/3462
1	D	0.37	0/2553	0.58	0/3462
1	E	0.36	0/2548	0.59	0/3455
1	F	0.35	0/2531	0.57	0/3433
1	G	0.38	0/2560	0.60	0/3470
1	H	0.38	0/2539	0.59	0/3443
All	All	0.37	0/20395	0.59	0/27653

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	297	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	297	ARG	Sidechain
1	E	297	ARG	Sidechain
1	F	297	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2506	0	2523	20	0
1	B	2516	0	2548	26	0
1	C	2514	0	2535	12	0
1	D	2510	0	2530	16	0
1	E	2508	0	2526	18	0
1	F	2492	0	2507	18	0
1	G	2517	0	2540	15	0
1	H	2499	0	2517	15	0
2	A	10	0	5	1	0
2	B	10	0	5	1	0
2	C	10	0	5	0	0
2	D	10	0	5	0	0
2	E	10	0	5	0	0
2	F	10	0	5	0	0
2	G	10	0	5	1	0
2	H	10	0	5	0	0
3	A	14	0	20	1	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0
3	D	7	0	10	2	0
3	E	7	0	10	0	0
3	F	7	0	10	0	0
3	G	7	0	10	0	0
4	A	44	0	26	1	0
4	B	44	0	26	1	0
4	C	44	0	26	0	0
4	D	44	0	26	0	0
4	E	44	0	26	0	0
4	F	44	0	26	0	0
4	G	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	44	0	26	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	B	10	0	14	1	0
7	B	1	0	0	0	0
8	C	6	0	8	0	0
8	D	6	0	8	0	0
9	D	15	0	18	0	0
9	H	15	0	18	0	0
10	A	177	0	0	3	0
10	B	169	0	0	2	0
10	C	160	0	0	0	0
10	D	176	0	0	0	0
10	E	143	0	0	1	0
10	F	156	0	0	0	0
10	G	155	0	0	0	0
10	H	162	0	0	3	0
All	All	21909	0	20620	130	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 130 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:A:27:ILE:HD11	1:A:328:GLU:HG2	1.29	1.06
1:B:36:THR:HG21	1:B:40[A]:MET:HG2	1.66	0.75
1:B:177:ILE:HD12	1:B:242:LEU:HD11	1.69	0.74
1:B:36:THR:HG22	1:B:37:PRO:HD2	1.70	0.73
1:D:83:LEU:HD13	1:D:85:TRP:CZ2	2.26	0.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/342 (97%)	322 (97%)	11 (3%)	0	100	100
1	B	335/342 (98%)	324 (97%)	11 (3%)	0	100	100
1	C	333/342 (97%)	320 (96%)	13 (4%)	0	100	100
1	D	333/342 (97%)	320 (96%)	13 (4%)	0	100	100
1	E	333/342 (97%)	323 (97%)	10 (3%)	0	100	100
1	F	331/342 (97%)	320 (97%)	11 (3%)	0	100	100
1	G	334/342 (98%)	320 (96%)	14 (4%)	0	100	100
1	H	332/342 (97%)	321 (97%)	11 (3%)	0	100	100
All	All	2664/2736 (97%)	2570 (96%)	94 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

Of 38 ligands modelled in this entry, 9 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	B	402	-	6,6,6	0.27	0	5,5,5	0.18	0
2	G3H	D	401	-	8,9,9	1.72	2 (25%)	7,12,12	1.38	1 (14%)
4	NAD	C	404	-	46,48,48	1.13	2 (4%)	64,73,73	0.90	3 (4%)
3	PEG	E	402	-	6,6,6	0.26	0	5,5,5	0.53	0
4	NAD	A	404	-	46,48,48	0.87	3 (6%)	64,73,73	1.02	5 (7%)
3	PEG	C	402	-	6,6,6	0.28	0	5,5,5	0.42	0
4	NAD	E	403	-	46,48,48	0.98	3 (6%)	64,73,73	1.07	5 (7%)
2	G3H	G	401	-	8,9,9	1.71	2 (25%)	7,12,12	1.37	1 (14%)
3	PEG	A	402	-	6,6,6	0.29	0	5,5,5	0.44	0
4	NAD	B	403	-	46,48,48	0.99	2 (4%)	64,73,73	0.98	2 (3%)
2	G3H	F	401	-	8,9,9	1.85	3 (37%)	7,12,12	1.52	1 (14%)
2	G3H	H	401	-	8,9,9	1.83	2 (25%)	7,12,12	1.50	1 (14%)
2	G3H	B	401	-	8,9,9	1.68	1 (12%)	7,12,12	1.48	1 (14%)
3	PEG	G	402	-	6,6,6	0.27	0	5,5,5	0.43	0
8	GOL	C	403	-	5,5,5	0.26	0	5,5,5	0.43	0
9	EPE	H	402	-	15,15,15	0.82	1 (6%)	19,20,20	0.82	0
4	NAD	D	405	-	46,48,48	1.01	3 (6%)	64,73,73	0.92	5 (7%)
4	NAD	F	403	-	46,48,48	0.88	2 (4%)	64,73,73	0.95	2 (3%)
3	PEG	F	402	-	6,6,6	0.12	0	5,5,5	0.08	0
3	PEG	D	402	-	6,6,6	0.27	0	5,5,5	0.31	0
4	NAD	G	403	-	46,48,48	1.20	3 (6%)	64,73,73	1.02	4 (6%)
9	EPE	D	404	-	15,15,15	0.83	0	19,20,20	1.18	1 (5%)
4	NAD	H	403	-	46,48,48	1.19	3 (6%)	64,73,73	0.98	2 (3%)
2	G3H	E	401	-	8,9,9	1.84	3 (37%)	7,12,12	1.61	1 (14%)
2	G3H	A	401	-	8,9,9	1.78	2 (25%)	7,12,12	1.59	2 (28%)
3	PEG	A	403	-	6,6,6	0.22	0	5,5,5	0.27	0
6	PGE	B	405	-	9,9,9	0.33	0	8,8,8	0.64	0
2	G3H	C	401	-	8,9,9	1.76	2 (25%)	7,12,12	1.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	D	403	-	5,5,5	0.32	0	5,5,5	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	402	-	-	1/4/4/4	-
2	G3H	D	401	-	-	5/7/8/8	-
4	NAD	C	404	-	-	4/30/62/62	0/5/5/5
3	PEG	E	402	-	-	2/4/4/4	-
4	NAD	A	404	-	-	5/30/62/62	0/5/5/5
3	PEG	C	402	-	-	0/4/4/4	-
4	NAD	E	403	-	-	4/30/62/62	0/5/5/5
2	G3H	G	401	-	-	0/7/8/8	-
3	PEG	A	402	-	-	4/4/4/4	-
4	NAD	B	403	-	-	4/30/62/62	0/5/5/5
2	G3H	F	401	-	-	5/7/8/8	-
2	G3H	H	401	-	-	6/7/8/8	-
2	G3H	B	401	-	-	2/7/8/8	-
3	PEG	G	402	-	-	2/4/4/4	-
8	GOL	C	403	-	-	2/4/4/4	-
9	EPE	H	402	-	-	5/9/19/19	0/1/1/1
4	NAD	D	405	-	-	4/30/62/62	0/5/5/5
4	NAD	F	403	-	-	4/30/62/62	0/5/5/5
3	PEG	F	402	-	-	4/4/4/4	-
3	PEG	D	402	-	-	3/4/4/4	-
4	NAD	G	403	-	-	4/30/62/62	0/5/5/5
9	EPE	D	404	-	-	4/9/19/19	0/1/1/1
4	NAD	H	403	-	-	5/30/62/62	0/5/5/5
2	G3H	E	401	-	-	5/7/8/8	-
2	G3H	A	401	-	-	1/7/8/8	-
3	PEG	A	403	-	-	2/4/4/4	-
6	PGE	B	405	-	-	2/7/7/7	-
2	G3H	C	401	-	-	5/7/8/8	-
8	GOL	D	403	-	-	2/4/4/4	-

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	403	NAD	PA-O3	4.67	1.64	1.59
4	C	404	NAD	PA-O3	4.58	1.64	1.59
4	G	403	NAD	PA-O3	4.27	1.64	1.59
4	B	403	NAD	PA-O3	4.25	1.64	1.59
4	C	404	NAD	PN-O3	4.10	1.63	1.59

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	404	EPE	O2S-S-C10	-3.34	101.69	106.73
4	E	403	NAD	O3-PA-O1A	-3.12	101.32	110.70
4	G	403	NAD	O3-PA-O1A	-3.02	101.61	110.70
4	H	403	NAD	O3-PA-O1A	-2.93	101.89	110.70
2	E	401	G3H	O2-C2-C1	2.75	114.96	109.03

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	G3H	C1-C2-C3-O1P
2	B	401	G3H	O2-C2-C3-O1P
2	C	401	G3H	O1-C1-C2-C3
2	C	401	G3H	C1-C2-C3-O1P
2	C	401	G3H	O2-C2-C3-O1P

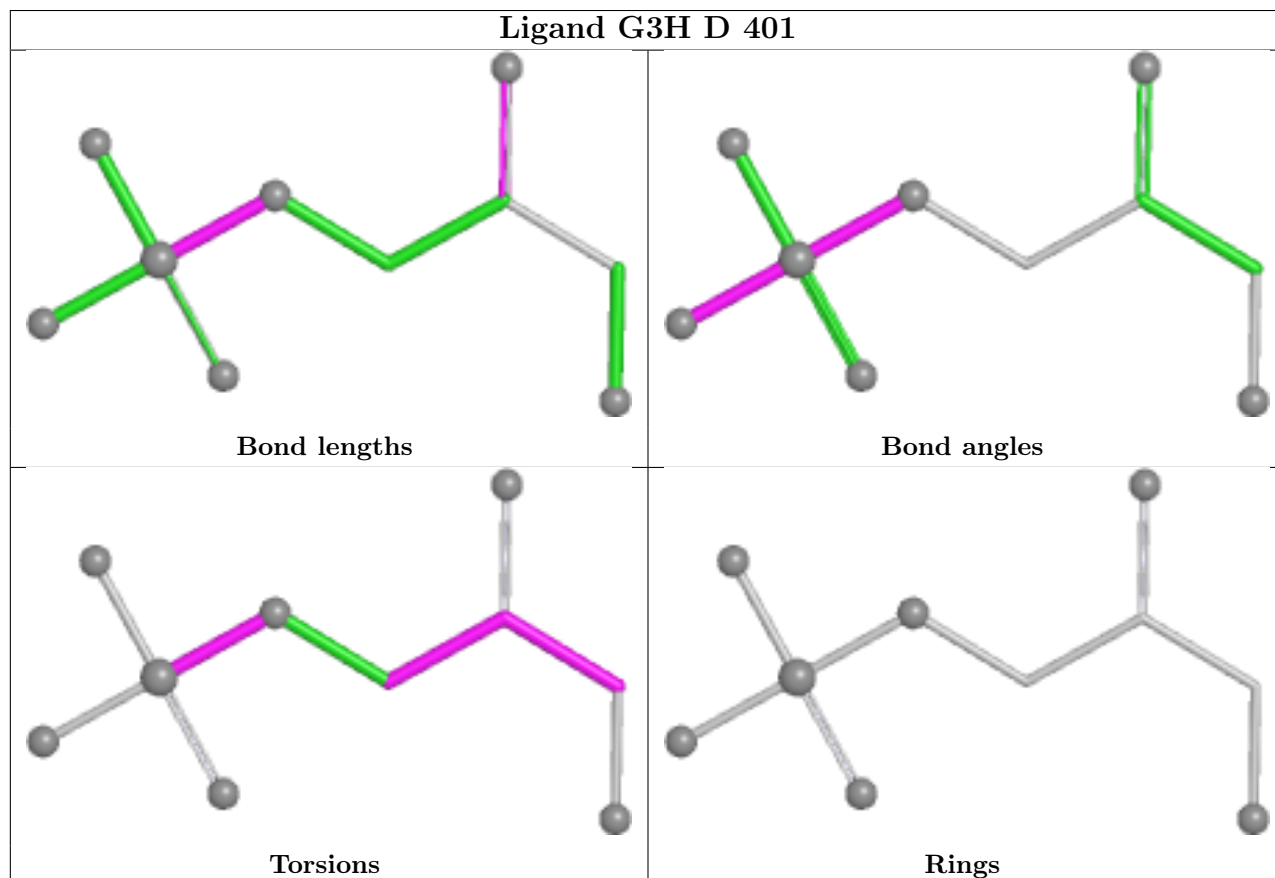
There are no ring outliers.

