



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2025 – 12:27 PM EST

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 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](#) ①) were used in the production of this report:

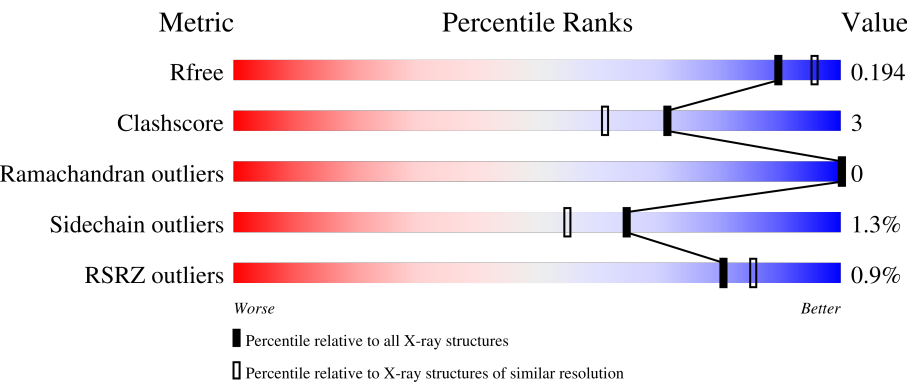
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance i

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}	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (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	<div><div>2%</div><div><div></div><div>90%</div><div>7%</div><div></div></div><div>...</div></div>
1	B	342	<div><div>%</div><div><div></div><div>90%</div><div>7%</div><div></div></div><div>.</div></div>
1	C	342	<div><div>%</div><div><div></div><div>92%</div><div>6%</div><div></div></div><div>.</div></div>
1	D	342	<div><div></div><div><div></div><div>89%</div><div>8%</div><div></div></div><div>.</div></div>
1	E	342	<div><div>2%</div><div><div></div><div>89%</div><div>8%</div><div></div></div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	F	342	<div><div></div><div>90%</div><div>7% •</div></div>
1	G	342	<div>%<div><div></div><div>92%</div><div>6% •</div></div></div>
1	H	342	<div><div></div><div>91%</div><div>7% •</div></div>

2 Entry composition

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
1	A	333	Total	C	N	O	S	0	2	0
			2506	1572	435	488	11			
1	B	334	Total	C	N	O	S	0	3	0
			2516	1581	434	489	12			
1	C	334	Total	C	N	O	S	0	1	0
			2514	1576	436	491	11			
1	D	333	Total	C	N	O	S	0	2	0
			2510	1574	435	491	10			
1	E	334	Total	C	N	O	S	0	1	0
			2508	1573	436	489	10			
1	F	332	Total	C	N	O	S	0	1	0
			2492	1562	432	488	10			
1	G	334	Total	C	N	O	S	0	2	0
			2517	1578	436	492	11			
1	H	333	Total	C	N	O	S	0	1	0
			2499	1568	435	486	10			

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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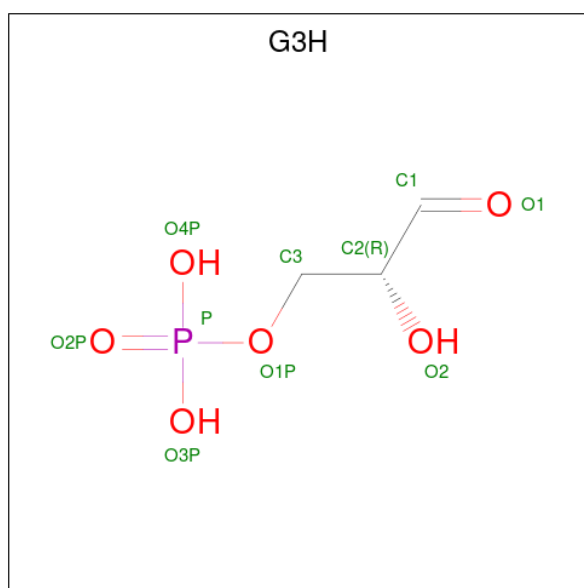
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP B4RPP8
B	-1	HIS	-	expression tag	UNP B4RPP8
B	0	HIS	-	expression tag	UNP B4RPP8
C	-7	MET	-	initiating methionine	UNP B4RPP8
C	-6	ALA	-	expression tag	UNP B4RPP8
C	-5	HIS	-	expression tag	UNP B4RPP8
C	-4	HIS	-	expression tag	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: $C_3H_7O_6P$) (labeled as "Ligand of Interest" by depositor).



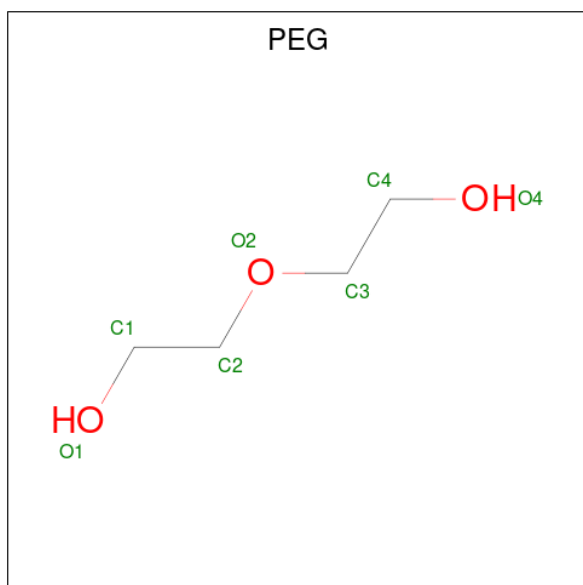
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	1	Total	C	O	P	0	0
			10	3	6	1		
2	C	1	Total	C	O	P	0	0
			10	3	6	1		
2	D	1	Total	C	O	P	0	0
			10	3	6	1		
2	E	1	Total	C	O	P	0	0
			10	3	6	1		
2	F	1	Total	C	O	P	0	0
			10	3	6	1		

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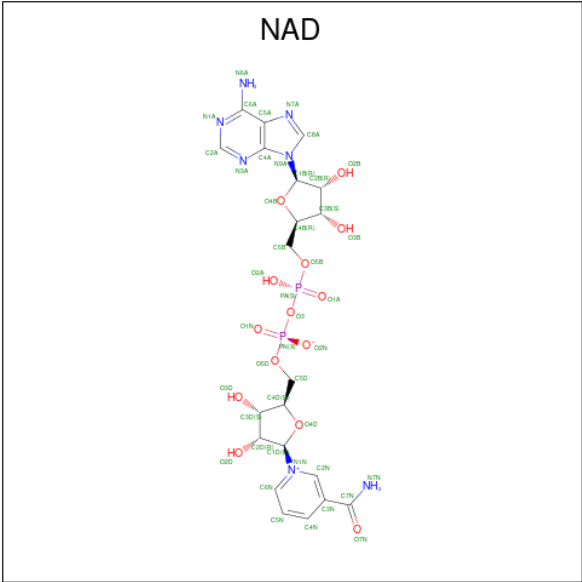
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	O	P	0	0
			10	3	6	1		
2	H	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

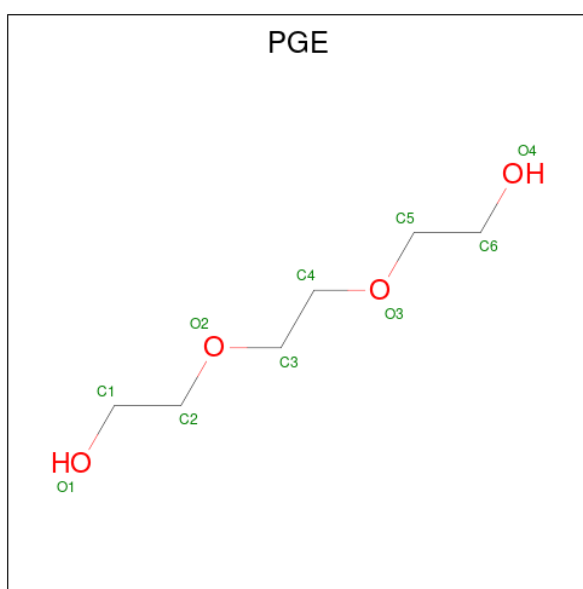
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

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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: $C_6H_{14}O_4$).

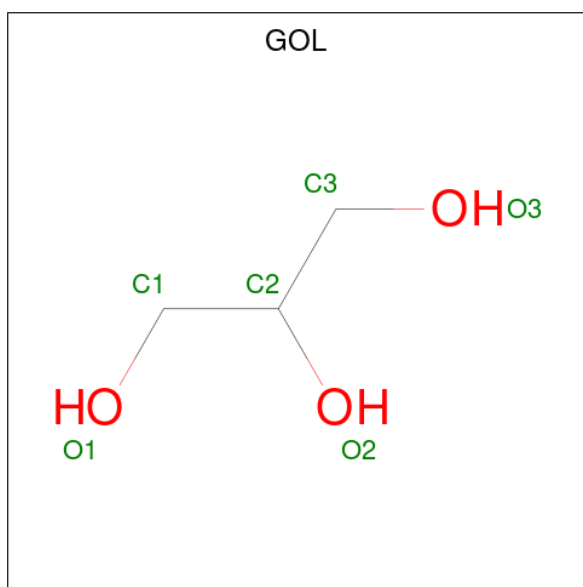


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

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

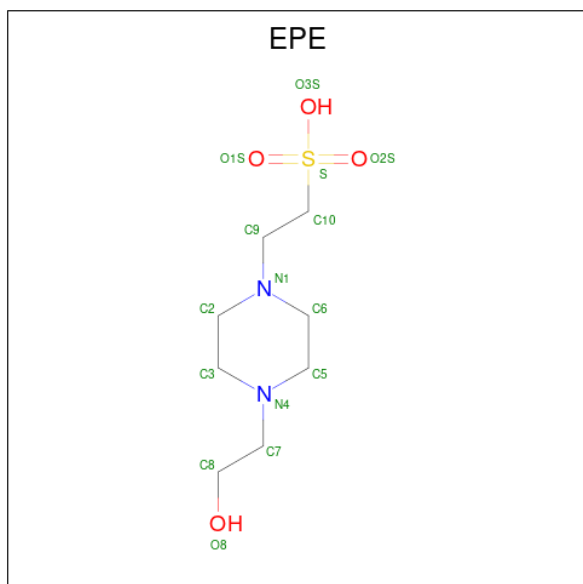
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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
9	H	1	Total 15	C 8	N 2	O 4	S 1	0	0

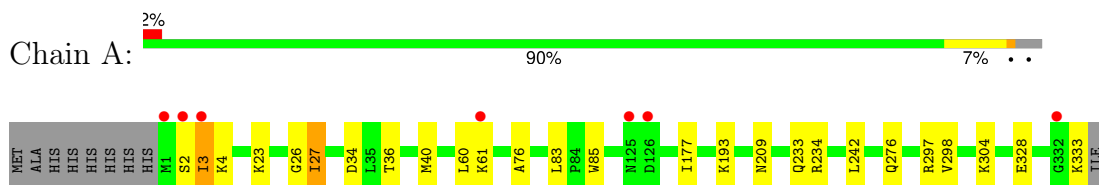
- Molecule 10 is water.

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

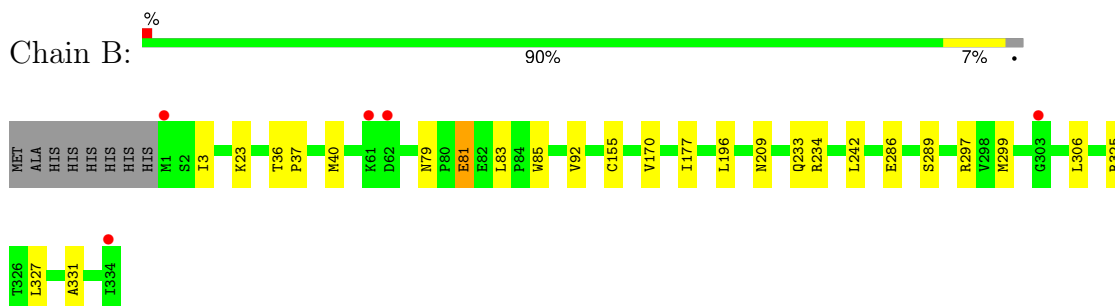
3 Residue-property plots

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.

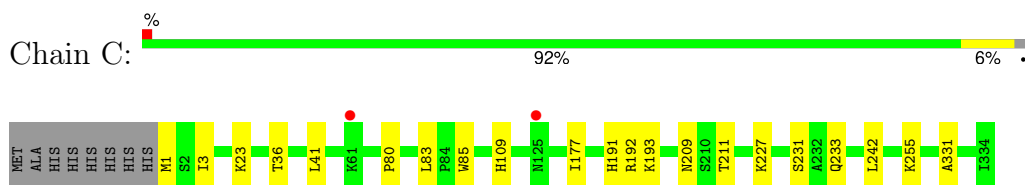
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



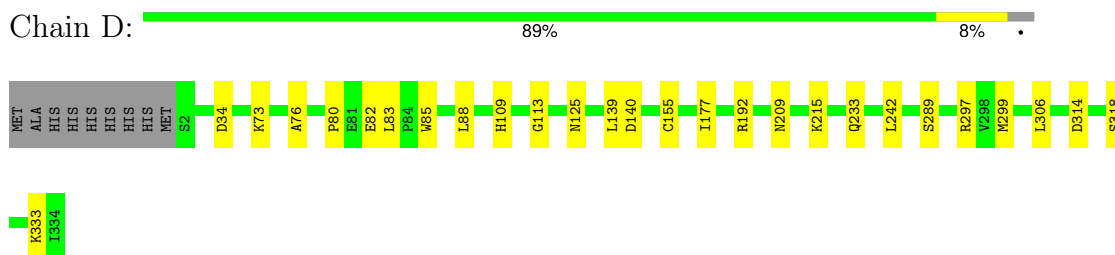
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



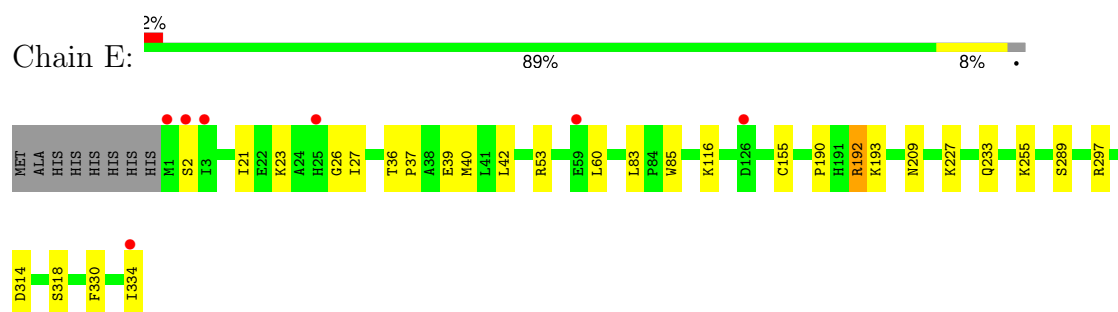
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



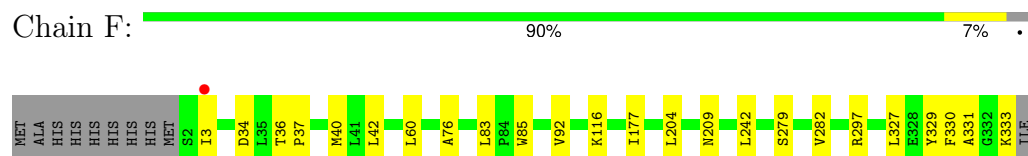
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



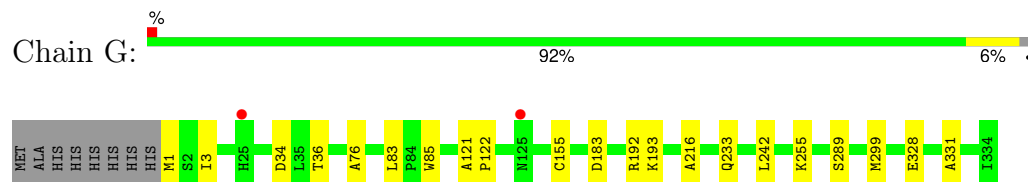
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



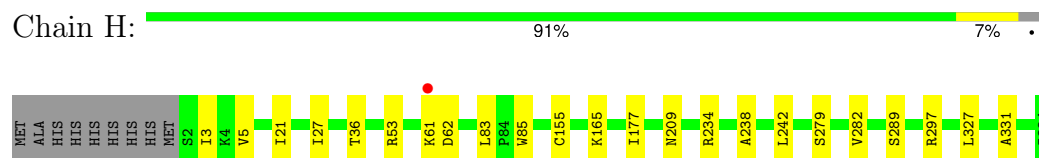
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- 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)	Xtriage
Refinement program	PHENIX (dev_5438: ???)	Depositor
R, R_{free}	0.155 , 0.187 0.163 , 0.194	Depositor DCC
R_{free} test set	9116 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	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

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.

All (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
1:G:3:ILE:HG13	1:G:331:ALA:HB1	1.72	0.70
1:F:36:THR:HG21	1:F:40:MET:HG2	1.74	0.70
1:F:36:THR:HG22	1:F:37:PRO:HD2	1.77	0.67
1:E:190:PRO:HB3	1:G:36:THR:HG21	1.76	0.66
1:A:27:ILE:CD1	1:A:328:GLU:HG2	2.17	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ASP:HA	1:D:333:LYS:HE3	1.80	0.63
1:D:140:ASP:HA	1:D:333:LYS:CE	2.31	0.61
1:B:83:LEU:HD13	1:B:85:TRP:CZ2	2.36	0.60
1:F:3:ILE:HD13	1:F:331:ALA:HB3	1.83	0.60
1:B:92:VAL:HG11	1:B:327[A]:LEU:CD1	2.31	0.60
1:E:83:LEU:HD13	1:E:85:TRP:CZ2	2.36	0.60
1:A:27:ILE:HD11	1:A:328:GLU:CG	2.19	0.59
1:C:83:LEU:HD13	1:C:85:TRP:CZ2	2.37	0.59
1:E:21:ILE:HG23	1:E:27:ILE:HG23	1.85	0.58
1:D:139:LEU:O	1:D:333:LYS:HE2	2.04	0.58
1:B:92:VAL:HG11	1:B:327[A]:LEU:HD12	1.86	0.56
1:B:92:VAL:HG11	1:B:327[B]:LEU:HD23	1.86	0.56
1:F:3:ILE:HD13	1:F:331:ALA:CB	2.36	0.56
1:G:1:MET:HE1	1:G:328:GLU:HG3	1.87	0.55
1:A:83:LEU:HD13	1:A:85:TRP:CZ2	2.42	0.55
1:F:83:LEU:HD13	1:F:85:TRP:CZ2	2.42	0.55
1:D:80:PRO:HB3	1:D:109:HIS:CE1	2.43	0.54
1:H:27:ILE:HD11	1:H:327:LEU:HD21	1.91	0.53
1:A:60:LEU:O	1:A:61:LYS:HD3	2.08	0.53
1:D:155:CYS:HA	1:D:289:SER:HB2	1.91	0.52
1:B:3:ILE:HD13	1:B:331:ALA:HB3	1.90	0.52
1:H:21:ILE:HG23	1:H:27:ILE:HG23	1.92	0.52
1:B:36:THR:HG22	1:B:37:PRO:CD	2.39	0.52
1:B:36:THR:HG21	1:B:40[B]:MET:SD	2.51	0.51
1:E:42:LEU:HD22	1:E:60:LEU:HB2	1.91	0.51
1:H:83:LEU:HD13	1:H:85:TRP:CZ2	2.44	0.51
1:G:83:LEU:HD13	1:G:85:TRP:CZ2	2.45	0.51
1:F:92:VAL:HG11	1:F:327:LEU:CD1	2.40	0.51
1:E:116:LYS:HG3	1:E:334:ILE:HG21	1.93	0.49
1:B:242:LEU:C	1:B:242:LEU:HD12	2.37	0.49
1:D:113:GLY:HA2	3:D:402:PEG:H11	1.94	0.49
1:G:34:ASP:O	1:G:76:ALA:HA	2.12	0.49
1:B:155:CYS:HA	1:B:289:SER:HB2	1.94	0.49
1:A:3:ILE:HG22	1:A:26:GLY:O	2.13	0.48
1:C:211:THR:HG22	1:C:231:SER:HA	1.94	0.48
1:E:233:GLN:HG3	1:F:177:ILE:CD1	2.43	0.48
1:H:3:ILE:HG13	1:H:331:ALA:HB1	1.95	0.48
1:H:165:LYS:HE3	10:H:618:HOH:O	2.13	0.48
1:B:234:ARG:CD	10:B:533:HOH:O	2.61	0.48
1:D:125:ASN:HB2	1:E:39:GLU:OE1	2.14	0.48
1:A:276:GLN:HG3	1:B:196:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LYS:NZ	1:D:88:LEU:HD21	2.29	0.47
1:E:36:THR:HG21	1:E:40:MET:HG2	1.95	0.47
1:C:36:THR:HG22	1:C:41:LEU:HD21	1.95	0.47
1:F:242:LEU:C	1:F:242:LEU:HD12	2.40	0.47
1:F:329:TYR:CE2	1:F:333:LYS:HE2	2.50	0.47
1:E:2:SER:HG	1:E:26:GLY:C	2.23	0.46
1:C:227:LYS:C	1:D:299:MET:CE	2.89	0.46
1:D:242:LEU:C	1:D:242:LEU:HD12	2.41	0.46
1:E:36:THR:HG22	1:E:37:PRO:HD2	1.97	0.46
1:F:36:THR:HG22	1:F:37:PRO:CD	2.44	0.45
1:A:177:ILE:HD12	1:A:242:LEU:HD11	1.98	0.45
1:H:234:ARG:HD2	10:H:571:HOH:O	2.16	0.45
1:B:92:VAL:HB	1:B:327[A]:LEU:HD11	1.99	0.45
1:E:227:LYS:NZ	10:E:1206:HOH:O	2.49	0.45
1:F:34:ASP:O	1:F:76:ALA:HA	2.17	0.45
1:H:155:CYS:HA	1:H:289:SER:HB2	1.99	0.45
1:C:233:GLN:HG3	1:D:177:ILE:HD12	1.98	0.45
1:C:191:HIS:CE1	1:C:193:LYS:HB2	2.52	0.45
3:D:402:PEG:H22	1:G:216:ALA:HB2	1.99	0.45
1:F:204:LEU:HD11	1:H:238:ALA:CB	2.47	0.45
1:A:36:THR:CG2	1:A:40[A]:MET:HG2	2.47	0.45
1:A:234:ARG:HD2	10:A:516:HOH:O	2.16	0.45
2:A:401:G3H:H32	4:A:404:NAD:H2D	1.98	0.45
1:H:242:LEU:C	1:H:242:LEU:HD12	2.42	0.45
1:H:234:ARG:CD	10:H:571:HOH:O	2.65	0.44
1:G:299:MET:HE2	1:G:299:MET:HB3	1.92	0.44
3:A:402:PEG:H41	10:A:625:HOH:O	2.18	0.43
1:B:234:ARG:HD2	10:B:533:HOH:O	2.17	0.43
1:D:82:GLU:HG2	1:H:297:ARG:NH1	2.33	0.43
1:E:314:ASP:O	1:E:318:SER:HB2	2.18	0.43
1:A:34:ASP:O	1:A:76:ALA:HA	2.18	0.43
1:A:36:THR:HG21	1:A:40[A]:MET:HG2	2.00	0.43
1:E:85:TRP:HE3	1:E:85:TRP:HA	1.84	0.43
1:C:177:ILE:CD1	1:D:233:GLN:HG3	2.49	0.43
1:E:85:TRP:HA	1:E:85:TRP:CE3	2.54	0.43
1:F:329:TYR:CZ	1:F:333:LYS:HE2	2.53	0.43
1:A:177:ILE:CD1	1:B:233:GLN:HG3	2.48	0.43
1:B:92:VAL:CG1	1:B:327[A]:LEU:CD1	2.96	0.43
1:D:34:ASP:O	1:D:76:ALA:HA	2.19	0.43
1:A:2:SER:HB2	1:A:4:LYS:NZ	2.32	0.43
1:C:80:PRO:HB3	1:C:109:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:CD	10:A:516:HOH:O	2.68	0.42
1:B:3:ILE:HD13	1:B:331:ALA:CB	2.50	0.42
1:G:183:ASP:HB3	2:G:401:G3H:H31	2.01	0.42
1:H:5:VAL:HG21	1:H:27:ILE:HD11	2.01	0.42
2:B:401:G3H:H2	4:B:403:NAD:O3	2.19	0.42
1:G:233:GLN:HG3	1:H:177:ILE:CD1	2.49	0.42
1:C:242:LEU:HD12	1:C:242:LEU:C	2.44	0.42
1:B:79:ASN:OD1	1:B:81:GLU:HG2	2.18	0.42
1:F:36:THR:CG2	1:F:37:PRO:HD2	2.47	0.42
1:G:192:ARG:HG3	1:G:193:LYS:HG2	2.01	0.42
1:A:3:ILE:HG23	1:A:27:ILE:HA	2.01	0.42
1:A:297:ARG:NH1	1:A:298:VAL:O	2.53	0.41
1:B:325:ARG:HG3	6:B:405:PGE:H3	2.02	0.41
1:G:155:CYS:HA	1:G:289:SER:HB2	2.01	0.41
1:H:61:LYS:O	1:H:62:ASP:C	2.62	0.41
1:C:3:ILE:HD13	1:C:331:ALA:CB	2.50	0.41
1:E:155:CYS:HA	1:E:289:SER:HB2	2.03	0.41
1:G:85:TRP:HA	1:G:85:TRP:CE3	2.55	0.41
1:E:192:ARG:HG3	1:E:193:LYS:N	2.34	0.41
1:E:330:PHE:O	1:E:334:ILE:HG23	2.20	0.41
1:A:233:GLN:HG3	1:B:177:ILE:HD13	2.02	0.41
1:B:306:LEU:HD12	1:B:306:LEU:HA	1.93	0.41
1:C:3:ILE:HG21	1:C:331:ALA:HB1	2.01	0.41
1:H:279:SER:O	1:H:282:VAL:HG22	2.20	0.41
1:A:27:ILE:HD12	1:A:27:ILE:HG21	1.89	0.41
1:A:304:LYS:HD2	1:B:170:VAL:HG11	2.03	0.41
1:B:242:LEU:HD12	1:B:242:LEU:O	2.21	0.41
1:E:2:SER:OG	1:E:26:GLY:C	2.63	0.41
1:B:23:LYS:NZ	1:B:286:GLU:OE2	2.54	0.40
1:F:279:SER:O	1:F:282:VAL:HG22	2.21	0.40
1:G:242:LEU:HD12	1:G:242:LEU:C	2.46	0.40
1:F:42:LEU:HD22	1:F:60:LEU:HB2	2.03	0.40
1:F:116:LYS:HB3	1:F:330:PHE:CE2	2.57	0.40
1:F:177:ILE:HD12	1:F:242:LEU:HD11	2.02	0.40
1:G:121:ALA:HB1	1:G:122:PRO:HD2	2.03	0.40
1:G:85:TRP:HA	1:G:85:TRP:HE3	1.85	0.40
1:C:85:TRP:HA	1:C:85:TRP:CE3	2.56	0.40
1:D:314:ASP:O	1:D:318:SER:HB2	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	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

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	265/273 (97%)	259 (98%)	6 (2%)	45	30
1	B	267/273 (98%)	264 (99%)	3 (1%)	70	63
1	C	267/273 (98%)	262 (98%)	5 (2%)	52	39
1	D	267/273 (98%)	263 (98%)	4 (2%)	60	49
1	E	265/273 (97%)	260 (98%)	5 (2%)	52	39
1	F	264/273 (97%)	263 (100%)	1 (0%)	89	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	268/273 (98%)	267 (100%)	1 (0%)	89	88
1	H	264/273 (97%)	261 (99%)	3 (1%)	70	63
All	All	2127/2184 (97%)	2099 (99%)	28 (1%)	65	55

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	23	LYS
1	A	27	ILE
1	A	193	LYS
1	A	209	ASN
1	A	333	LYS
1	B	81	GLU
1	B	209	ASN
1	B	299	MET
1	C	1	MET
1	C	23	LYS
1	C	192	ARG
1	C	209	ASN
1	C	255	LYS
1	D	192	ARG
1	D	209	ASN
1	D	215	LYS
1	D	306	LEU
1	E	23	LYS
1	E	53	ARG
1	E	192	ARG
1	E	209	ASN
1	E	255	LYS
1	F	209	ASN
1	G	255	LYS
1	H	36	THR
1	H	53	ARG
1	H	209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN

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Mol	Chain	Res	Type
1	B	233	GLN
1	B	276	GLN
1	D	125	ASN
1	E	125	ASN
1	E	209	ASN
1	H	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	E	402	-	6,6,6	0.26	0	5,5,5	0.53	0
3	PEG	B	402	-	6,6,6	0.27	0	5,5,5	0.18	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
9	EPE	D	404	-	15,15,15	0.83	0	19,20,20	1.18	1 (5%)
4	NAD	H	403	-	42,48,48	1.37	5 (11%)	50,73,73	1.15	4 (8%)
2	G3H	H	401	-	8,9,9	1.83	2 (25%)	7,12,12	1.50	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G3H	E	401	-	8,9,9	1.84	3 (37%)	7,12,12	1.61	1 (14%)
4	NAD	B	403	-	42,48,48	1.17	4 (9%)	50,73,73	1.11	3 (6%)
4	NAD	C	404	-	42,48,48	1.29	4 (9%)	50,73,73	1.02	3 (6%)
8	GOL	C	403	-	5,5,5	0.26	0	5,5,5	0.43	0
2	G3H	A	401	-	8,9,9	1.78	2 (25%)	7,12,12	1.59	2 (28%)
8	GOL	D	403	-	5,5,5	0.32	0	5,5,5	0.59	0
2	G3H	F	401	-	8,9,9	1.85	3 (37%)	7,12,12	1.52	1 (14%)
4	NAD	D	405	-	42,48,48	1.19	5 (11%)	50,73,73	1.06	5 (10%)
4	NAD	G	403	-	42,48,48	1.34	5 (11%)	50,73,73	1.15	4 (8%)
9	EPE	H	402	-	15,15,15	0.82	1 (6%)	19,20,20	0.82	0
3	PEG	C	402	-	6,6,6	0.28	0	5,5,5	0.42	0
3	PEG	A	403	-	6,6,6	0.22	0	5,5,5	0.27	0
3	PEG	D	402	-	6,6,6	0.27	0	5,5,5	0.31	0
2	G3H	B	401	-	8,9,9	1.68	1 (12%)	7,12,12	1.48	1 (14%)
2	G3H	G	401	-	8,9,9	1.71	2 (25%)	7,12,12	1.37	1 (14%)
3	PEG	F	402	-	6,6,6	0.12	0	5,5,5	0.08	0
4	NAD	E	403	-	42,48,48	1.16	5 (11%)	50,73,73	1.26	6 (12%)
4	NAD	A	404	-	42,48,48	1.04	4 (9%)	50,73,73	1.21	6 (12%)
3	PEG	A	402	-	6,6,6	0.29	0	5,5,5	0.44	0
4	NAD	F	403	-	42,48,48	1.06	4 (9%)	50,73,73	1.05	2 (4%)
2	G3H	D	401	-	8,9,9	1.72	2 (25%)	7,12,12	1.38	1 (14%)
3	PEG	G	402	-	6,6,6	0.27	0	5,5,5	0.43	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	E	402	-	-	2/4/4/4	-
3	PEG	B	402	-	-	1/4/4/4	-
6	PGE	B	405	-	-	2/7/7/7	-
2	G3H	C	401	-	-	5/7/8/8	-
9	EPE	D	404	-	-	4/9/19/19	0/1/1/1
4	NAD	H	403	-	-	5/26/62/62	0/5/5/5
2	G3H	H	401	-	-	6/7/8/8	-
2	G3H	E	401	-	-	5/7/8/8	-
4	NAD	B	403	-	-	4/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	C	404	-	-	4/26/62/62	0/5/5/5
8	GOL	C	403	-	-	2/4/4/4	-
2	G3H	A	401	-	-	1/7/8/8	-
8	GOL	D	403	-	-	2/4/4/4	-
2	G3H	F	401	-	-	5/7/8/8	-
4	NAD	D	405	-	-	4/26/62/62	0/5/5/5
4	NAD	G	403	-	-	4/26/62/62	0/5/5/5
9	EPE	H	402	-	-	5/9/19/19	0/1/1/1
3	PEG	C	402	-	-	0/4/4/4	-
3	PEG	A	403	-	-	2/4/4/4	-
3	PEG	D	402	-	-	3/4/4/4	-
2	G3H	B	401	-	-	2/7/8/8	-
2	G3H	G	401	-	-	0/7/8/8	-
3	PEG	F	402	-	-	4/4/4/4	-
4	NAD	E	403	-	-	4/26/62/62	0/5/5/5
4	NAD	A	404	-	-	4/26/62/62	0/5/5/5
3	PEG	A	402	-	-	4/4/4/4	-
4	NAD	F	403	-	-	4/26/62/62	0/5/5/5
2	G3H	D	401	-	-	5/7/8/8	-
3	PEG	G	402	-	-	2/4/4/4	-