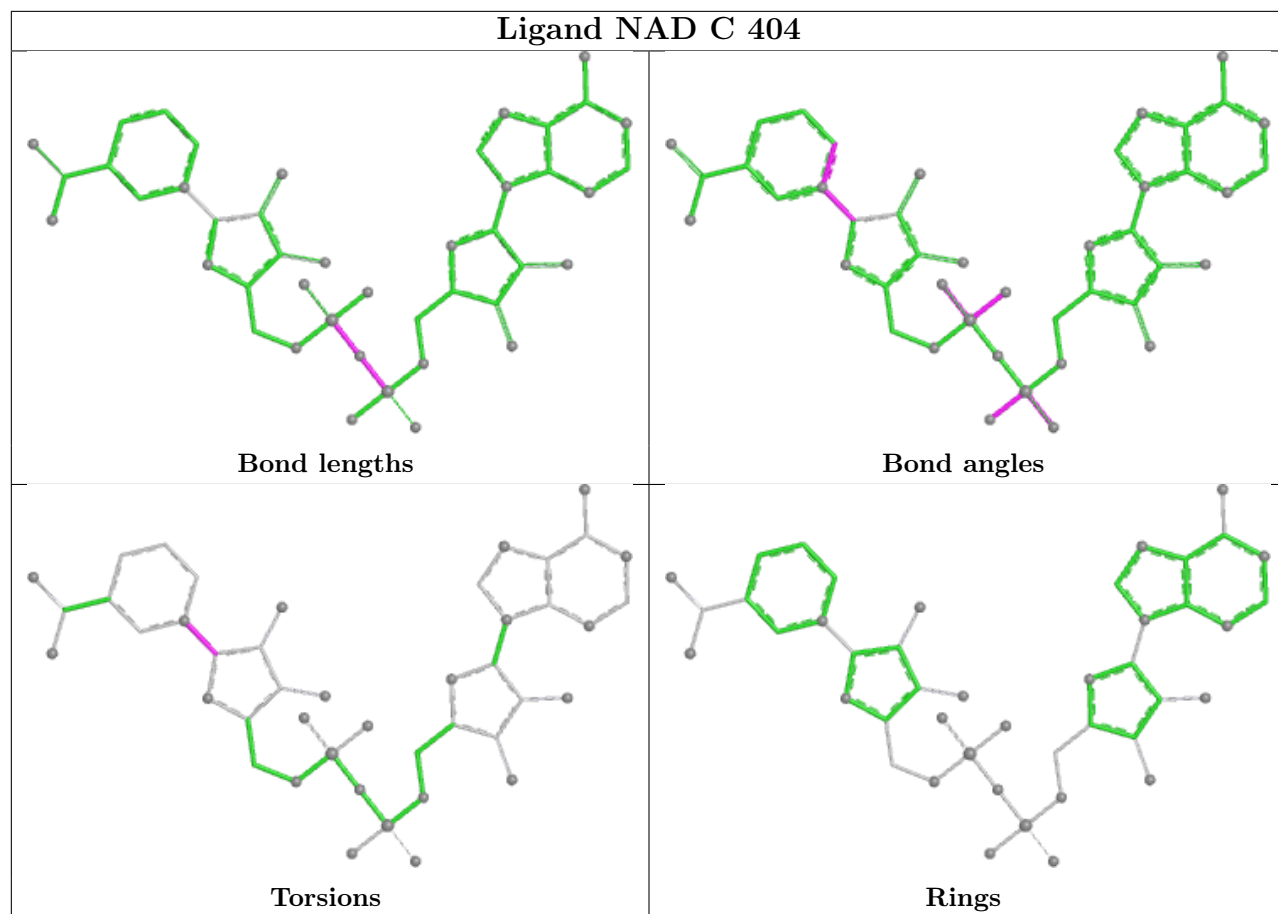
8 monomers are involved in 7 short contacts:

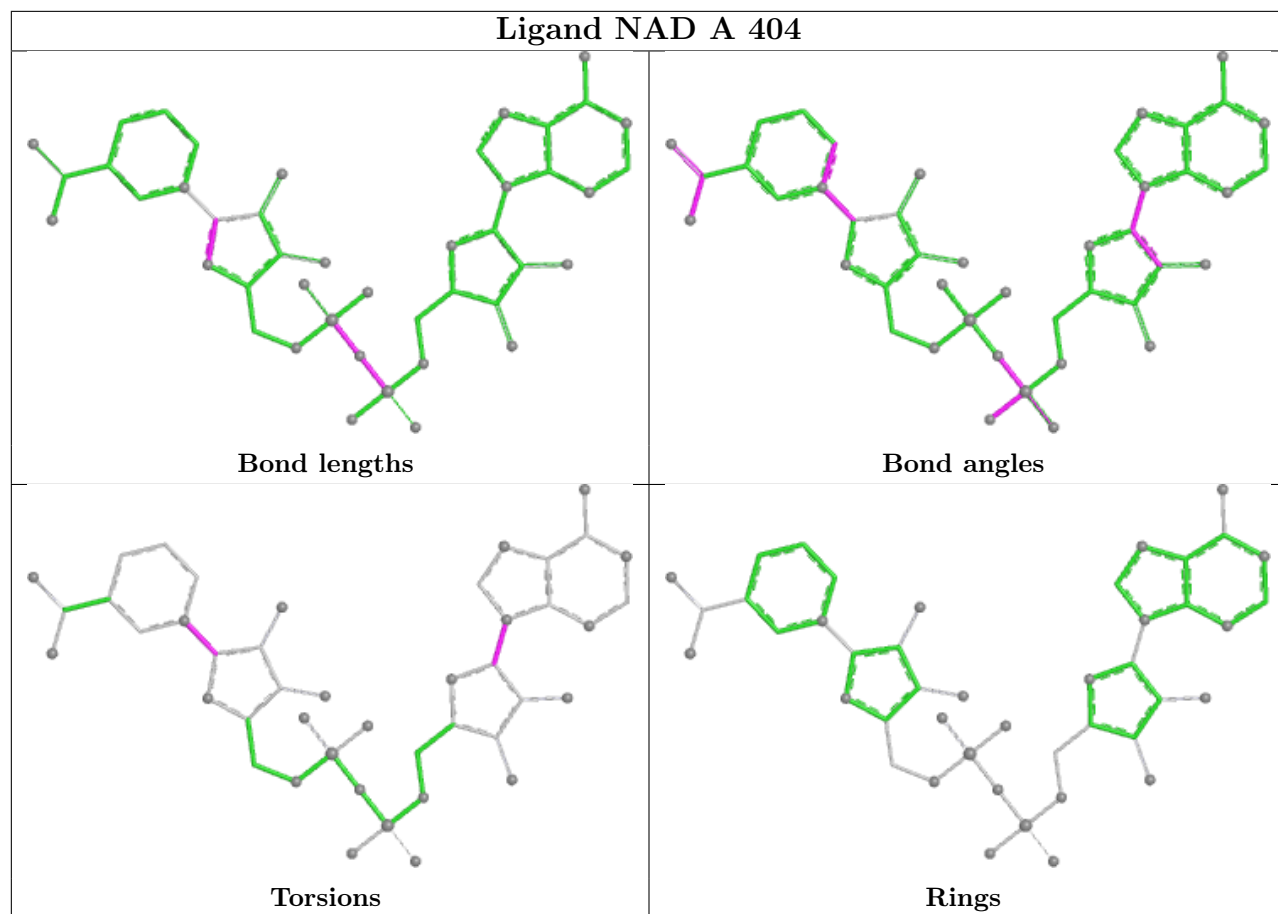
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	NAD	1	0
2	G	401	G3H	1	0
3	A	402	PEG	1	0
4	B	403	NAD	1	0
2	B	401	G3H	1	0
3	D	402	PEG	2	0
2	A	401	G3H	1	0
6	B	405	PGE	1	0

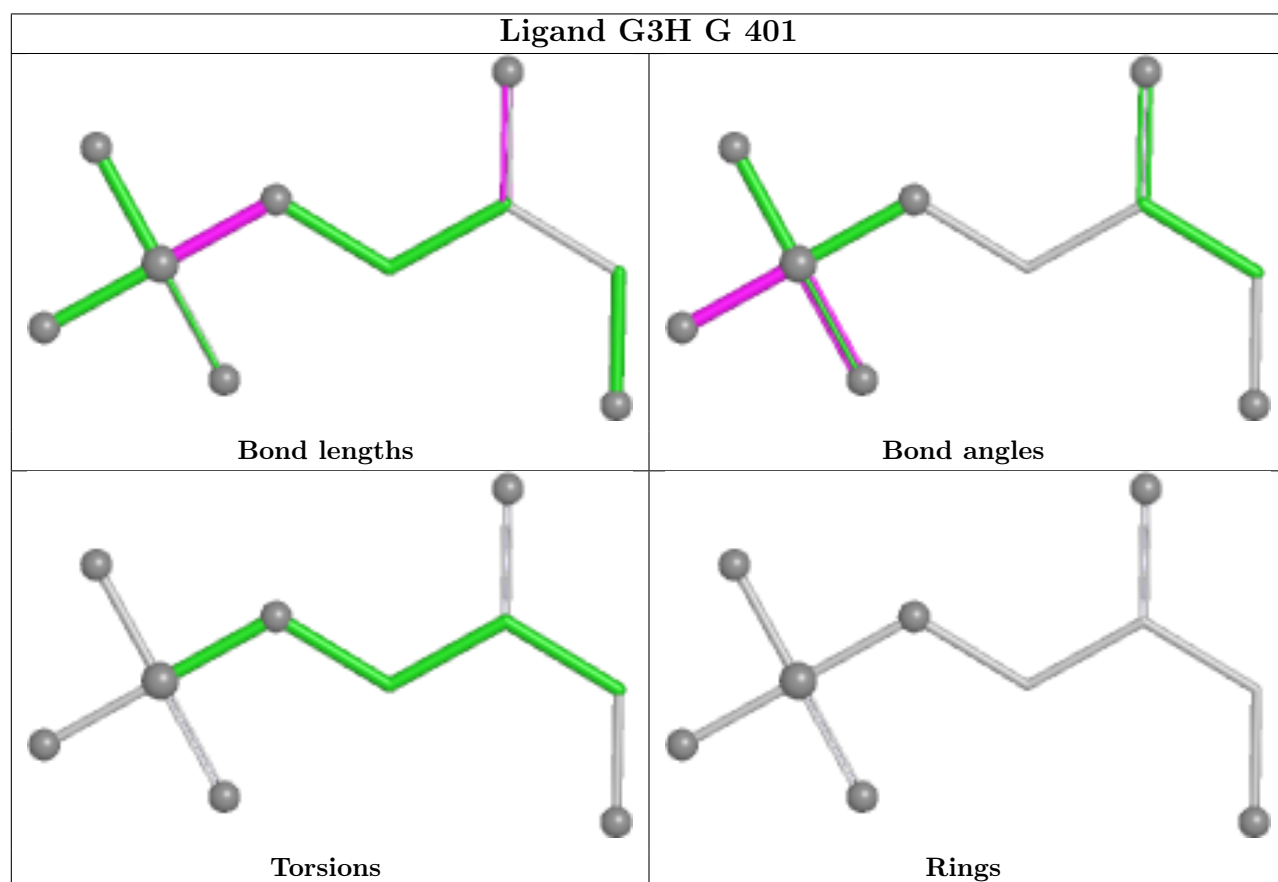
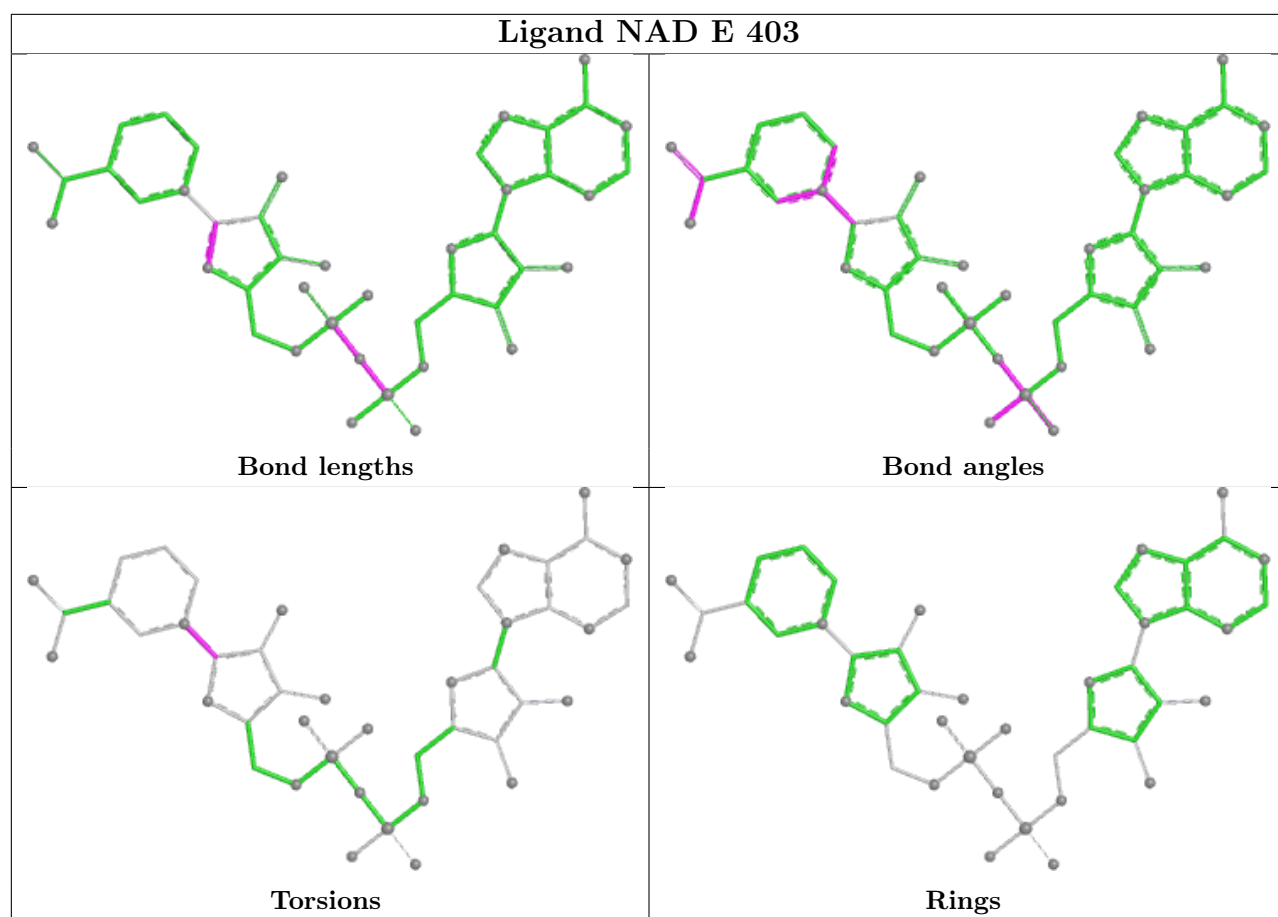
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