All (54) 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
4	D	405	NAD	PA-O3	4.04	1.63	1.59
2	H	401	G3H	P-O1P	4.00	1.72	1.60
2	E	401	G3H	P-O1P	3.95	1.72	1.60
2	F	401	G3H	P-O1P	3.93	1.72	1.60
2	A	401	G3H	P-O1P	3.92	1.72	1.60
2	C	401	G3H	P-O1P	3.84	1.72	1.60
2	B	401	G3H	P-O1P	3.83	1.72	1.60
4	E	403	NAD	PA-O3	3.83	1.63	1.59
4	H	403	NAD	PN-O3	3.79	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	G3H	P-O1P	3.76	1.72	1.60
2	G	401	G3H	P-O1P	3.64	1.71	1.60
4	G	403	NAD	O4D-C1D	-3.52	1.36	1.40
4	G	403	NAD	PN-O3	3.51	1.63	1.59
4	D	405	NAD	PN-O3	3.05	1.62	1.59
4	H	403	NAD	O4D-C1D	-2.91	1.37	1.40
4	A	404	NAD	PA-O3	2.86	1.62	1.59
4	B	403	NAD	PN-O3	2.83	1.62	1.59
4	F	403	NAD	PN-O3	2.81	1.62	1.59
4	E	403	NAD	O4D-C1D	-2.74	1.37	1.40
4	A	404	NAD	O4D-C1D	-2.68	1.37	1.40
4	F	403	NAD	PA-O3	2.64	1.62	1.59
4	C	404	NAD	C8A-N7A	-2.63	1.29	1.34
4	B	403	NAD	C1B-N9A	-2.62	1.43	1.49
4	H	403	NAD	C8A-N7A	-2.58	1.30	1.34
4	F	403	NAD	C1B-N9A	-2.39	1.44	1.49
4	H	403	NAD	C1B-N9A	-2.39	1.44	1.49
4	A	404	NAD	C1B-N9A	-2.38	1.44	1.49
2	A	401	G3H	C3-C2	2.35	1.54	1.51
4	F	403	NAD	C8A-N7A	-2.33	1.30	1.34
9	H	402	EPE	C10-S	2.30	1.80	1.77
2	F	401	G3H	C3-C2	2.30	1.54	1.51
4	E	403	NAD	C1B-N9A	-2.29	1.44	1.49
4	B	403	NAD	C8A-N7A	-2.27	1.30	1.34
4	C	404	NAD	C1B-N9A	-2.26	1.44	1.49
4	D	405	NAD	C8A-N7A	-2.23	1.30	1.34
4	G	403	NAD	C1B-N9A	-2.20	1.44	1.49
2	E	401	G3H	C3-C2	2.13	1.54	1.51
2	G	401	G3H	O2-C2	-2.11	1.40	1.43
4	A	404	NAD	PN-O3	2.11	1.61	1.59
2	H	401	G3H	C3-C2	2.11	1.54	1.51
2	E	401	G3H	O2-C2	-2.09	1.40	1.43
2	D	401	G3H	O2-C2	-2.09	1.40	1.43
4	E	403	NAD	C8A-N7A	-2.08	1.30	1.34
4	D	405	NAD	O4D-C1D	-2.08	1.38	1.40
4	E	403	NAD	PN-O3	2.06	1.61	1.59
2	F	401	G3H	O2-C2	-2.03	1.40	1.43
4	G	403	NAD	C8A-N7A	-2.02	1.31	1.34
4	D	405	NAD	C1B-N9A	-2.01	1.45	1.49
2	C	401	G3H	C3-C2	2.00	1.54	1.51

All (42) 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
4	G	403	NAD	C6N-N1N-C1D	-2.69	114.46	119.73
2	F	401	G3H	O3P-P-O1P	-2.67	99.72	106.67
4	H	403	NAD	C4A-C5A-N7A	2.65	112.14	109.34
4	A	404	NAD	C5A-C6A-N6A	2.64	124.33	120.31
4	F	403	NAD	O3-PA-O1A	-2.61	102.84	110.70
4	H	403	NAD	O4B-C1B-N9A	-2.61	105.29	108.75
4	A	404	NAD	O2A-PA-O3	2.58	114.25	107.27
2	A	401	G3H	O2-C2-C1	2.55	114.52	109.03
2	D	401	G3H	O3P-P-O1P	-2.51	100.14	106.67
4	D	405	NAD	O4B-C1B-N9A	-2.48	105.45	108.75
4	E	403	NAD	O7N-C7N-N7N	2.46	126.17	122.62
4	A	404	NAD	C6N-N1N-C1D	-2.43	114.96	119.73
2	B	401	G3H	O2-C2-C1	2.41	114.22	109.03
4	A	404	NAD	O3-PA-O1A	-2.38	103.54	110.70
2	A	401	G3H	O3P-P-O1P	-2.38	100.46	106.67
2	H	401	G3H	O2-C2-C1	2.33	114.05	109.03
4	F	403	NAD	O2A-PA-O1A	2.30	123.13	112.44
4	B	403	NAD	O7N-C7N-N7N	2.29	125.92	122.62
4	E	403	NAD	C6N-N1N-C1D	-2.26	115.29	119.73
4	G	403	NAD	O2A-PA-O1A	2.25	122.93	112.44
4	C	404	NAD	O2N-PN-O1N	2.24	122.86	112.44
4	E	403	NAD	O2A-PA-O1A	2.24	122.85	112.44
4	E	403	NAD	C4B-O4B-C1B	-2.22	107.89	109.92
4	D	405	NAD	O3-PA-O1A	-2.21	104.05	110.70
4	A	404	NAD	O4B-C1B-N9A	-2.21	105.81	108.75
4	G	403	NAD	O4B-C1B-N9A	-2.19	105.84	108.75
4	H	403	NAD	C6N-N1N-C1D	-2.19	115.44	119.73
4	C	404	NAD	O2A-PA-O1A	2.18	122.58	112.44
4	D	405	NAD	O3B-C3B-C4B	-2.10	105.05	111.08
4	C	404	NAD	C6N-N1N-C1D	-2.09	115.63	119.73
4	B	403	NAD	O3-PA-O1A	-2.08	104.44	110.70
4	E	403	NAD	C2N-N1N-C1D	2.07	123.70	119.13
4	A	404	NAD	O7N-C7N-N7N	2.05	125.57	122.62
4	D	405	NAD	O2A-PA-O1A	2.03	121.88	112.44
4	B	403	NAD	C4A-C5A-N7A	2.02	111.47	109.34
4	D	405	NAD	O2N-PN-O3	2.02	112.73	107.27
2	G	401	G3H	O4P-P-O3P	2.02	115.38	107.80

There are no chirality outliers.

All (95) 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
2	C	401	G3H	C3-O1P-P-O3P
2	C	401	G3H	C3-O1P-P-O4P
2	D	401	G3H	O1-C1-C2-C3
2	D	401	G3H	C1-C2-C3-O1P
2	D	401	G3H	O2-C2-C3-O1P
2	D	401	G3H	C3-O1P-P-O3P
2	D	401	G3H	C3-O1P-P-O4P
2	E	401	G3H	O1-C1-C2-C3
2	E	401	G3H	C1-C2-C3-O1P
2	E	401	G3H	O2-C2-C3-O1P
2	E	401	G3H	C3-O1P-P-O3P
2	E	401	G3H	C3-O1P-P-O4P
2	F	401	G3H	C1-C2-C3-O1P
2	F	401	G3H	O2-C2-C3-O1P
2	F	401	G3H	C3-O1P-P-O3P
2	F	401	G3H	C3-O1P-P-O4P
2	H	401	G3H	O1-C1-C2-C3
2	H	401	G3H	C1-C2-C3-O1P
2	H	401	G3H	O2-C2-C3-O1P
2	H	401	G3H	C3-O1P-P-O2P
2	H	401	G3H	C3-O1P-P-O3P
2	H	401	G3H	C3-O1P-P-O4P
4	A	404	NAD	O4D-C1D-N1N-C2N
4	A	404	NAD	O4D-C1D-N1N-C6N
4	A	404	NAD	C2D-C1D-N1N-C6N
4	B	403	NAD	O4D-C1D-N1N-C2N
4	B	403	NAD	O4D-C1D-N1N-C6N
4	B	403	NAD	C2D-C1D-N1N-C2N
4	B	403	NAD	C2D-C1D-N1N-C6N
4	C	404	NAD	O4D-C1D-N1N-C2N
4	C	404	NAD	O4D-C1D-N1N-C6N
4	C	404	NAD	C2D-C1D-N1N-C6N
4	D	405	NAD	O4D-C1D-N1N-C2N
4	D	405	NAD	O4D-C1D-N1N-C6N
4	D	405	NAD	C2D-C1D-N1N-C6N
4	E	403	NAD	O4D-C1D-N1N-C2N
4	E	403	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
4	E	403	NAD	C2D-C1D-N1N-C6N
4	F	403	NAD	O4D-C1D-N1N-C2N
4	F	403	NAD	O4D-C1D-N1N-C6N
4	F	403	NAD	C2D-C1D-N1N-C2N
4	F	403	NAD	C2D-C1D-N1N-C6N
4	G	403	NAD	O4D-C1D-N1N-C2N
4	G	403	NAD	O4D-C1D-N1N-C6N
4	G	403	NAD	C2D-C1D-N1N-C6N
4	H	403	NAD	O4D-C1D-N1N-C2N
4	H	403	NAD	O4D-C1D-N1N-C6N
4	H	403	NAD	C2D-C1D-N1N-C6N
8	C	403	GOL	C1-C2-C3-O3
8	D	403	GOL	C1-C2-C3-O3
8	D	403	GOL	O2-C2-C3-O3
9	D	404	EPE	C10-C9-N1-C6
9	D	404	EPE	C9-C10-S-O2S
9	D	404	EPE	C9-C10-S-O3S
9	H	402	EPE	C9-C10-S-O3S
9	H	402	EPE	N4-C7-C8-O8
3	A	403	PEG	O2-C3-C4-O4
3	D	402	PEG	O1-C1-C2-O2
3	E	402	PEG	O2-C3-C4-O4
3	G	402	PEG	O1-C1-C2-O2
3	F	402	PEG	O1-C1-C2-O2
8	C	403	GOL	O2-C2-C3-O3
3	A	402	PEG	O2-C3-C4-O4
3	B	402	PEG	O2-C3-C4-O4
3	G	402	PEG	O2-C3-C4-O4
3	F	402	PEG	O2-C3-C4-O4
6	B	405	PGE	O2-C3-C4-O3
9	H	402	EPE	C8-C7-N4-C3
9	D	404	EPE	C9-C10-S-O1S
9	H	402	EPE	C9-C10-S-O1S
9	H	402	EPE	C9-C10-S-O2S
3	E	402	PEG	C4-C3-O2-C2
3	A	402	PEG	C4-C3-O2-C2
3	D	402	PEG	C4-C3-O2-C2
6	B	405	PGE	C4-C3-O2-C2
3	F	402	PEG	C4-C3-O2-C2
3	A	403	PEG	C1-C2-O2-C3
4	A	404	NAD	C2D-C1D-N1N-C2N
4	C	404	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
4	D	405	NAD	C2D-C1D-N1N-C2N
4	E	403	NAD	C2D-C1D-N1N-C2N
4	G	403	NAD	C2D-C1D-N1N-C2N
4	H	403	NAD	C2D-C1D-N1N-C2N
3	F	402	PEG	C1-C2-O2-C3
2	F	401	G3H	C2-C3-O1P-P
3	D	402	PEG	C1-C2-O2-C3
3	A	402	PEG	O1-C1-C2-O2
4	H	403	NAD	O4B-C4B-C5B-O5B
2	A	401	G3H	C2-C3-O1P-P
3	A	402	PEG	C1-C2-O2-C3

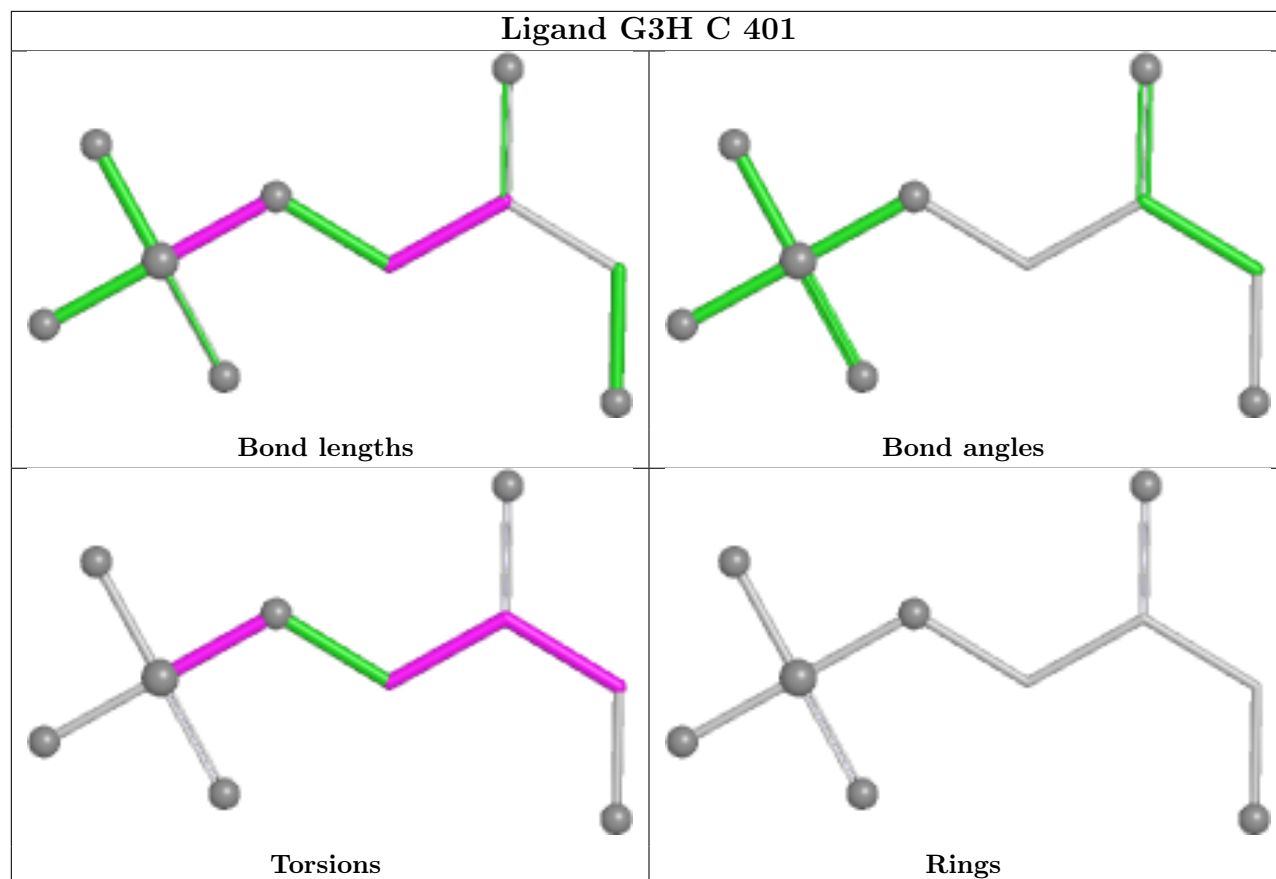
There are no ring outliers.