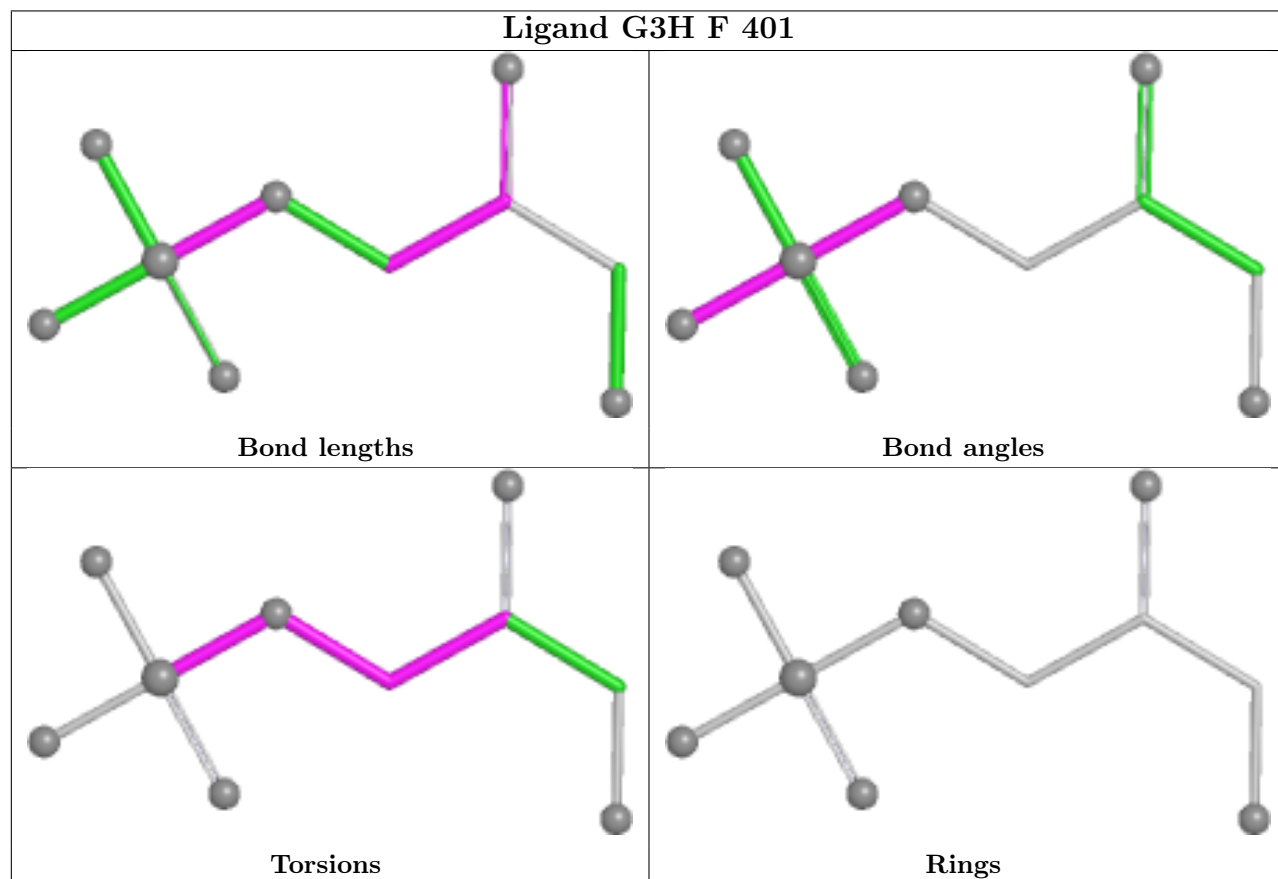
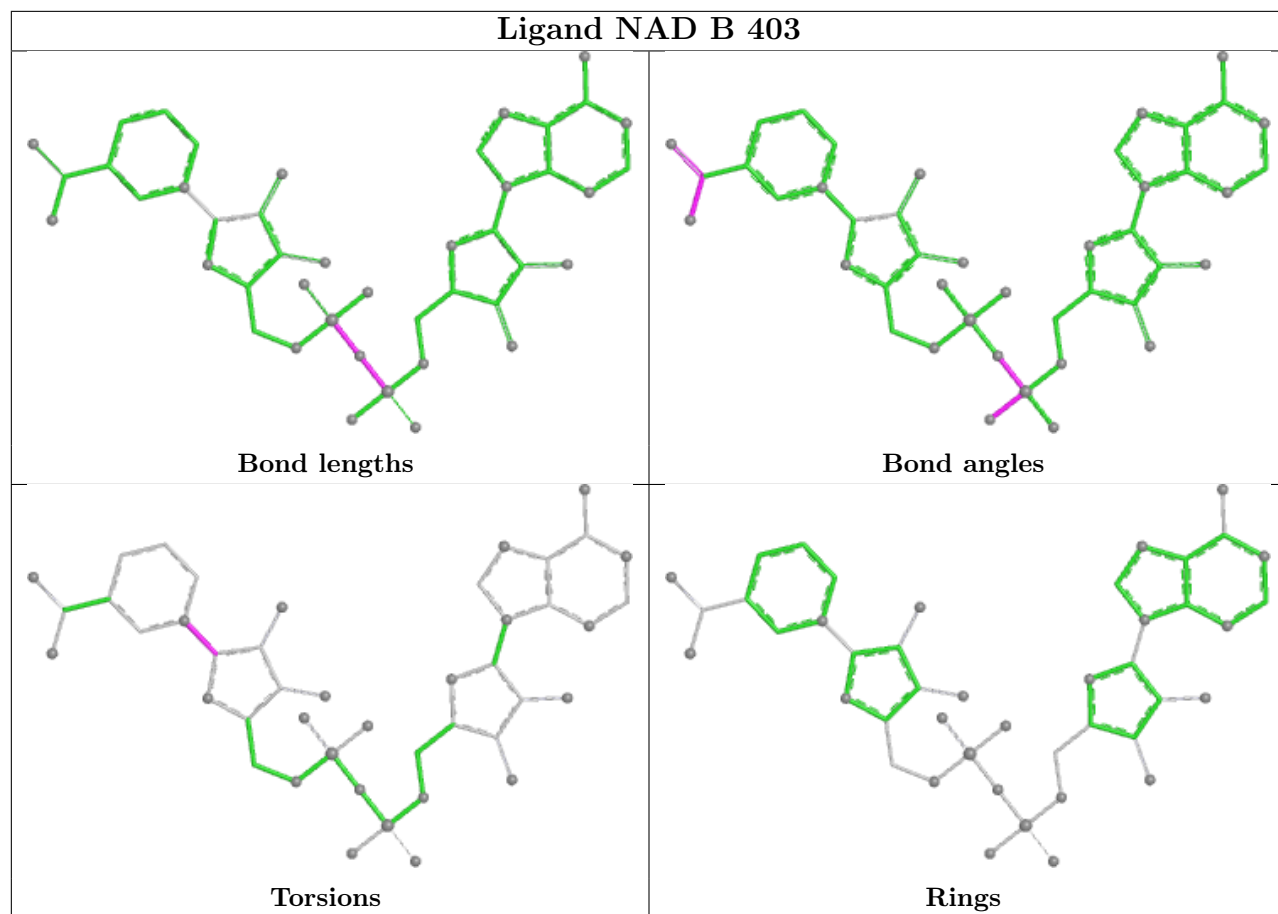
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