8 monomers are involved in 7 short contacts:

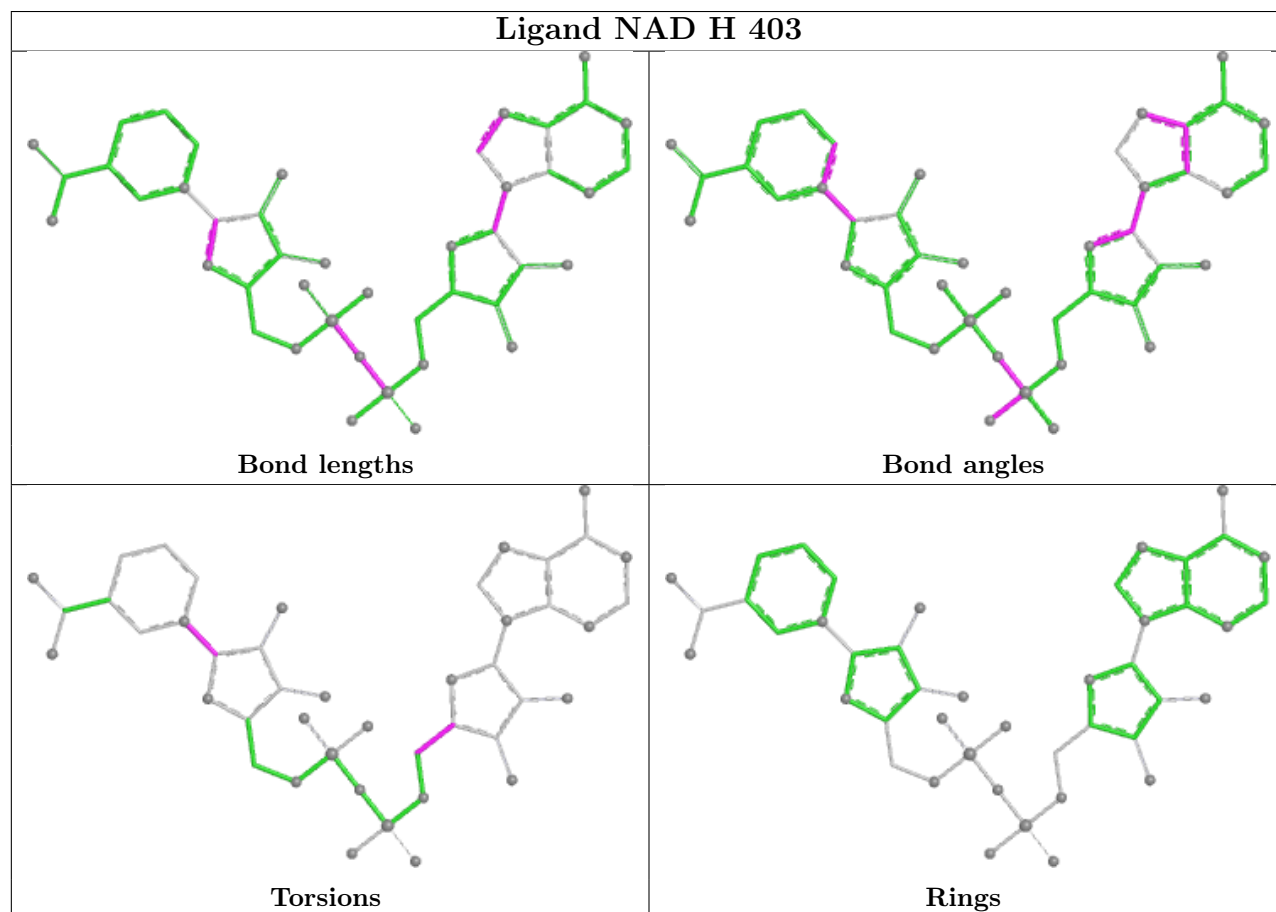
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	405	PGE	1	0
4	B	403	NAD	1	0
2	A	401	G3H	1	0
3	D	402	PEG	2	0
2	B	401	G3H	1	0
2	G	401	G3H	1	0
4	A	404	NAD	1	0
3	A	402	PEG	1	0

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.