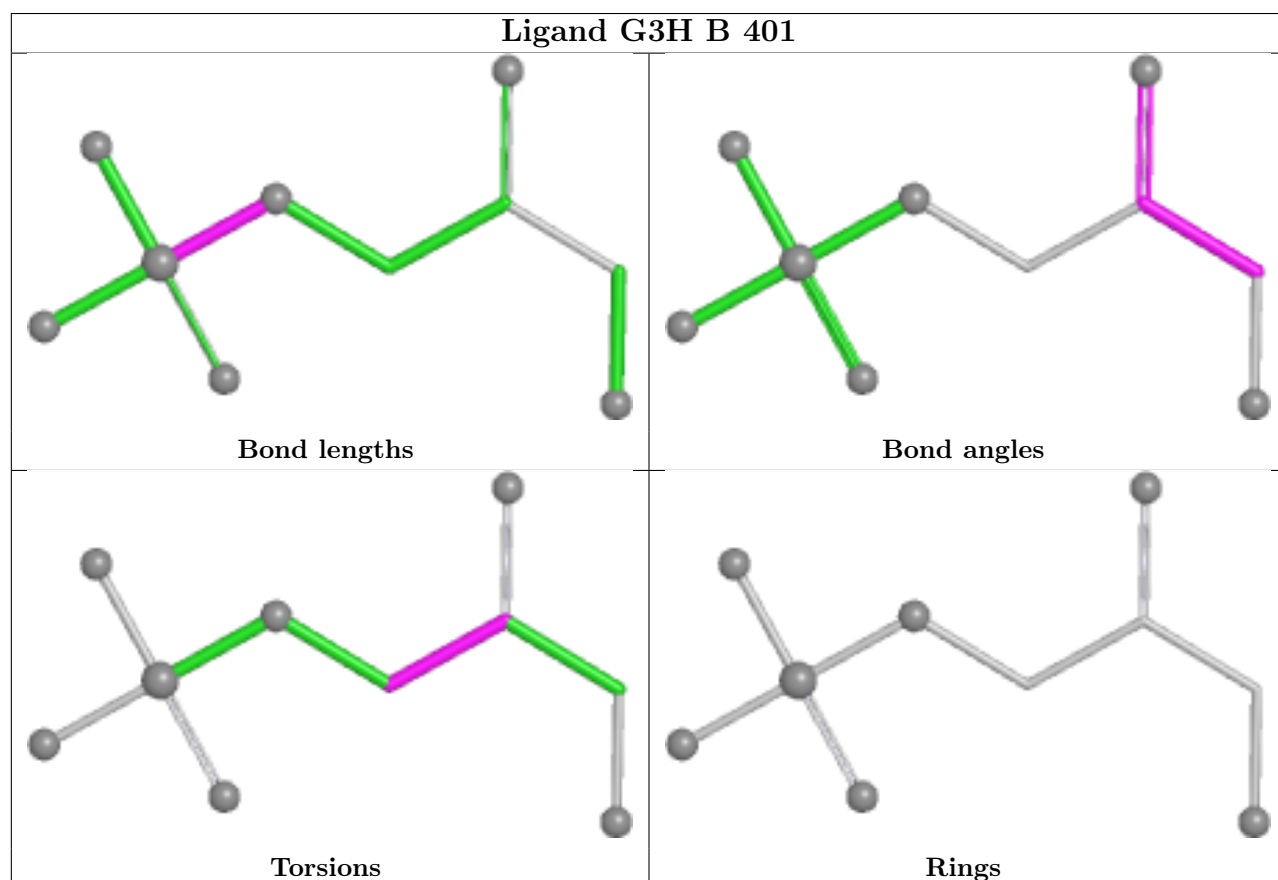
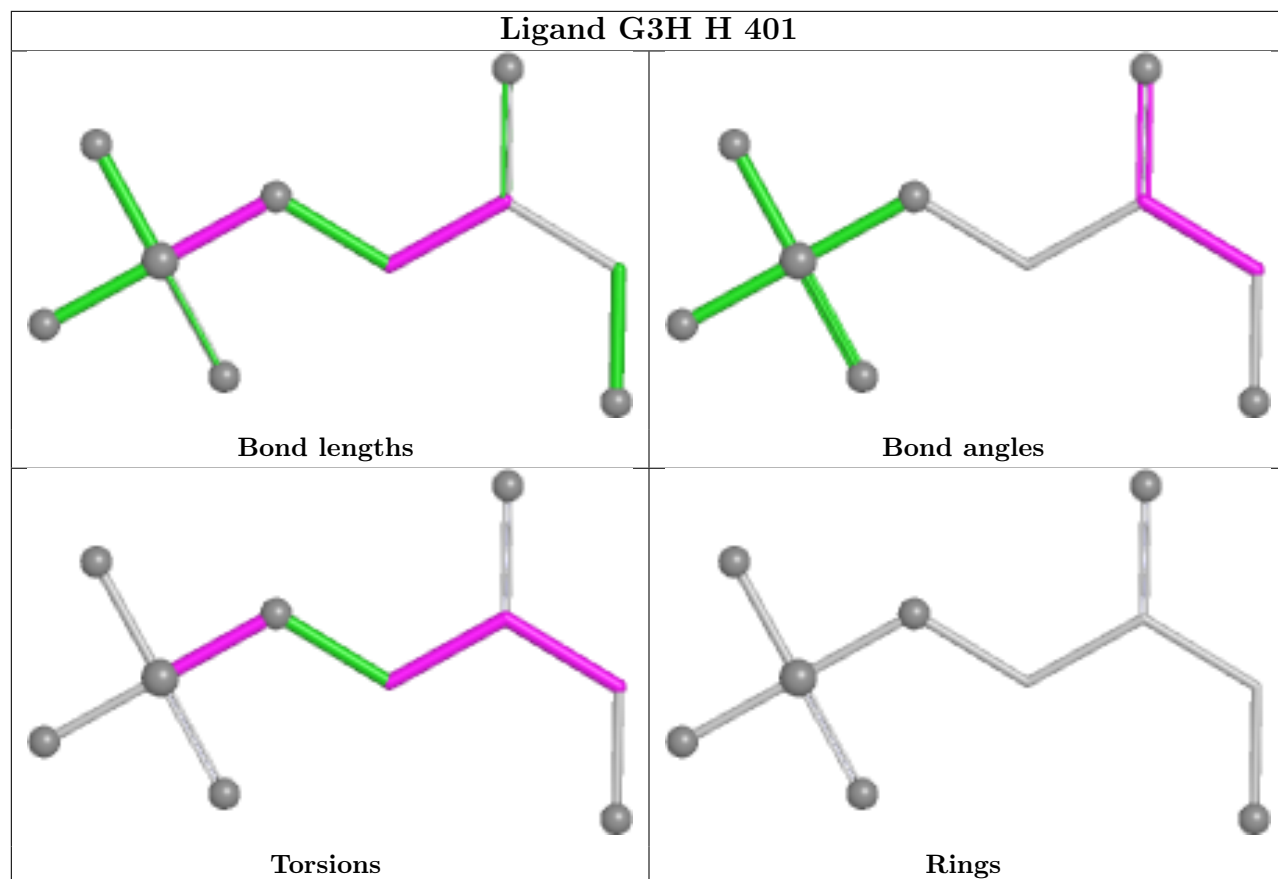


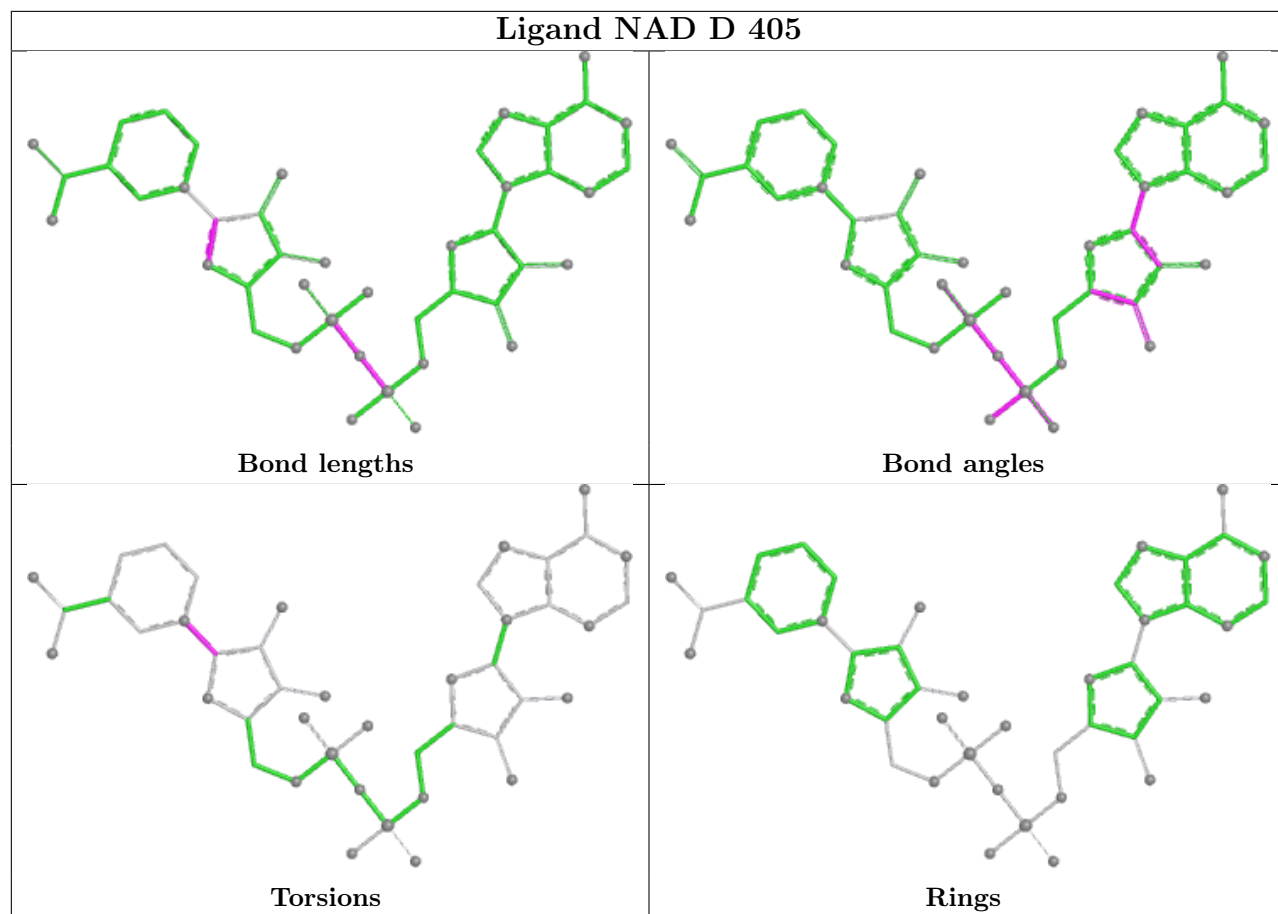


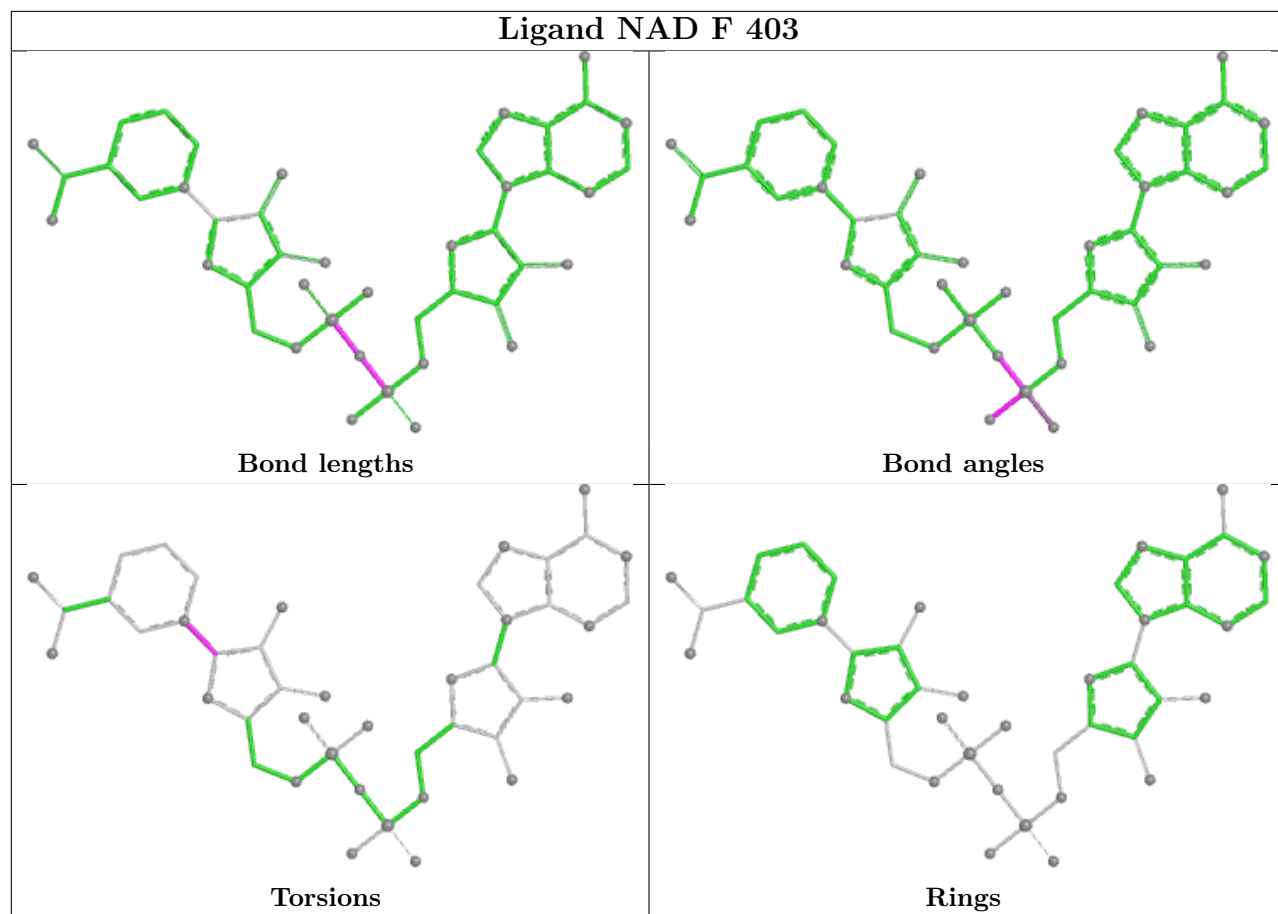


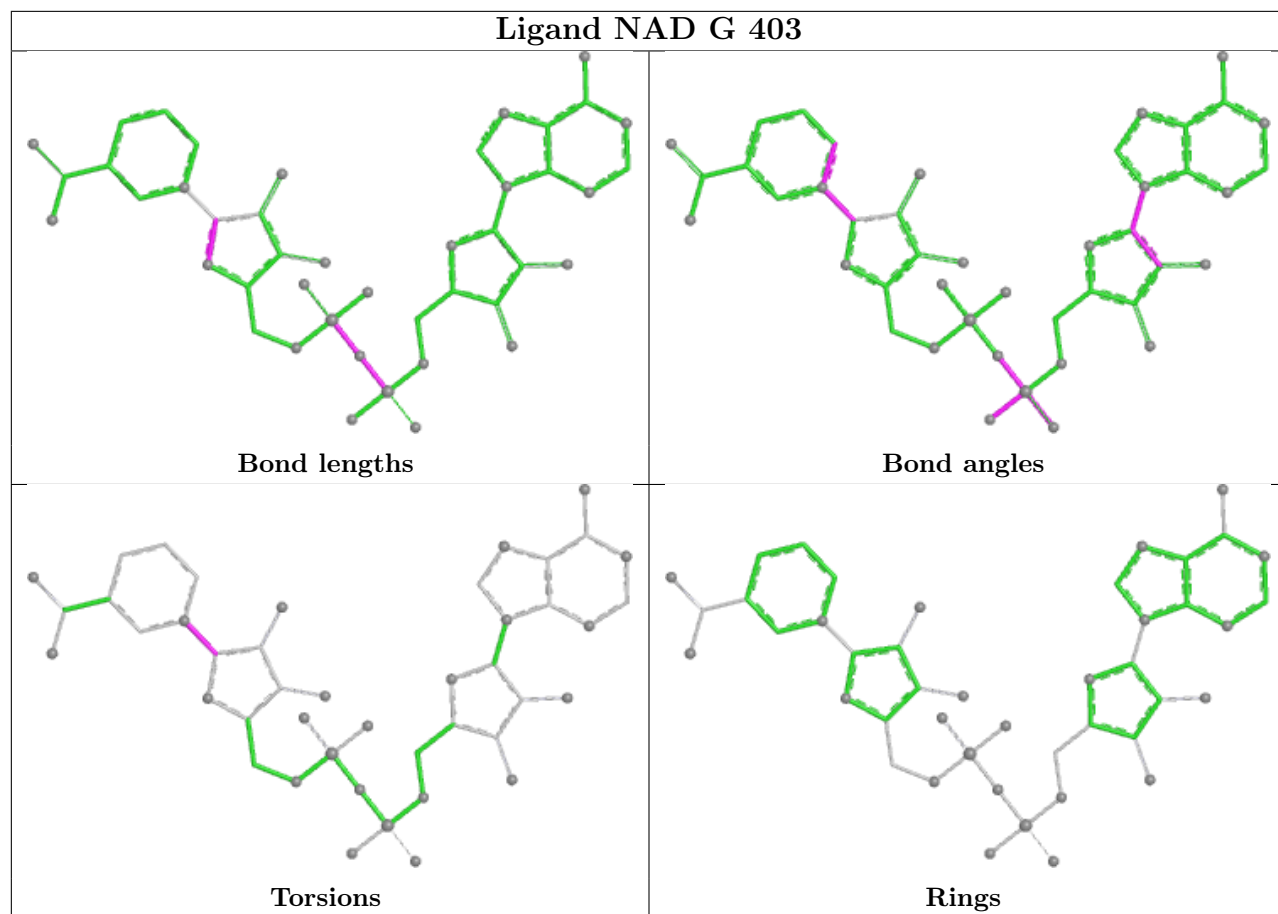


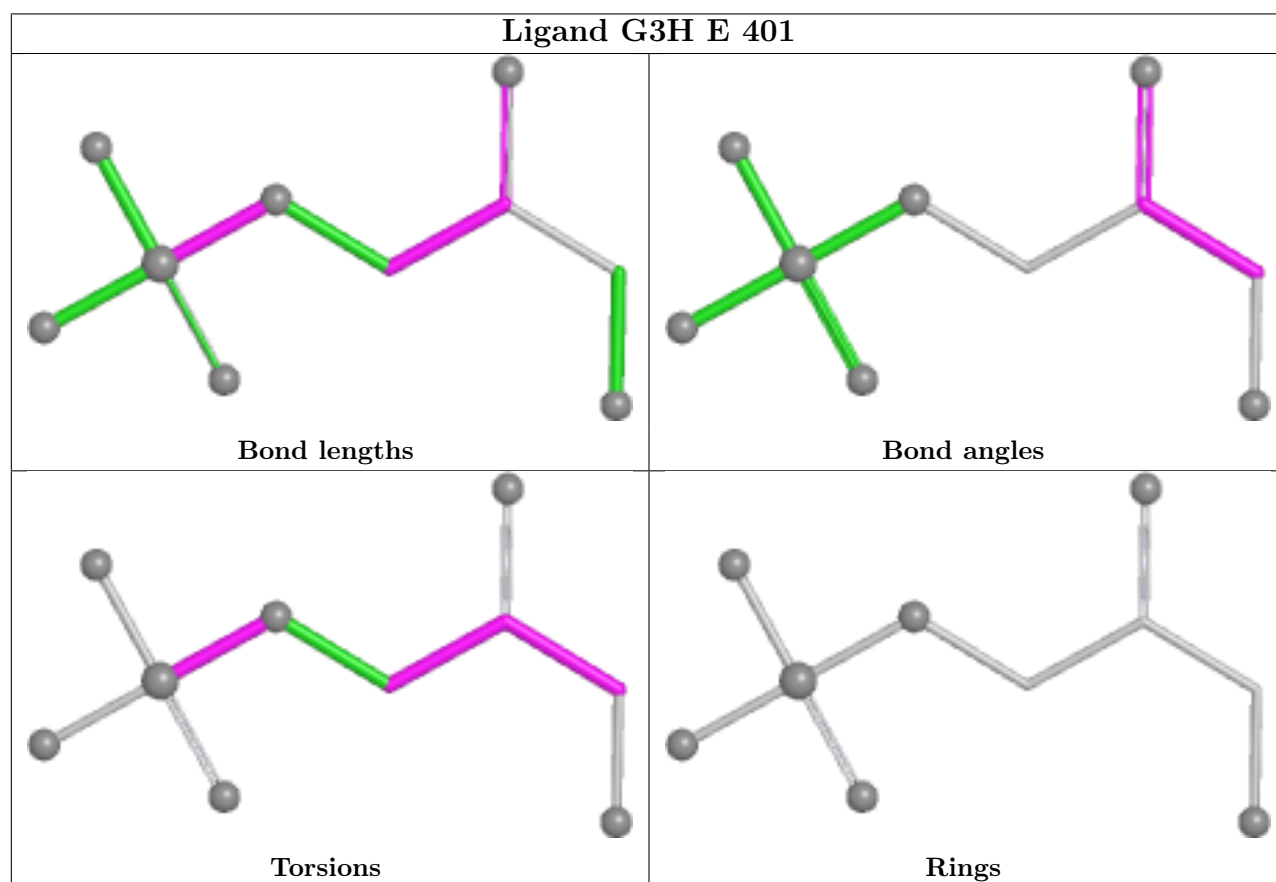
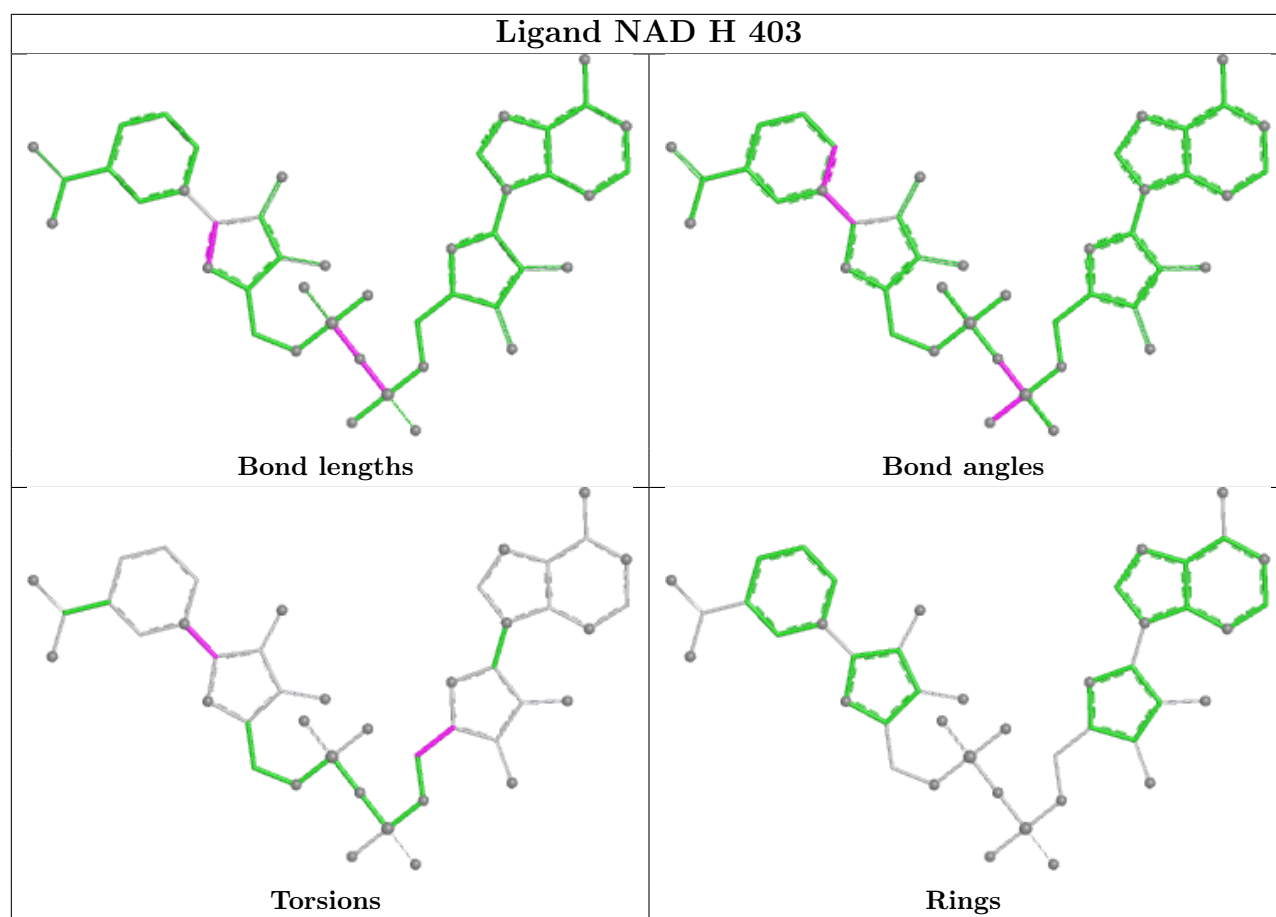