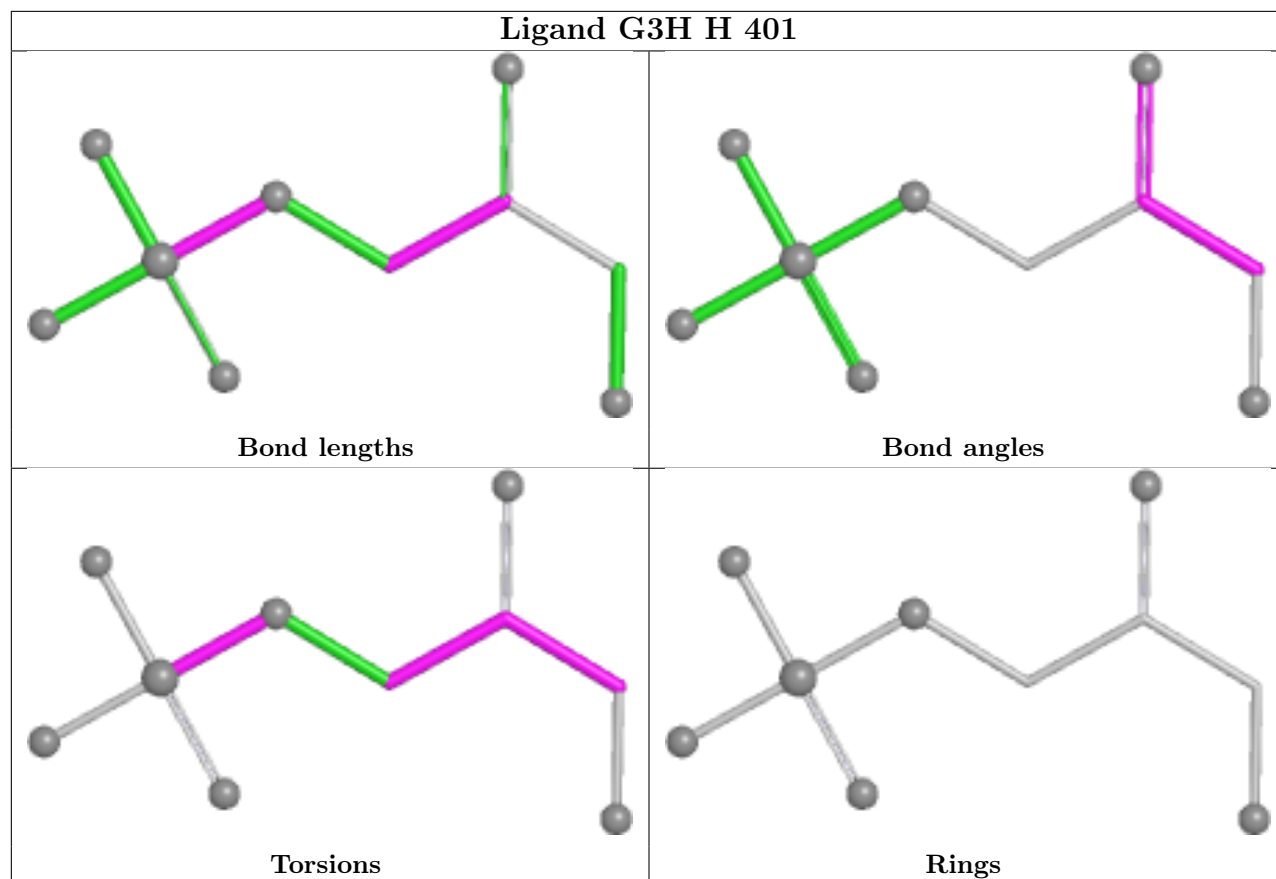
Ligand G3H C 401



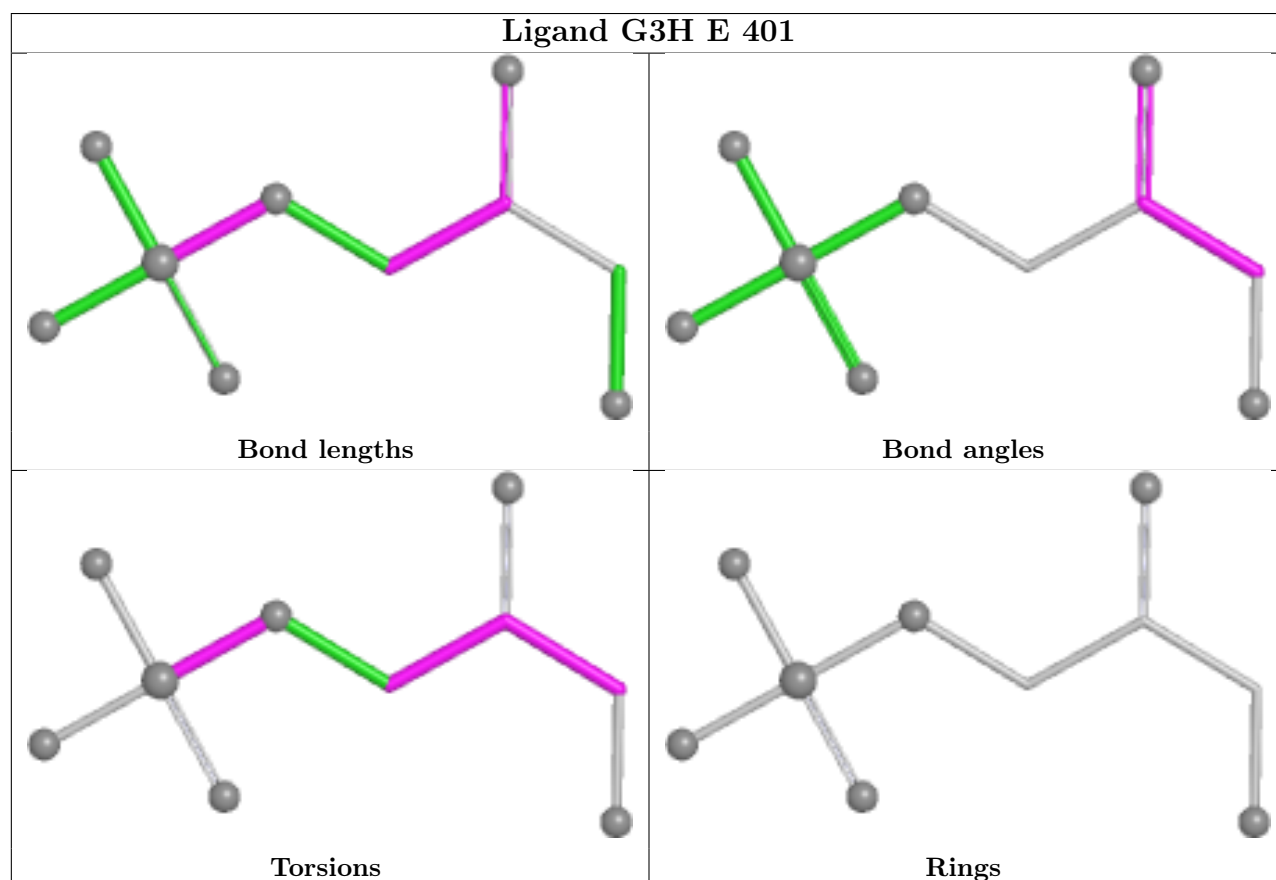
Ligand NAD H 403

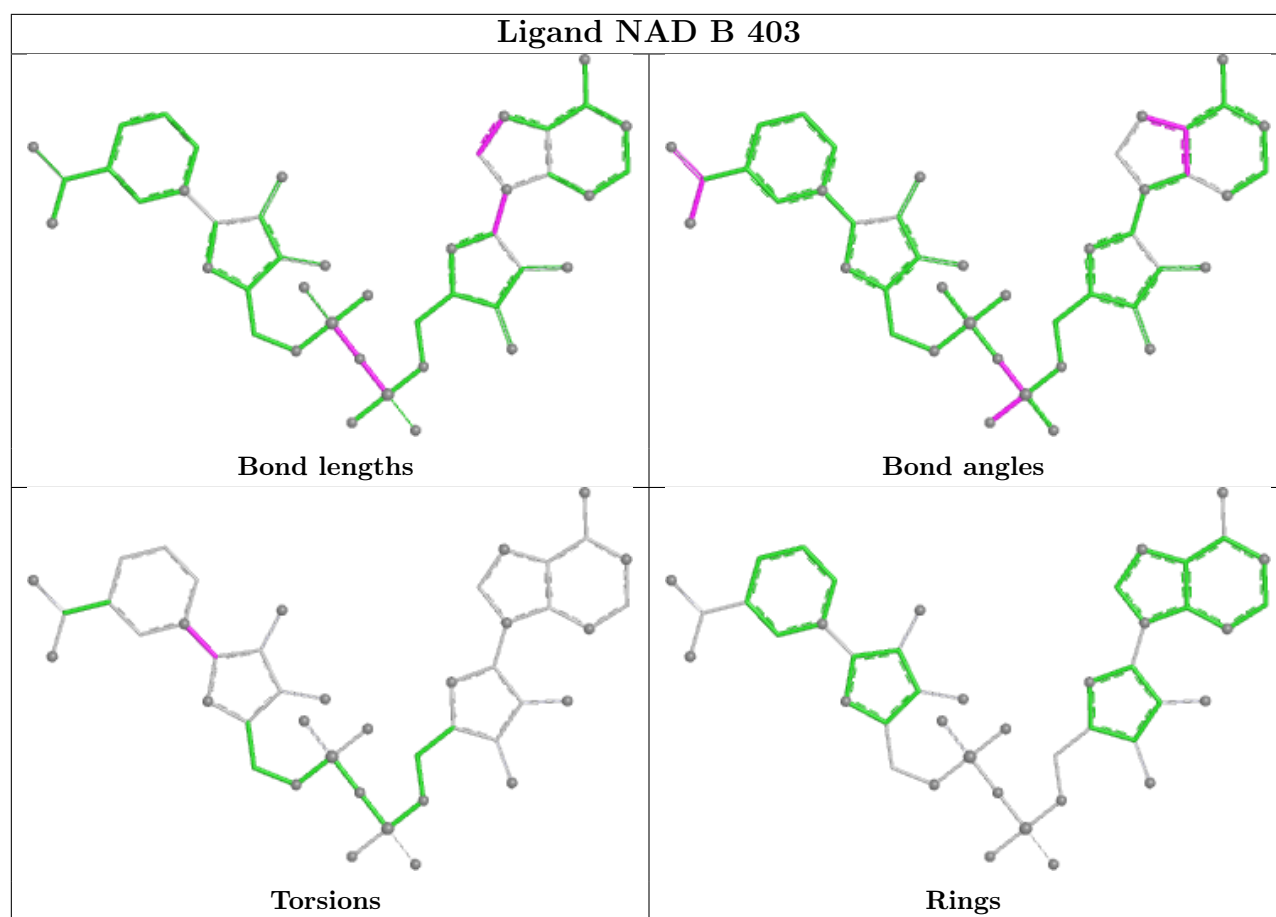


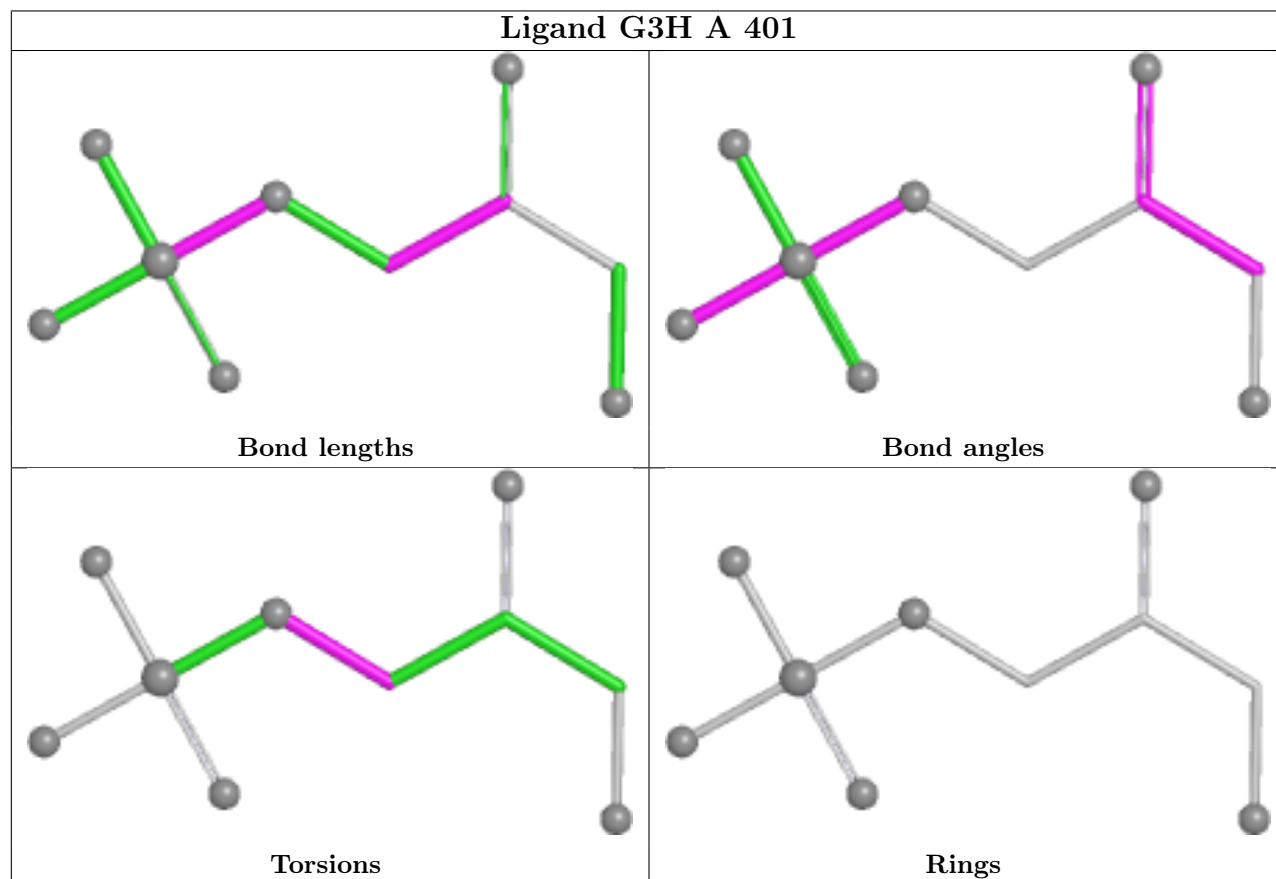
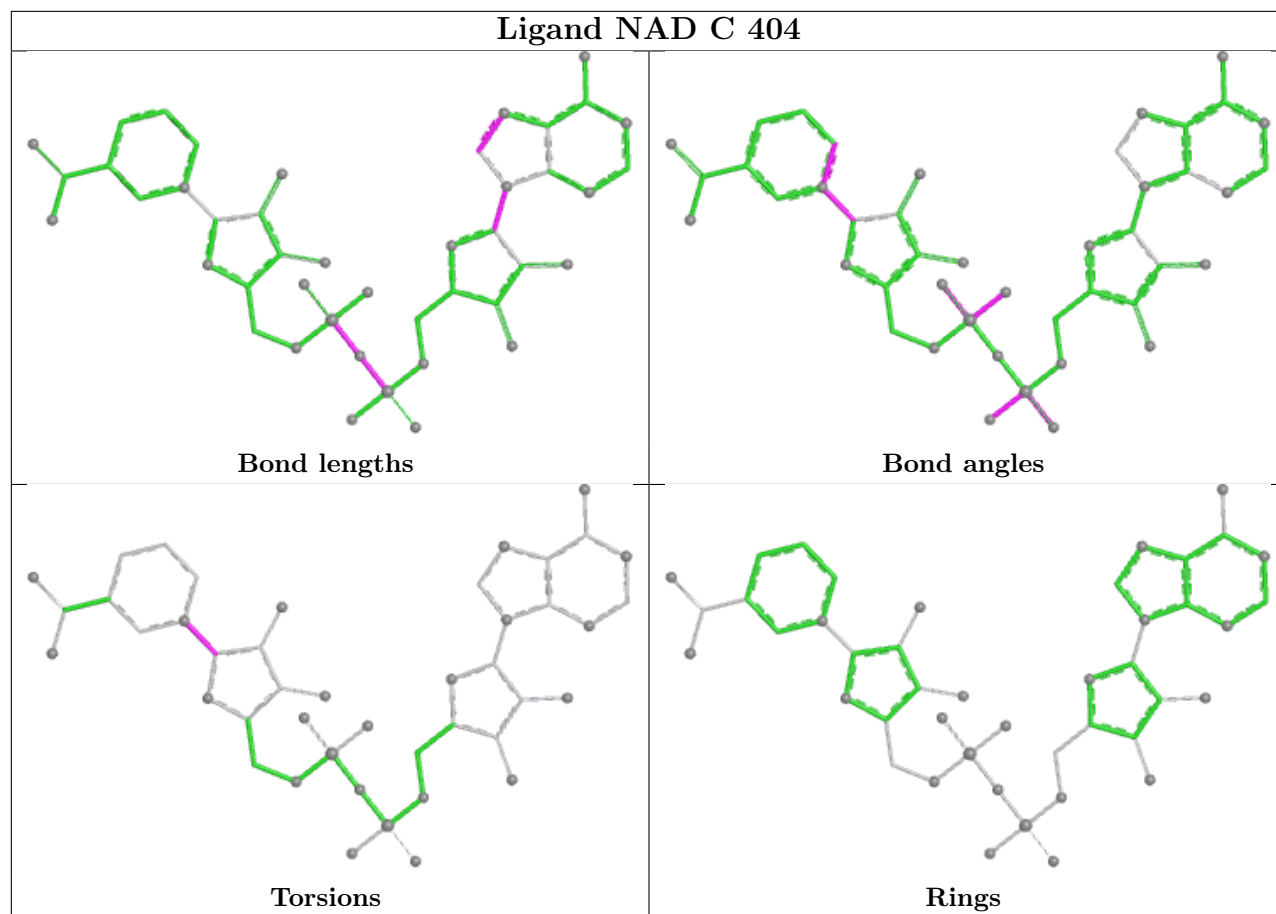
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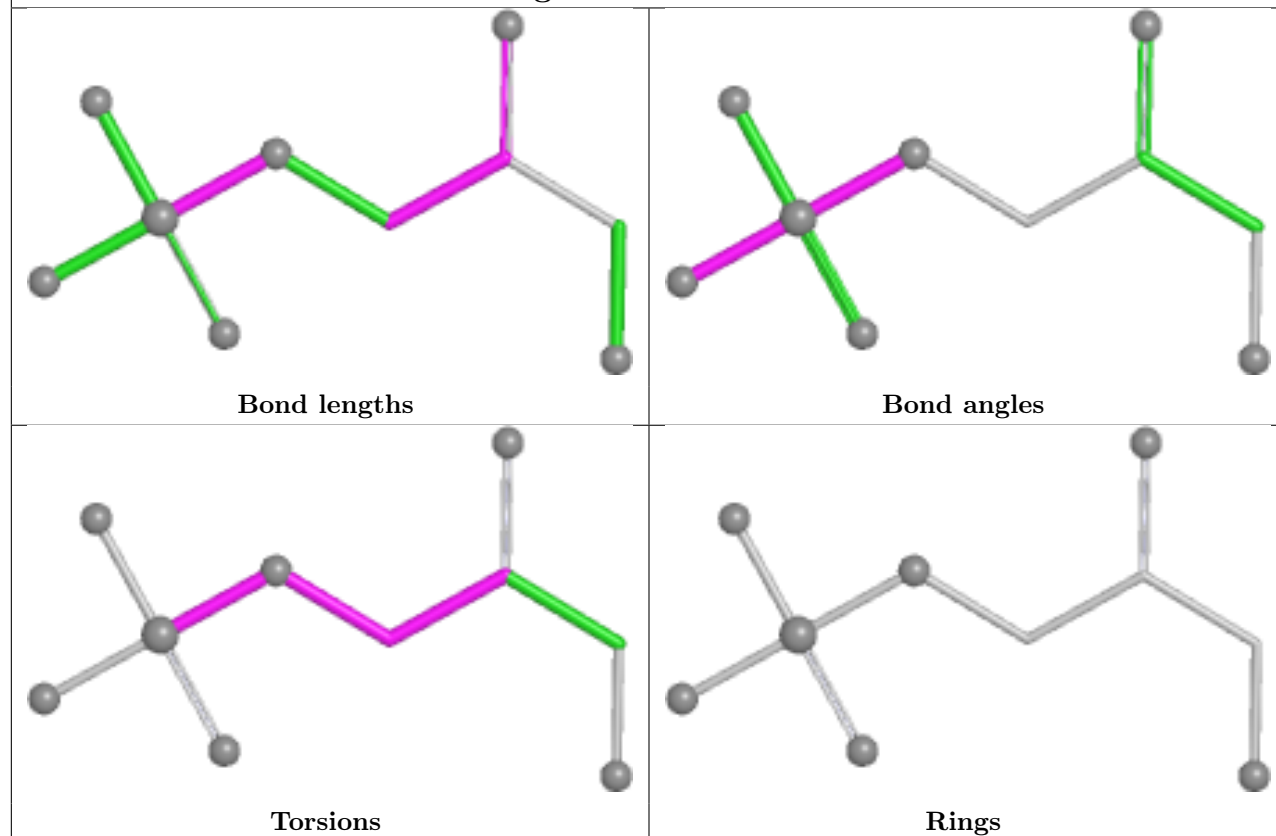
Ligand G3H E 401