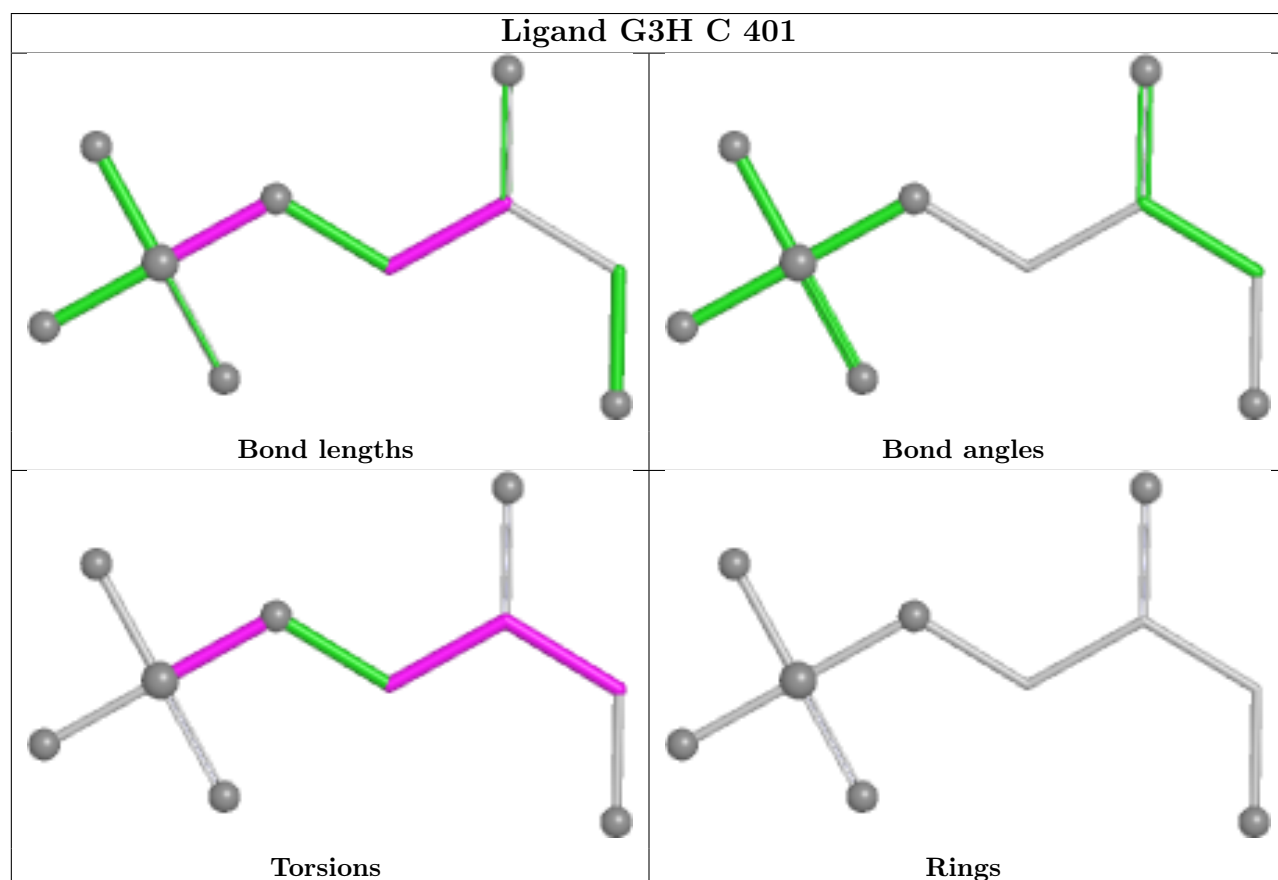
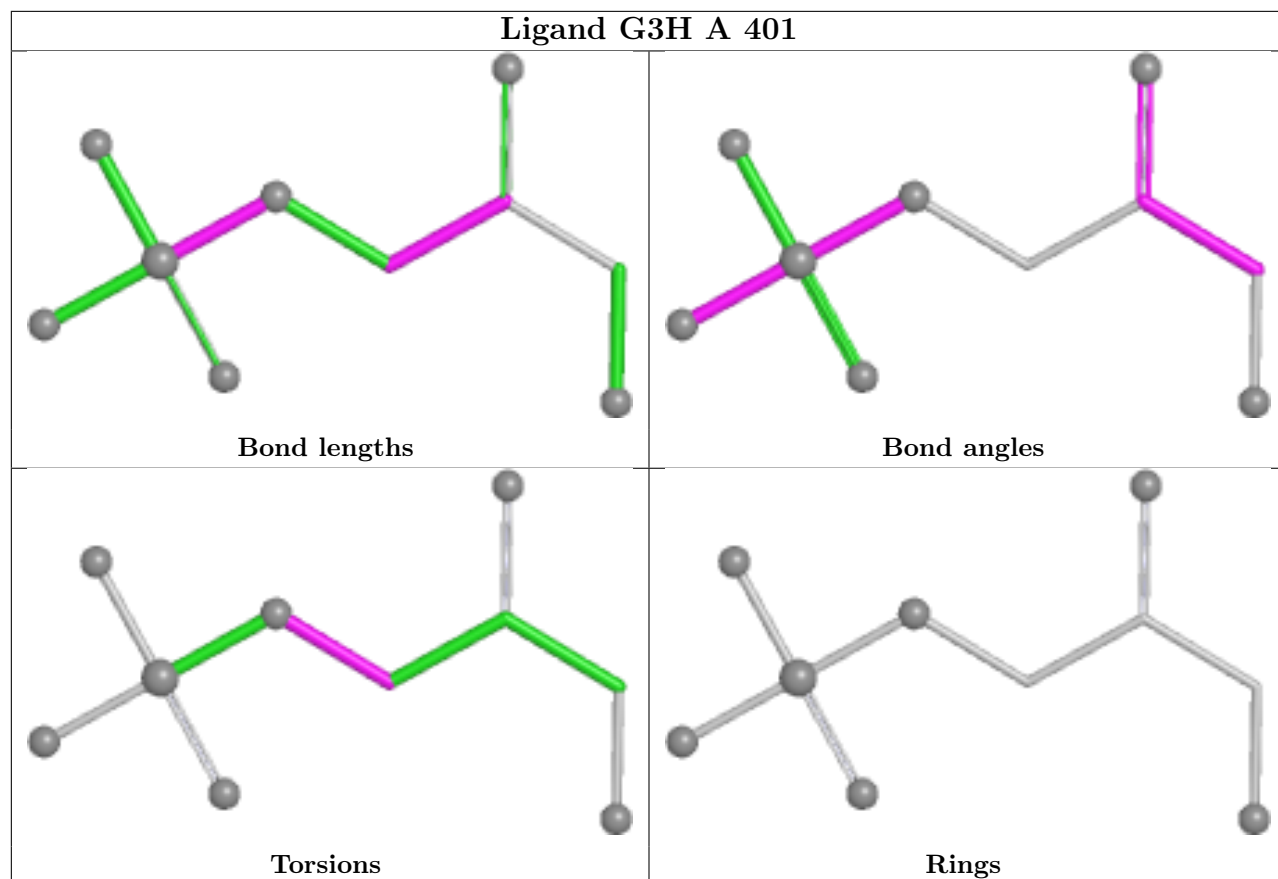












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/342 (97%)	-0.20	7 (2%) 63 70	12, 23, 46, 66	2 (0%)
1	B	334/342 (97%)	-0.25	5 (1%) 72 79	13, 22, 42, 69	3 (0%)
1	C	334/342 (97%)	-0.21	5 (1%) 72 79	13, 24, 42, 72	1 (0%)
1	D	333/342 (97%)	-0.28	2 (0%) 85 89	14, 23, 42, 69	2 (0%)
1	E	334/342 (97%)	-0.09	8 (2%) 59 66	15, 25, 51, 77	1 (0%)
1	F	332/342 (97%)	-0.15	1 (0%) 90 93	15, 27, 49, 63	1 (0%)
1	G	334/342 (97%)	-0.24	3 (0%) 81 86	13, 23, 42, 71	2 (0%)
1	H	333/342 (97%)	-0.19	4 (1%) 76 82	13, 23, 43, 73	1 (0%)
All	All	2667/2736 (97%)	-0.20	35 (1%) 75 82	12, 24, 45, 77	13 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	334	ILE	4.7
1	E	1	MET	4.1
1	A	332	GLY	3.5
1	C	125	ASN	3.4
1	E	3	ILE	3.3

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.

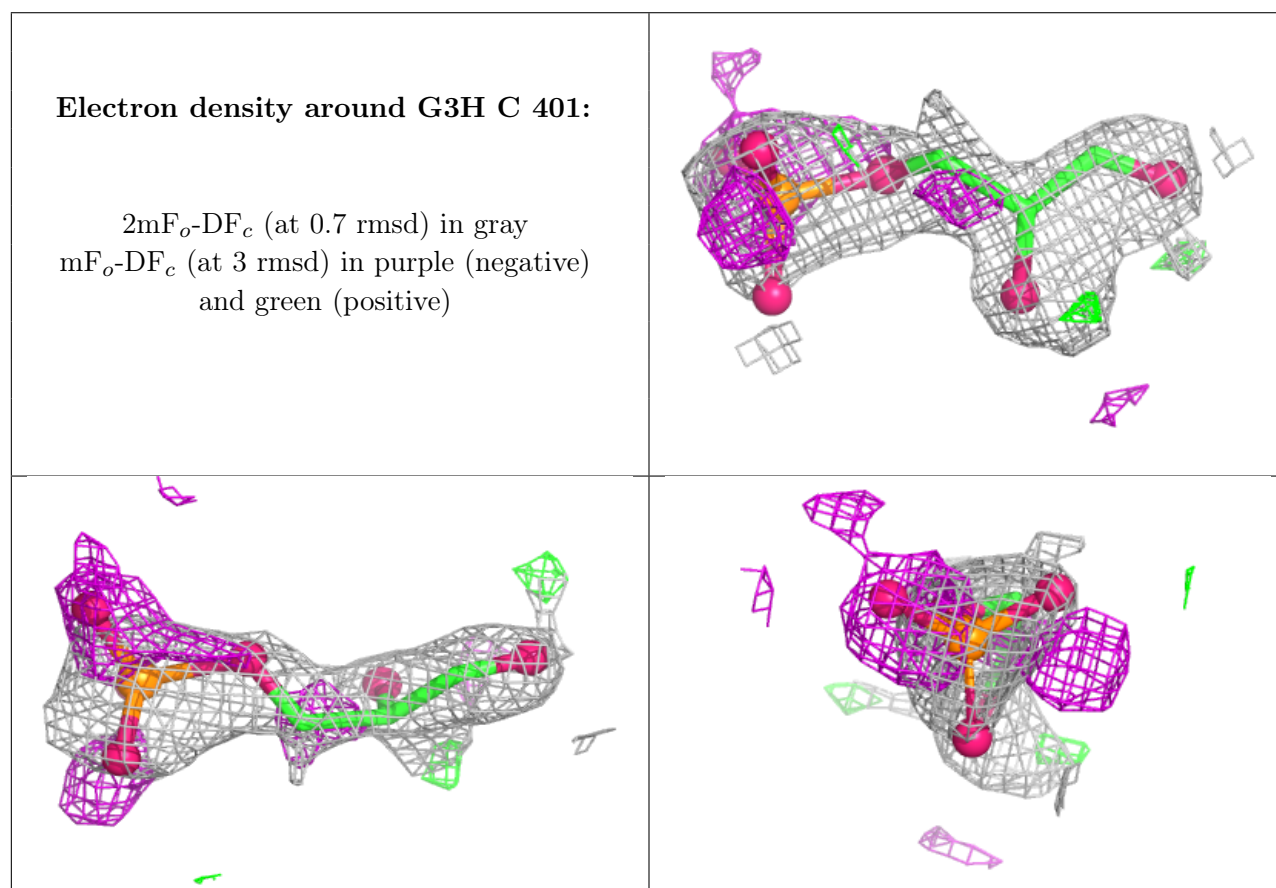
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	C	403	6/6	0.75	0.13	38,46,54,54	0
2	G3H	C	401	10/10	0.76	0.12	40,47,62,68	0
2	G3H	B	401	10/10	0.76	0.13	30,44,51,56	0
3	PEG	B	402	7/7	0.77	0.14	40,42,51,53	0
2	G3H	F	401	10/10	0.77	0.13	41,50,58,61	0
2	G3H	E	401	10/10	0.78	0.12	39,45,56,61	0
2	G3H	H	401	10/10	0.79	0.12	39,48,51,59	0
3	PEG	A	402	7/7	0.79	0.14	33,44,50,53	0
8	GOL	D	403	6/6	0.79	0.14	38,44,52,53	0
9	EPE	D	404	15/15	0.79	0.15	37,48,56,59	0
9	EPE	H	402	15/15	0.79	0.14	37,49,65,71	0
3	PEG	G	402	7/7	0.80	0.14	36,42,55,55	0
3	PEG	C	402	7/7	0.82	0.15	40,45,50,57	0
2	G3H	G	401	10/10	0.82	0.11	40,48,55,58	0
3	PEG	A	403	7/7	0.83	0.12	43,47,55,57	0
3	PEG	E	402	7/7	0.84	0.11	35,42,49,52	0
2	G3H	A	401	10/10	0.84	0.11	36,49,58,59	0
2	G3H	D	401	10/10	0.84	0.10	36,44,49,52	0
3	PEG	D	402	7/7	0.85	0.12	36,39,42,42	0
5	NA	F	404	1/1	0.88	0.08	40,40,40,40	0
6	PGE	B	405	10/10	0.88	0.12	32,38,46,52	0
3	PEG	F	402	7/7	0.91	0.09	34,41,46,46	0
7	CL	B	406	1/1	0.94	0.07	52,52,52,52	0
5	NA	D	406	1/1	0.95	0.06	32,32,32,32	0
5	NA	E	404	1/1	0.95	0.11	38,38,38,38	0
5	NA	A	405	1/1	0.95	0.11	35,35,35,35	0
5	NA	H	404	1/1	0.96	0.07	33,33,33,33	0
5	NA	G	404	1/1	0.97	0.05	29,29,29,29	0
4	NAD	C	404	44/44	0.98	0.05	14,19,25,27	0
4	NAD	D	405	44/44	0.98	0.05	13,18,21,24	0
4	NAD	E	403	44/44	0.98	0.04	15,20,24,24	0
4	NAD	F	403	44/44	0.98	0.05	18,22,29,30	0
4	NAD	G	403	44/44	0.98	0.04	14,19,22,24	0
4	NAD	H	403	44/44	0.98	0.05	17,21,26,28	0
4	NAD	A	404	44/44	0.98	0.04	15,20,25,29	0
5	NA	B	404	1/1	0.98	0.04	25,25,25,25	0
5	NA	C	405	1/1	0.98	0.03	29,29,29,29	0

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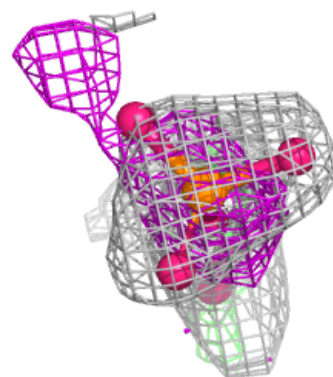
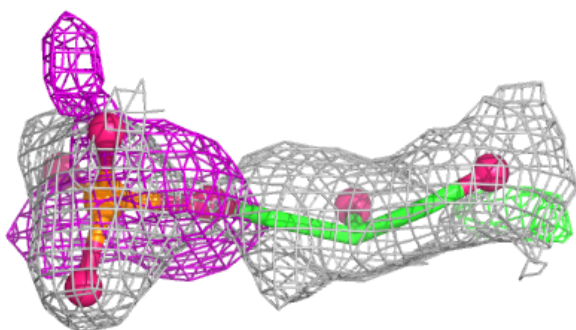
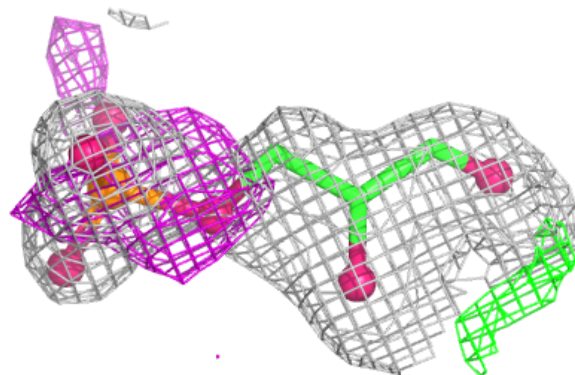
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAD	B	403	44/44	0.98	0.04	15,19,23,25	0

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.