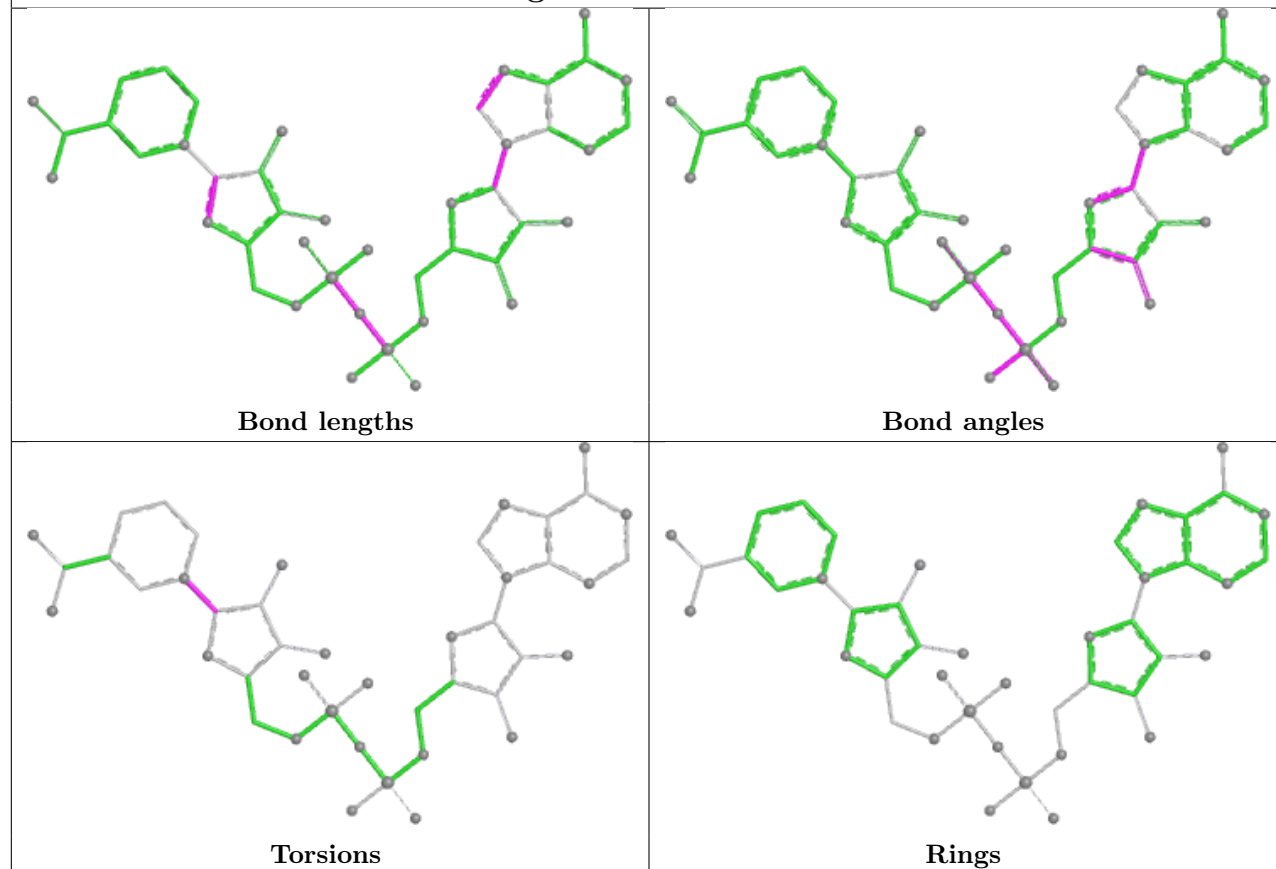


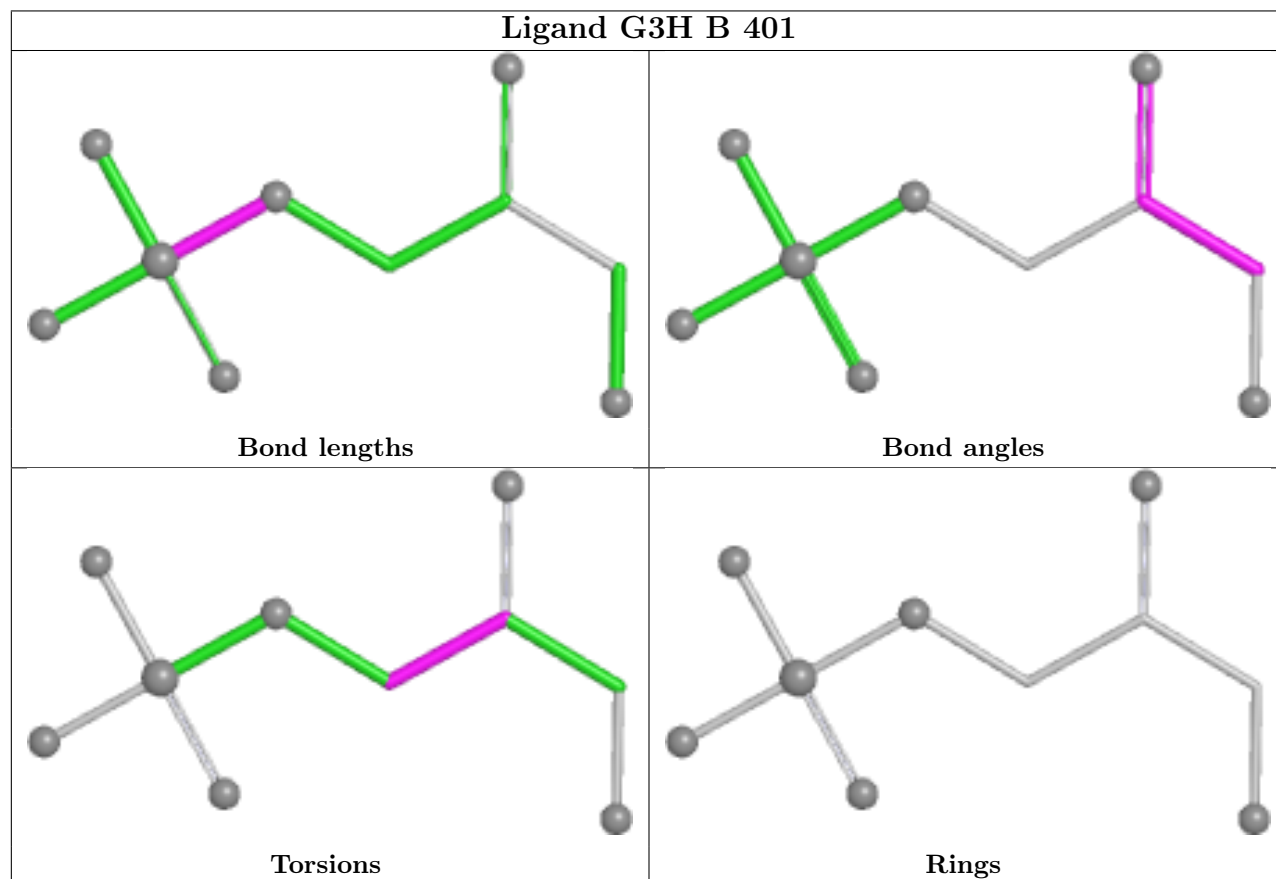
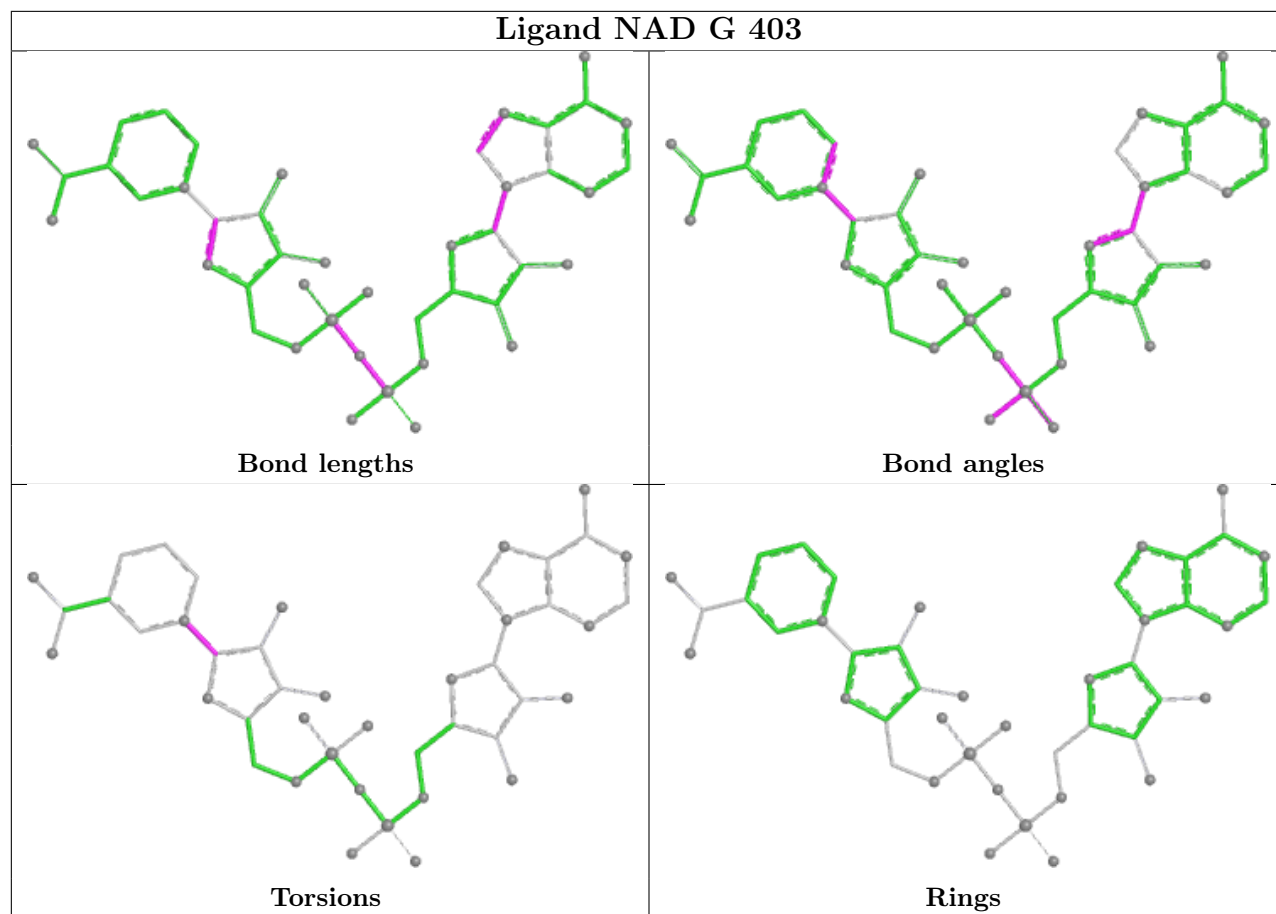


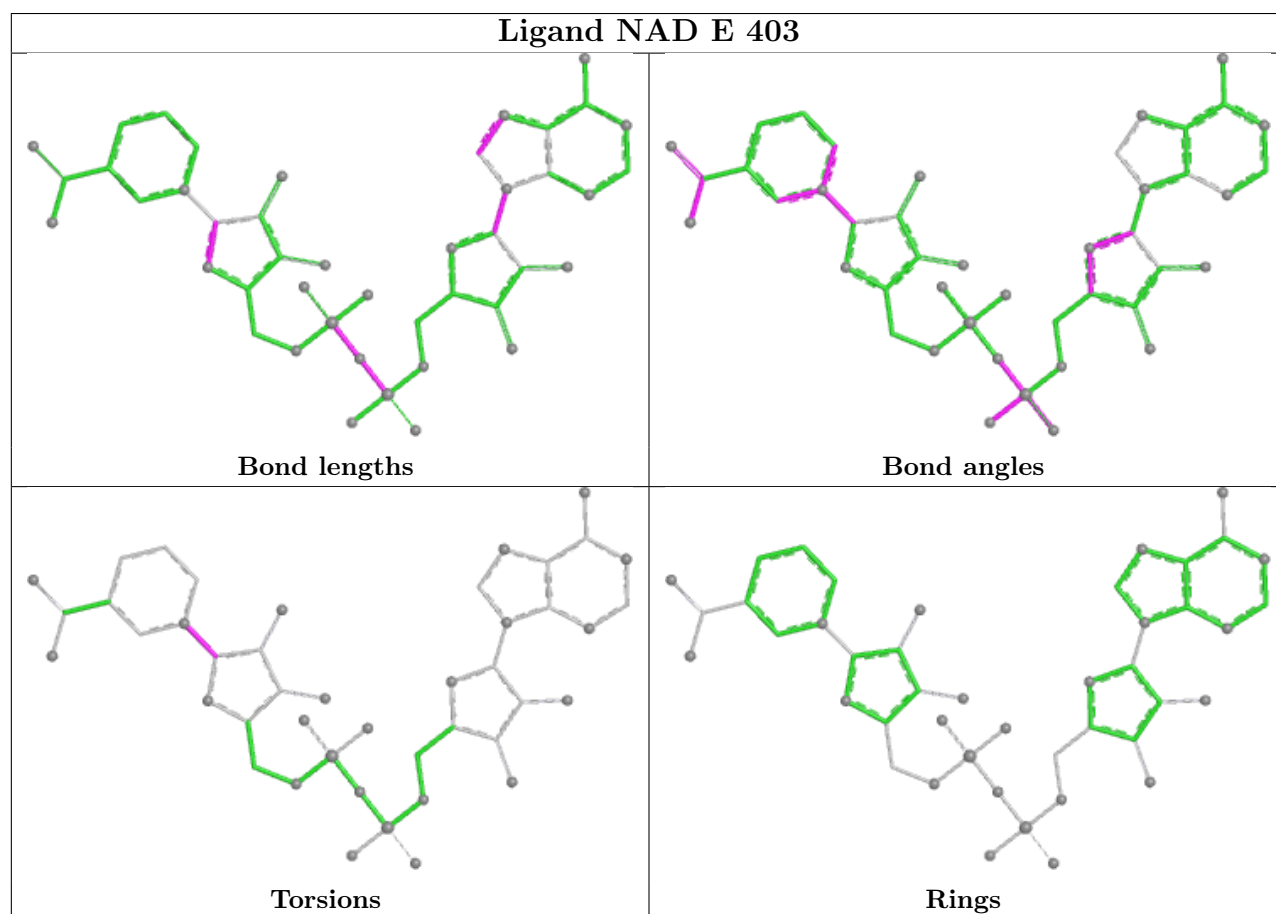
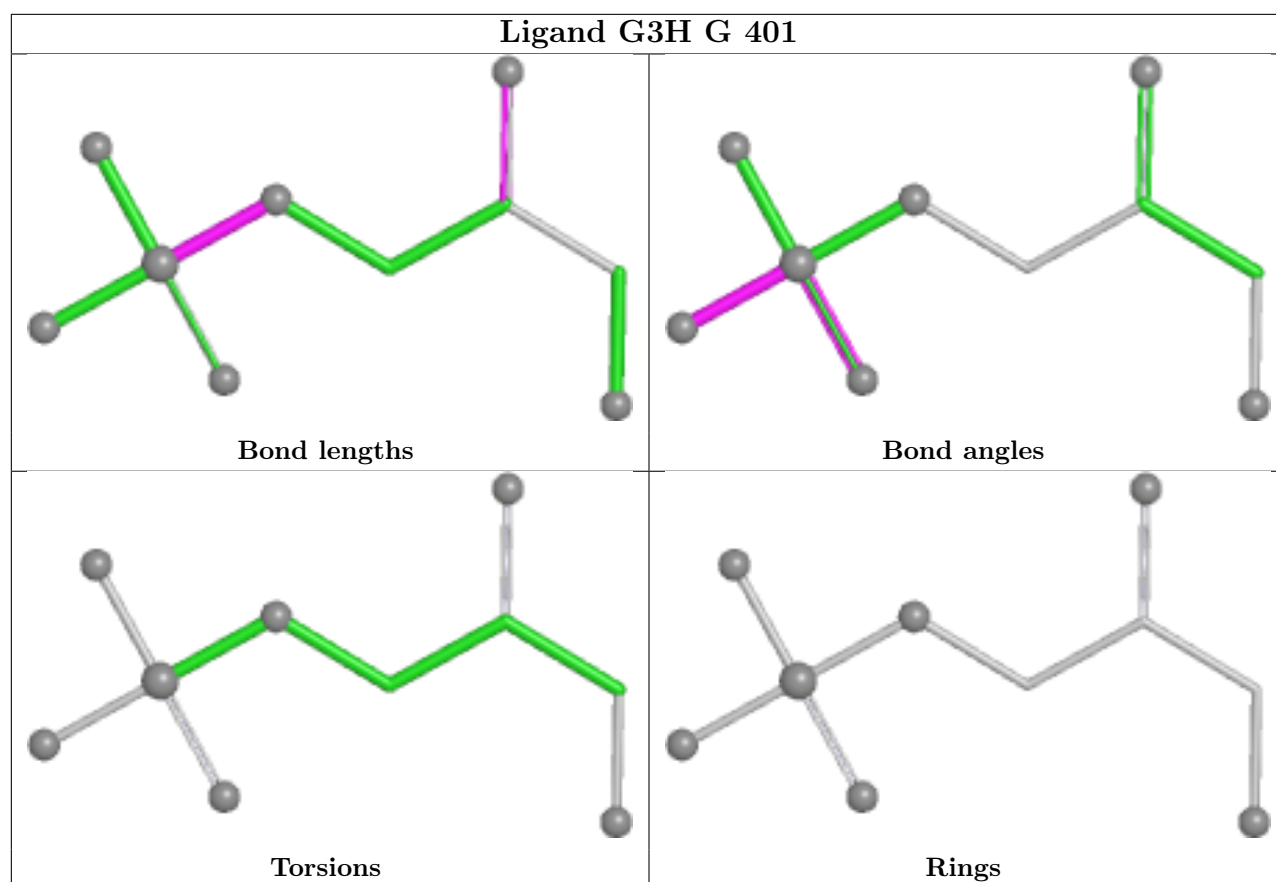
Ligand G3H F 401

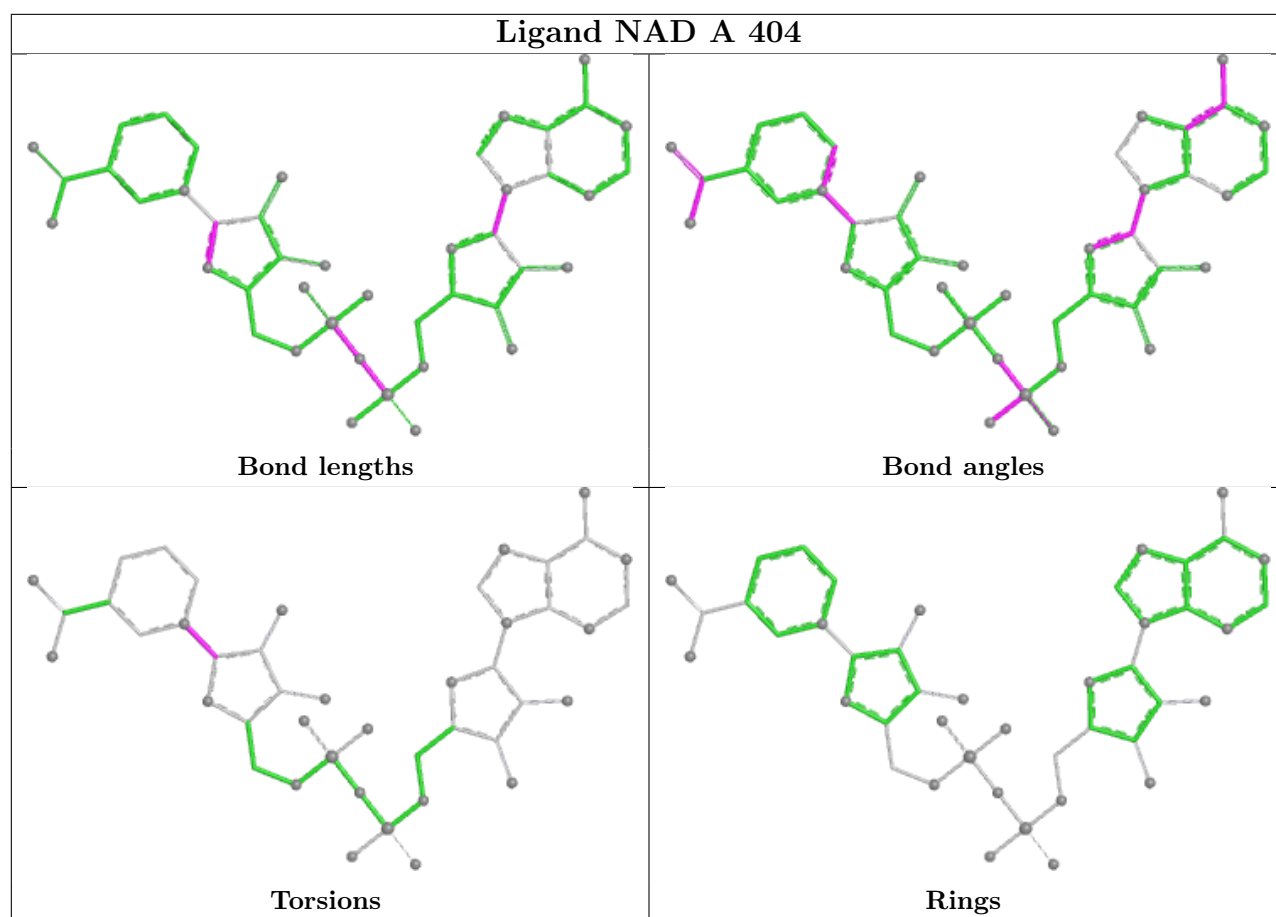


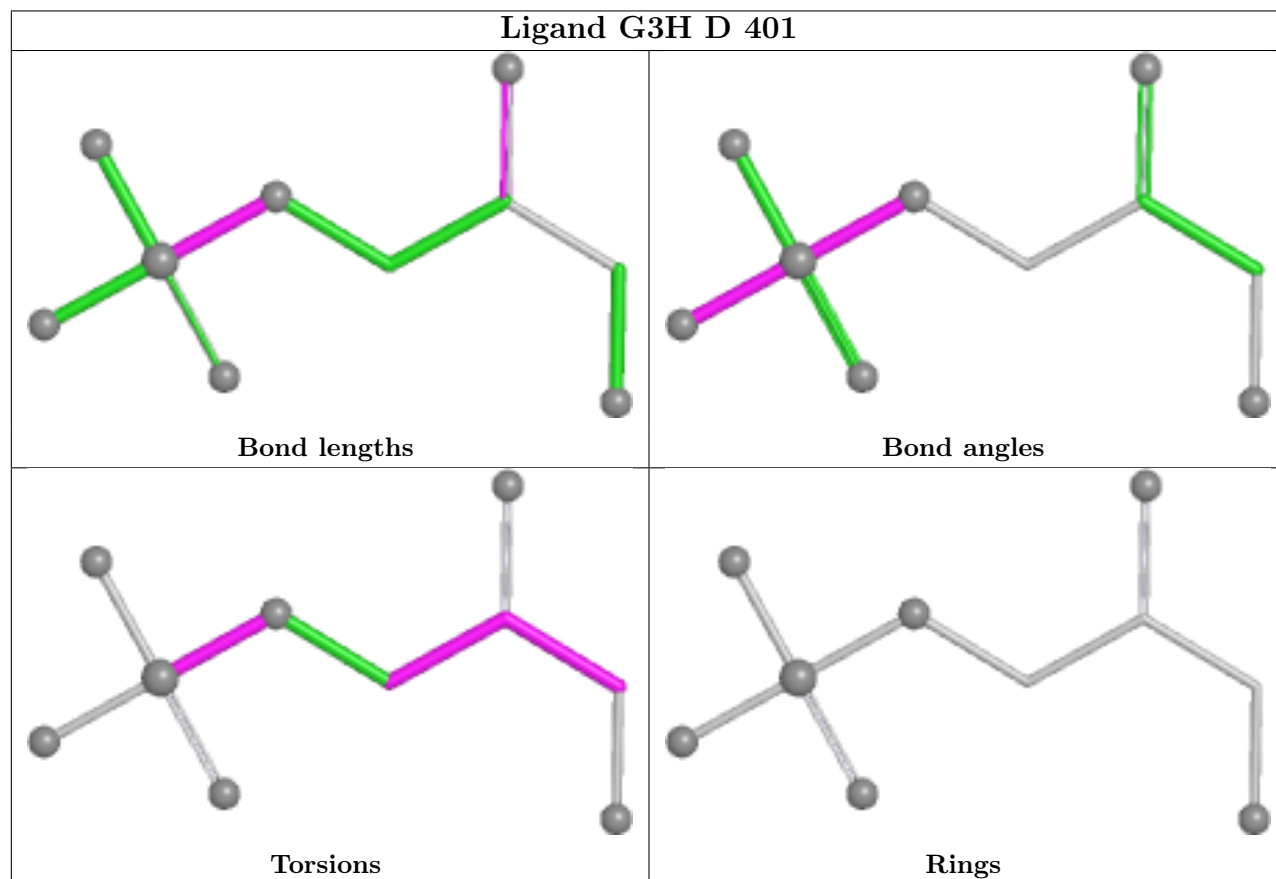
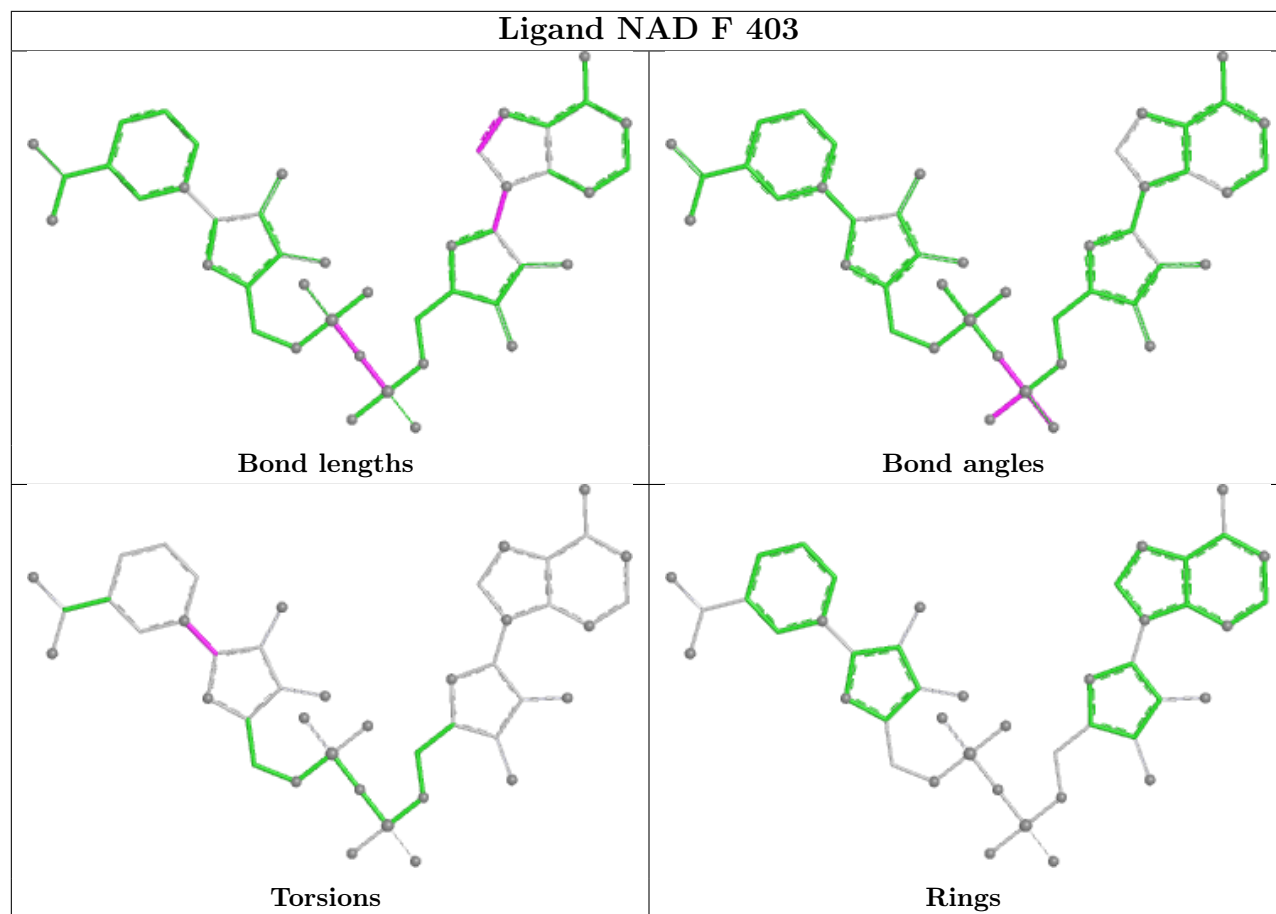
Ligand NAD D 405











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%)	-0.30	7 (2%) 63 69	12, 23, 46, 66	2 (0%)
1	B	334/342 (97%)	-0.35	5 (1%) 71 77	13, 22, 42, 69	3 (0%)
1	C	334/342 (97%)	-0.31	2 (0%) 85 89	13, 24, 42, 72	1 (0%)
1	D	333/342 (97%)	-0.38	0 100 100	14, 23, 42, 69	2 (0%)
1	E	334/342 (97%)	-0.18	7 (2%) 63 69	15, 25, 51, 77	1 (0%)
1	F	332/342 (97%)	-0.25	1 (0%) 90 93	15, 27, 49, 63	1 (0%)
1	G	334/342 (97%)	-0.34	2 (0%) 85 89	13, 23, 42, 71	2 (0%)
1	H	333/342 (97%)	-0.28	1 (0%) 90 93	13, 23, 43, 73	1 (0%)
All	All	2667/2736 (97%)	-0.30	25 (0%) 81 85	12, 24, 45, 77	13 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	334	ILE	4.5
1	E	1	MET	3.9
1	A	332	GLY	3.3
1	C	125	ASN	3.3
1	E	3	ILE	3.2
1	A	126	ASP	3.1
1	A	2	SER	2.9
1	F	3	ILE	2.9
1	A	125	ASN	2.8
1	B	1	MET	2.8
1	B	62	ASP	2.7
1	G	25	HIS	2.7
1	B	334	ILE	2.6
1	A	1	MET	2.5
1	H	61	LYS	2.4
1	A	61	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	61	LYS	2.3
1	B	303	GLY	2.3
1	E	126	ASP	2.2
1	C	61	LYS	2.2
1	G	125	ASN	2.1
1	E	2	SER	2.1
1	A	3	ILE	2.0
1	E	25	HIS	2.0
1	E	59	GLU	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
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

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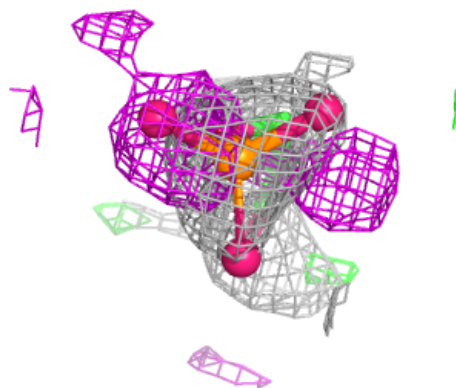
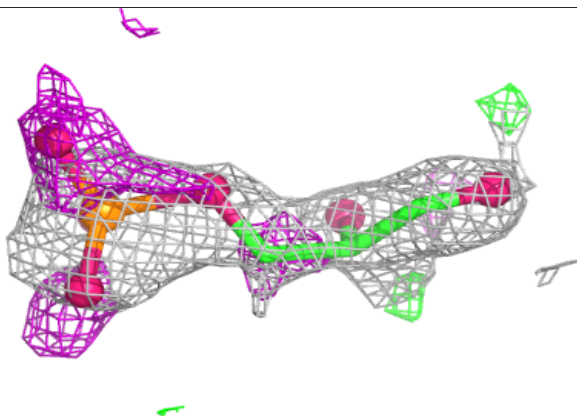
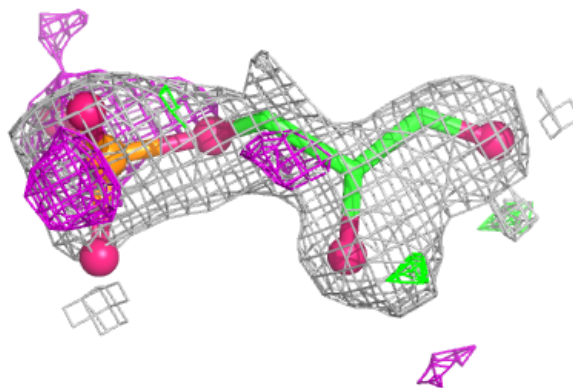
Continued from previous page...

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

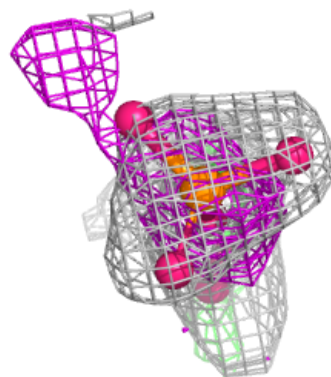
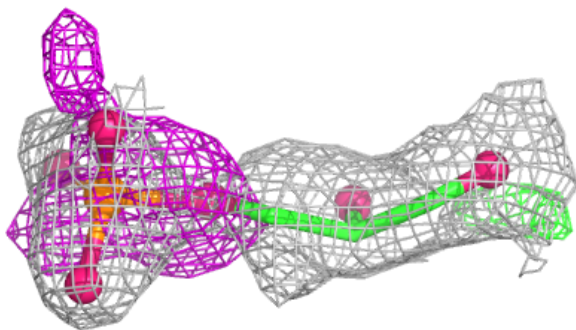
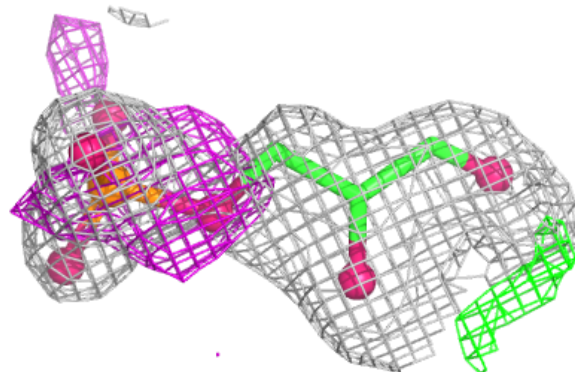
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G3H 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)