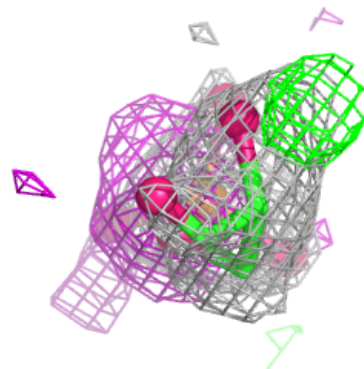
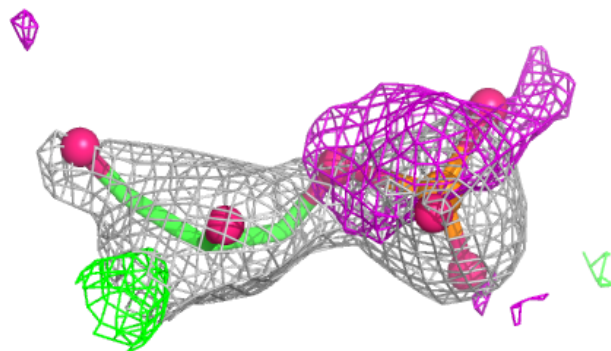
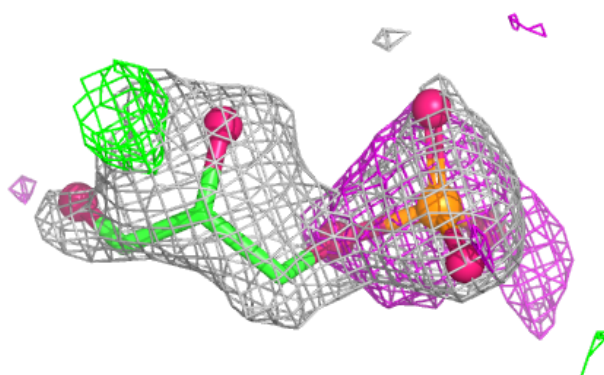


Electron density around G3H B 401:

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

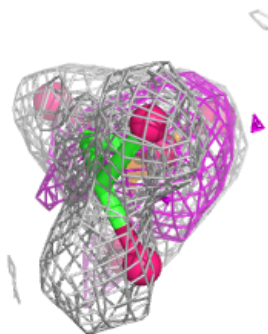
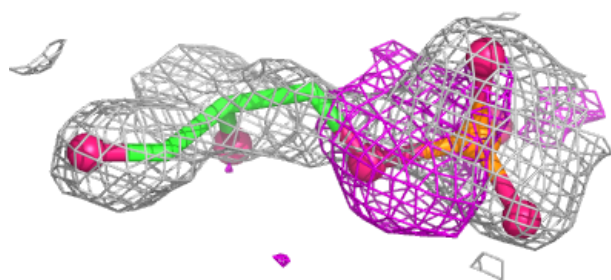
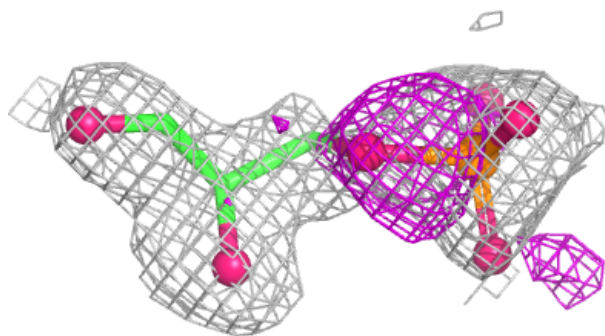
**Electron density around G3H F 401:**

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

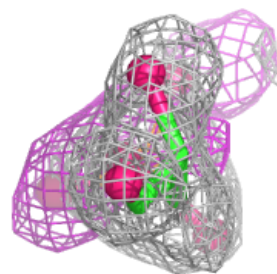
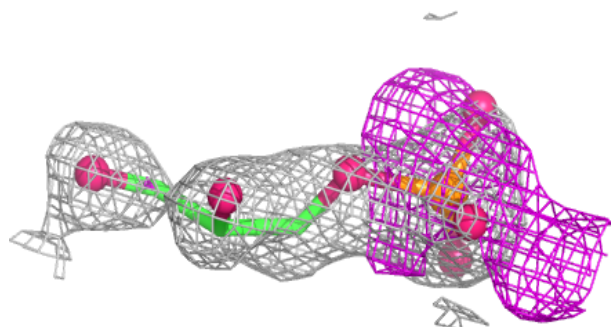
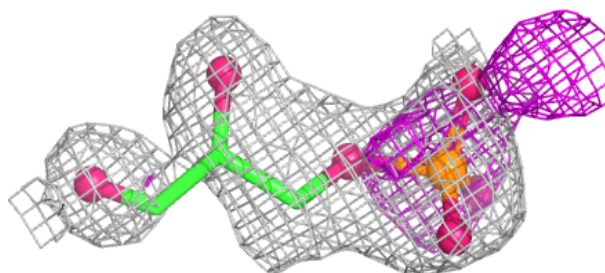


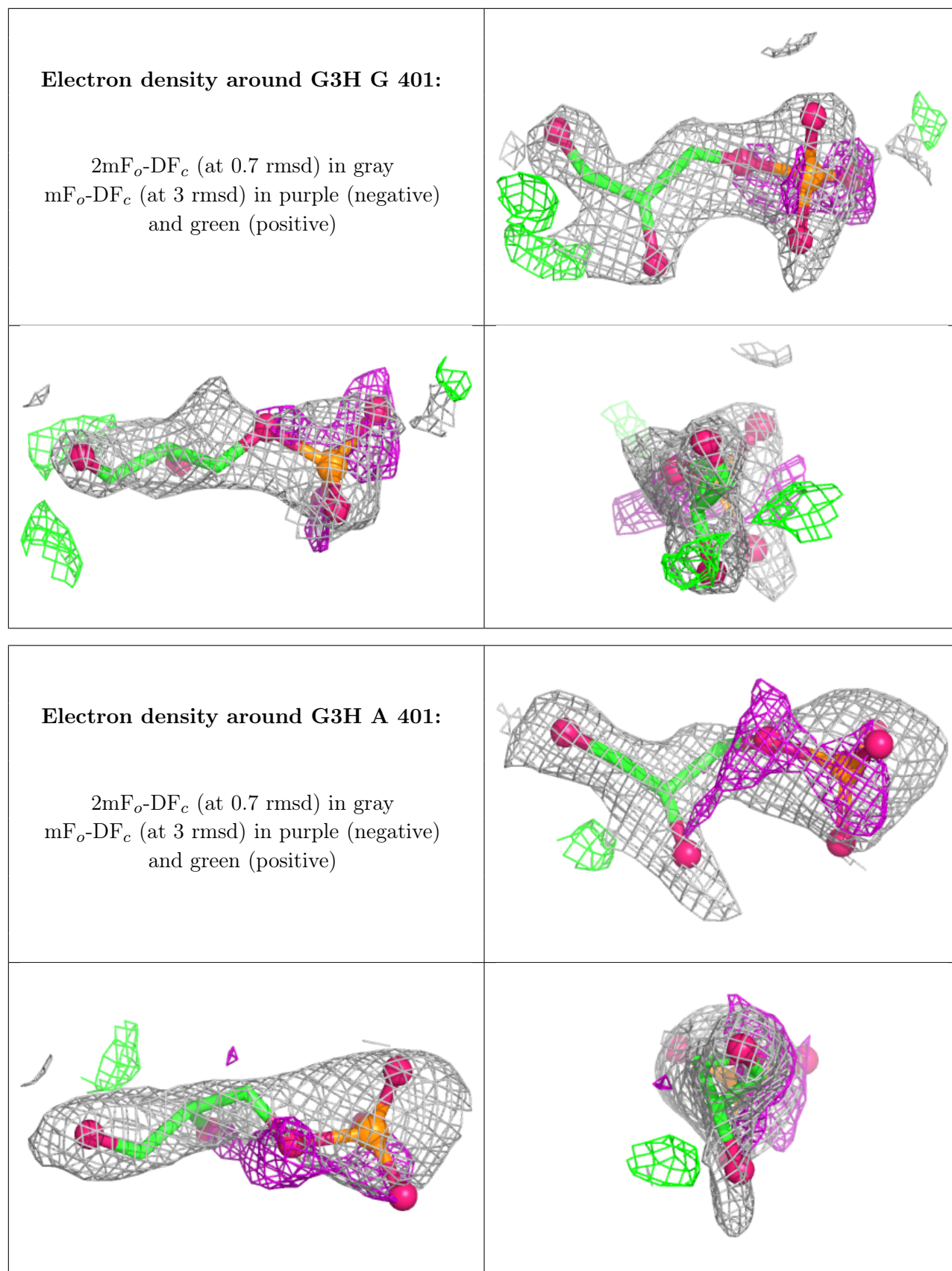
Electron density around G3H E 401:

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

**Electron density around G3H H 401:**

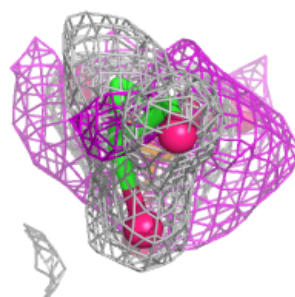
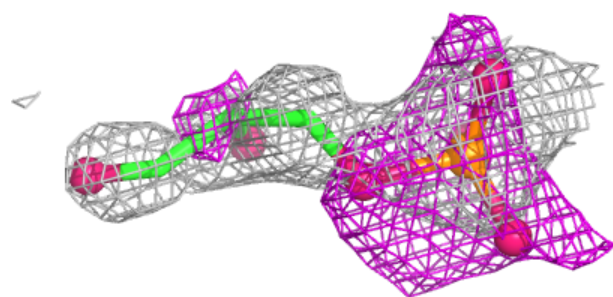
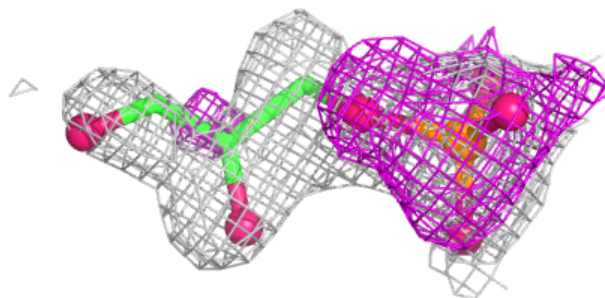
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



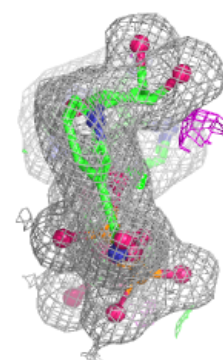
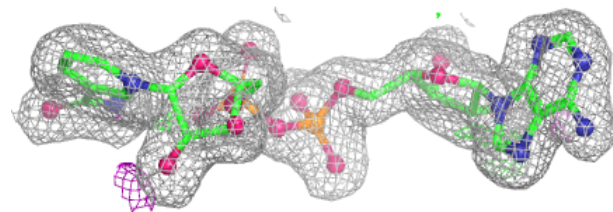
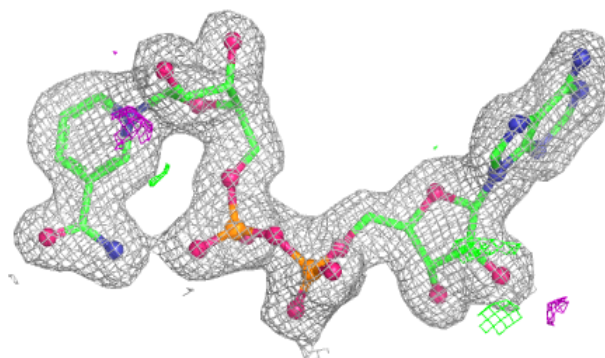


Electron density around G3H D 401:

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

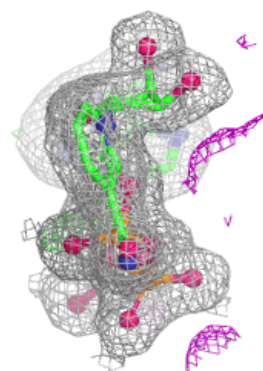
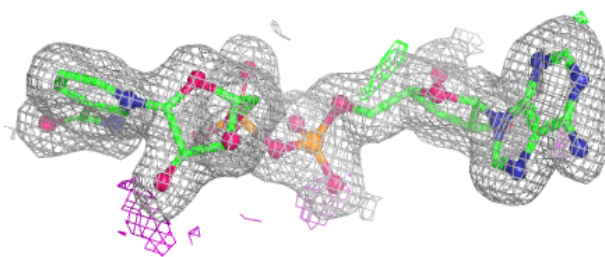
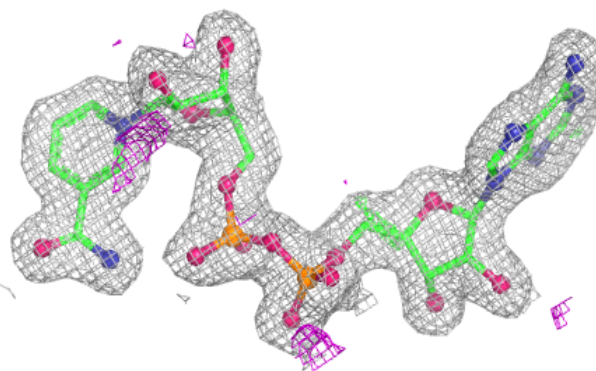
**Electron density around NAD C 404:**

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

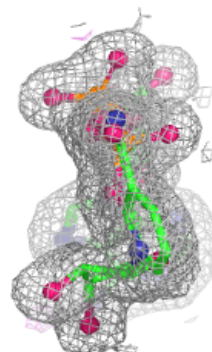
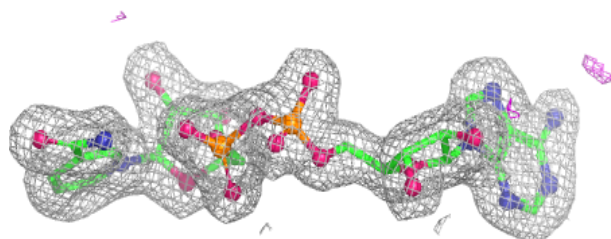
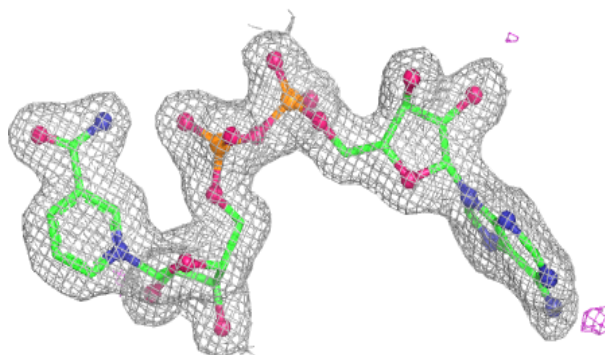


Electron density around NAD D 405:

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

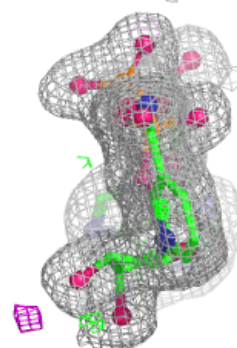
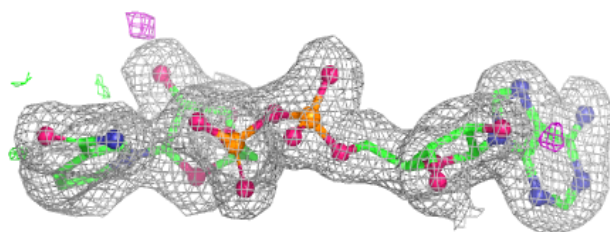
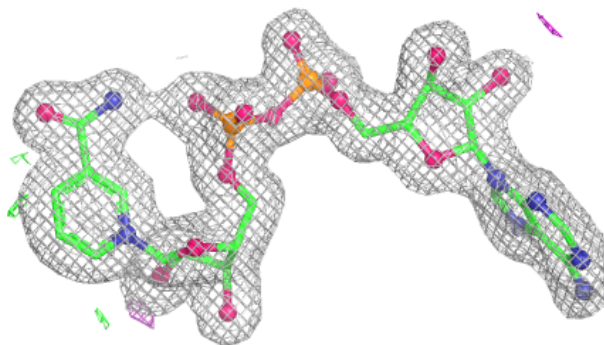
**Electron density around NAD E 403:**

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

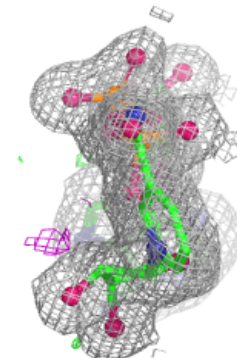
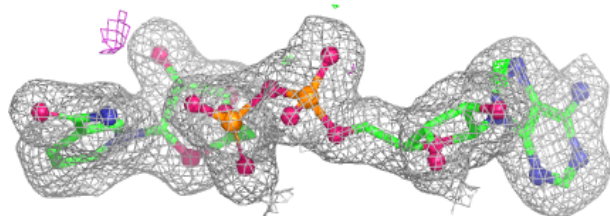
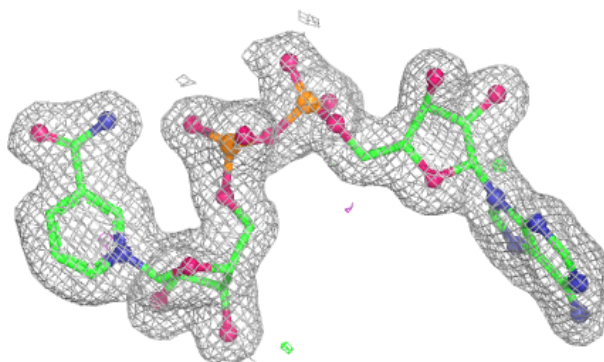


Electron density around NAD F 403:

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

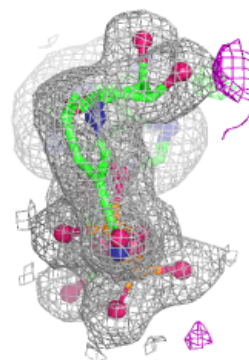
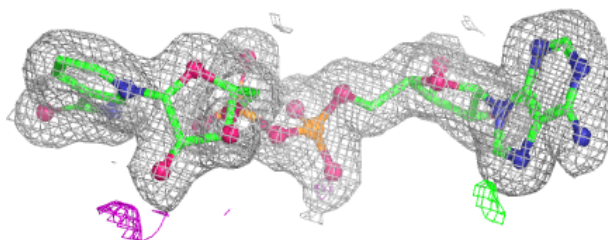
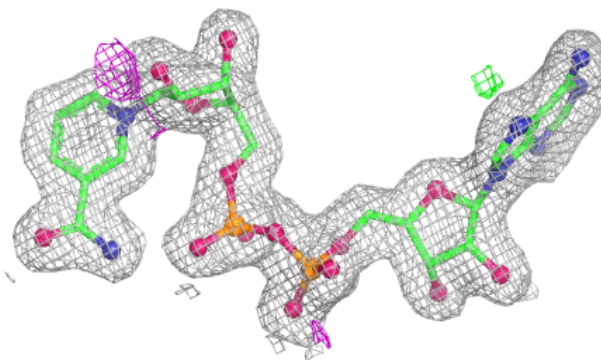
**Electron density around NAD G 403:**

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

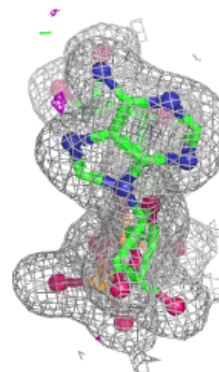
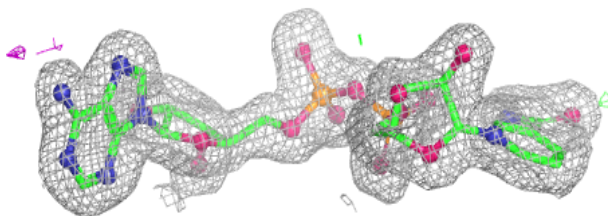
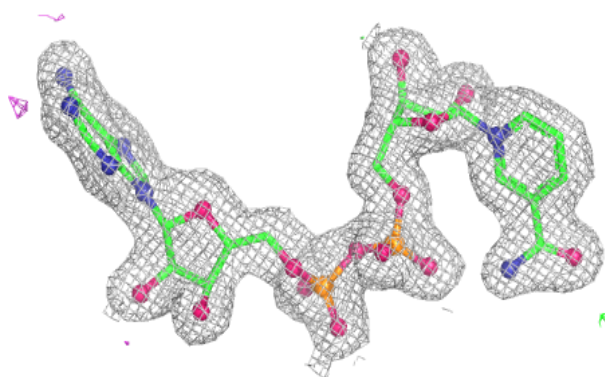


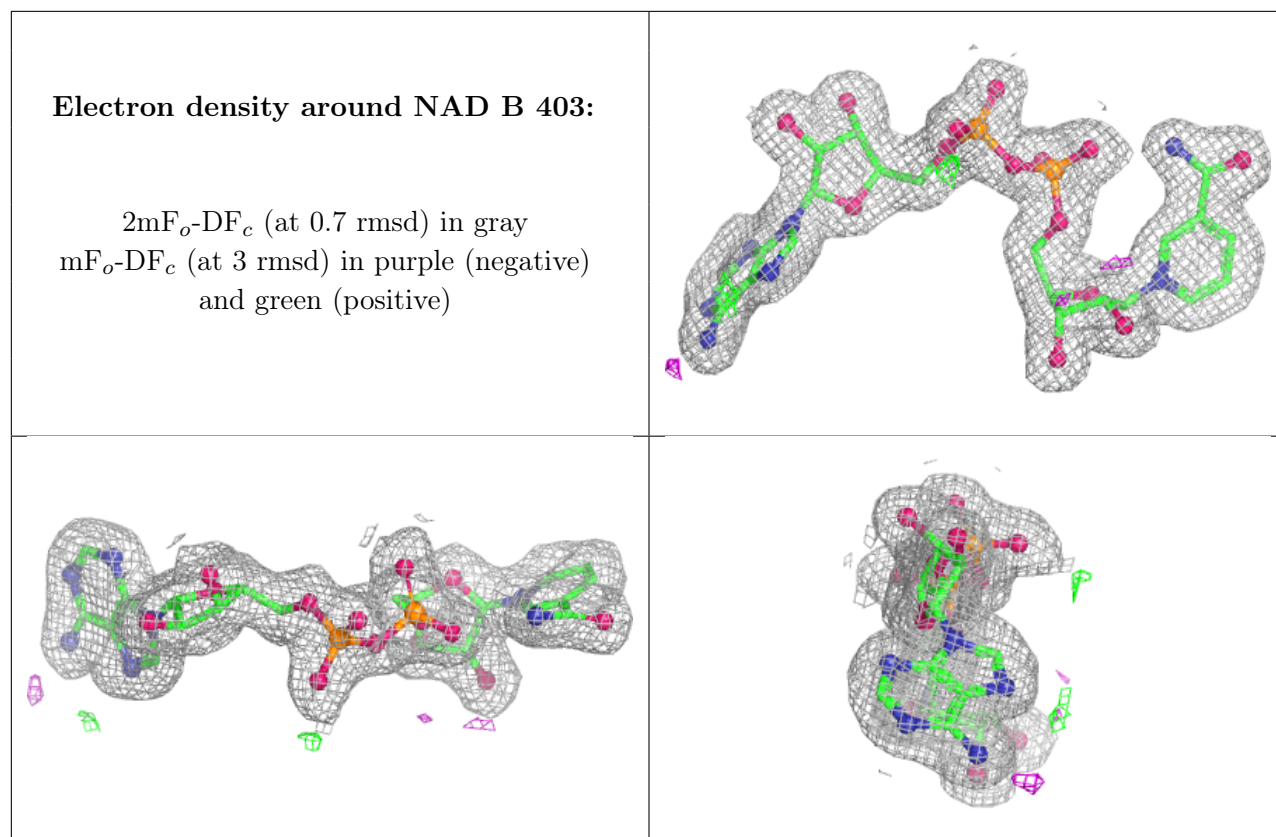
Electron density around NAD H 403:

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

**Electron density around NAD A 404:**

$2mF_o-DF_c$ (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.