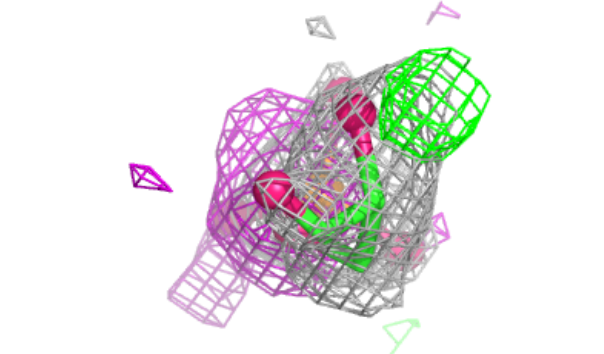
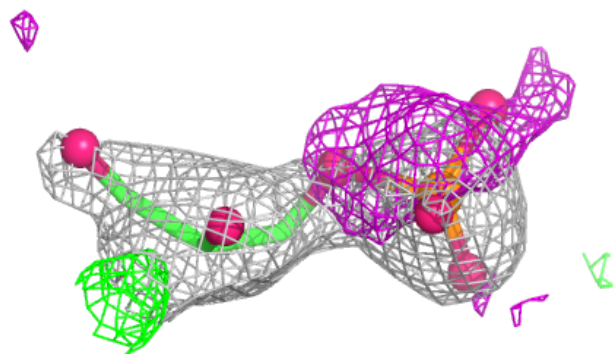
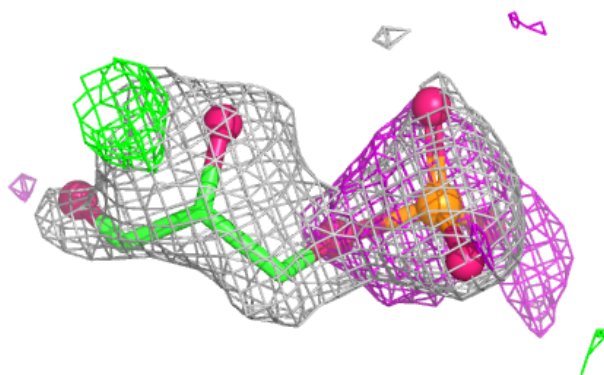
**Electron density around G3H B 401:**

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

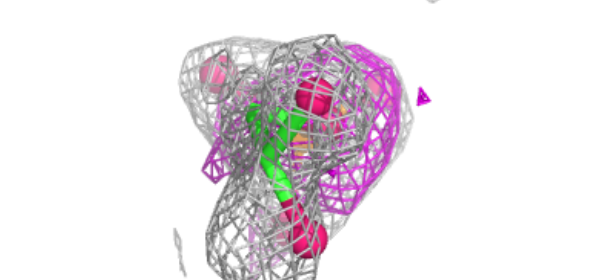
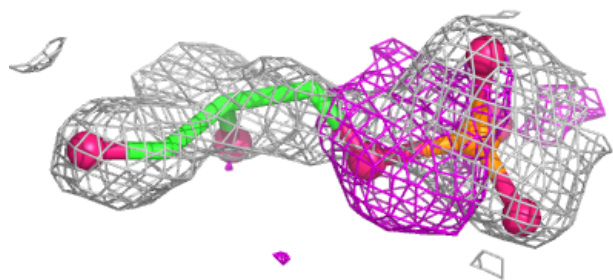
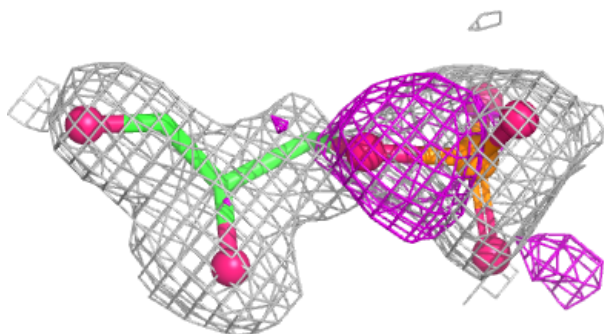


Electron density around G3H F 401:

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

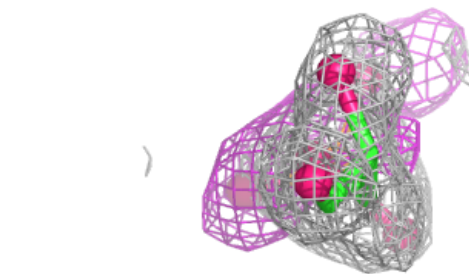
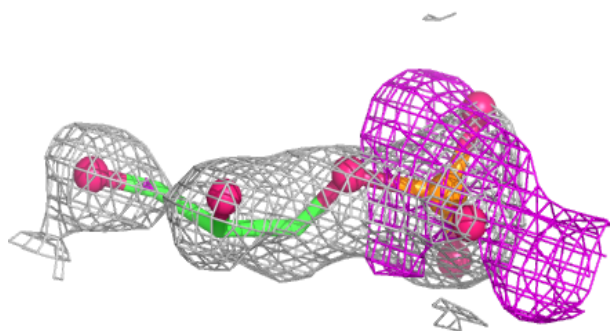
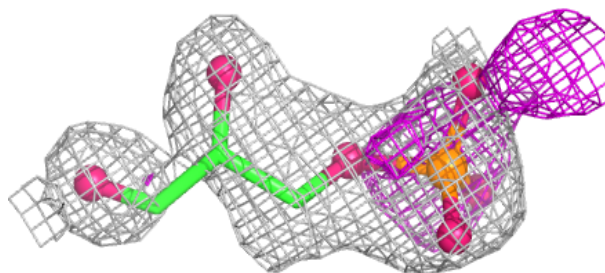
**Electron density around G3H E 401:**

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

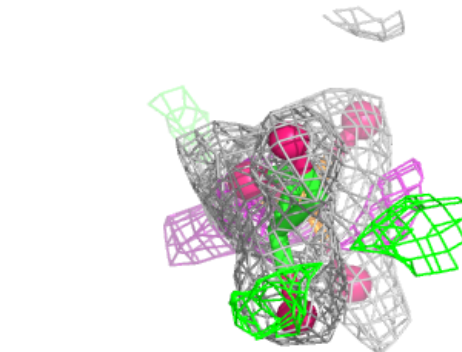
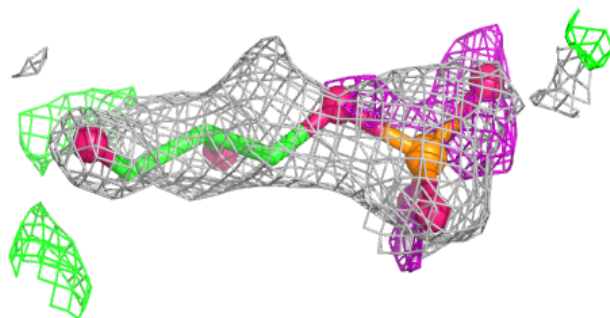
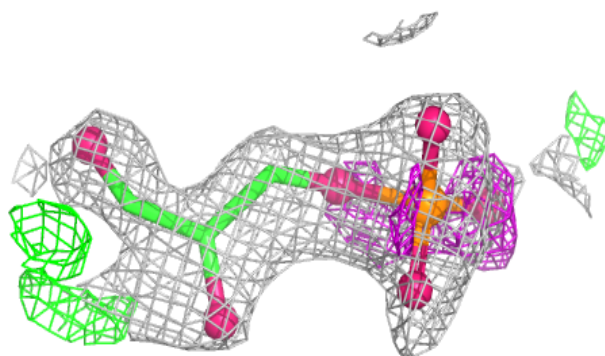


Electron density around G3H H 401:

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

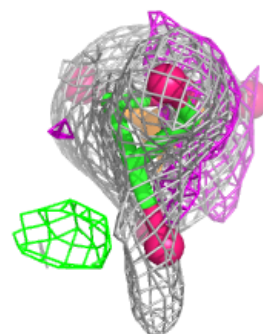
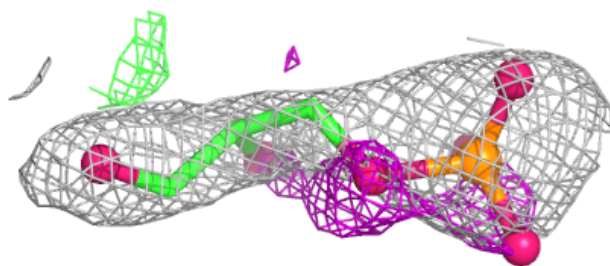
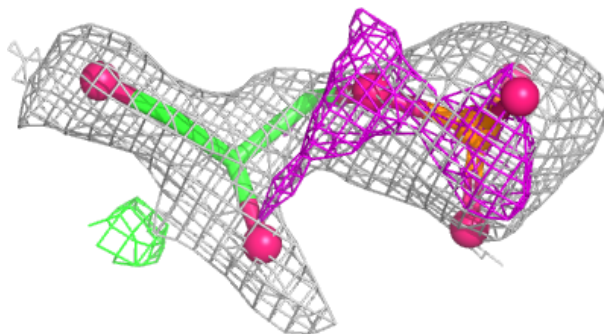
**Electron density around G3H G 401:**

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

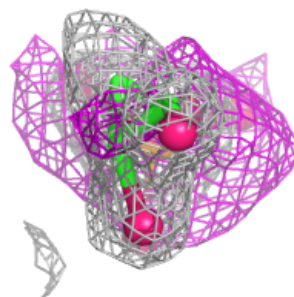
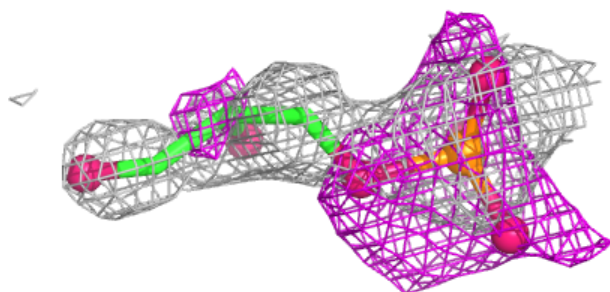
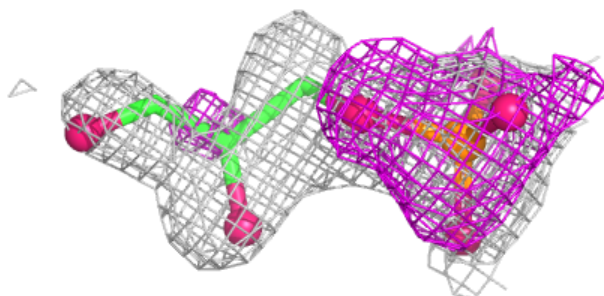


Electron density around G3H A 401:

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

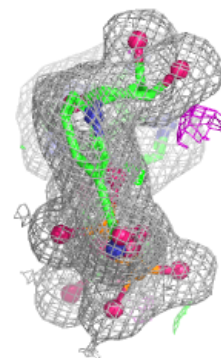
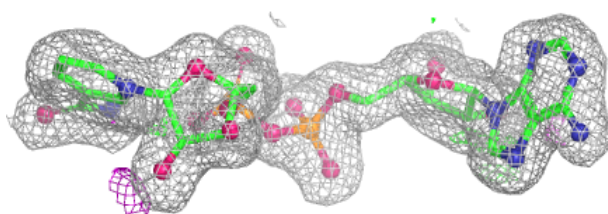
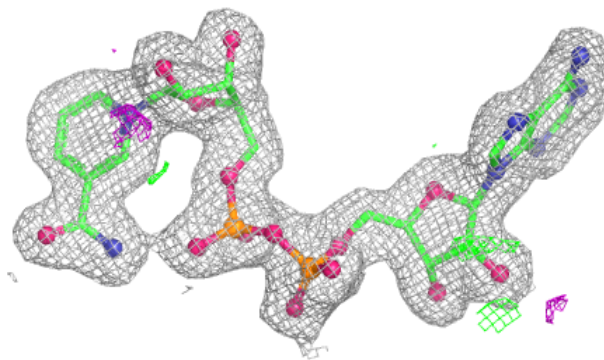
**Electron density around G3H D 401:**

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

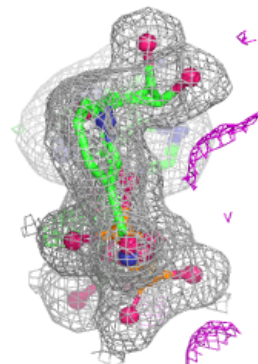
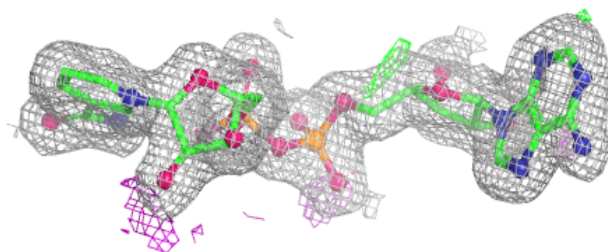
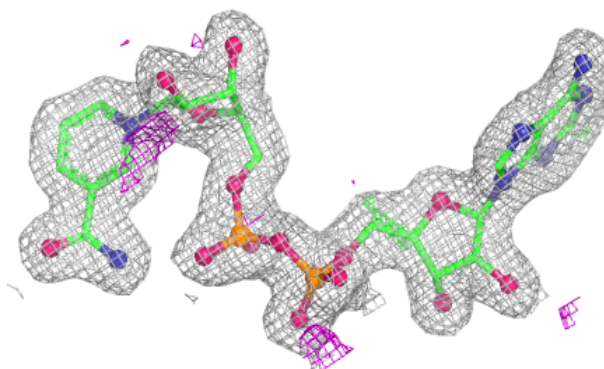


Electron density around NAD C 404:

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

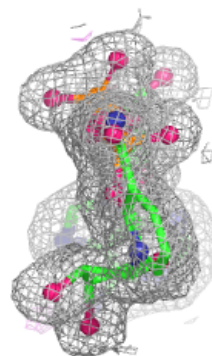
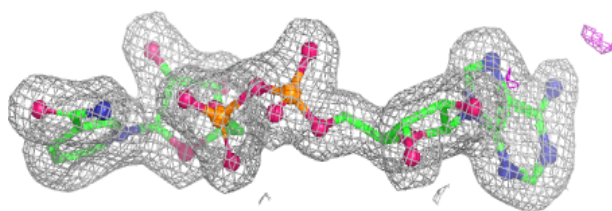
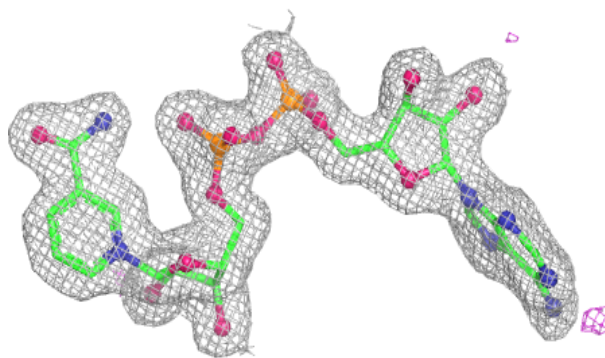
**Electron density around NAD D 405:**

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

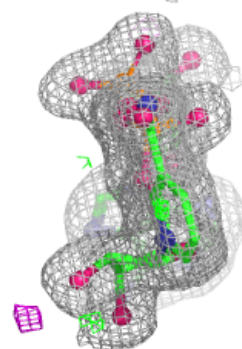
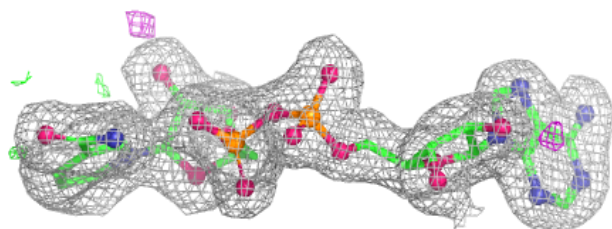
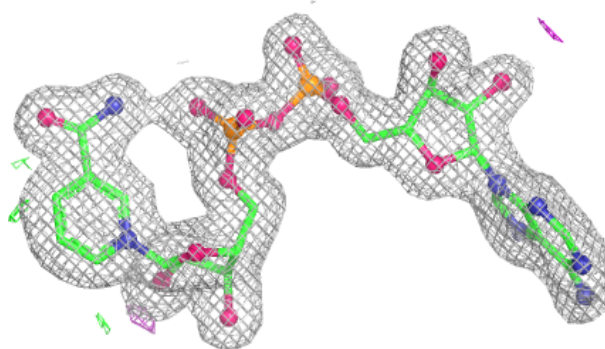


Electron density around NAD E 403:

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

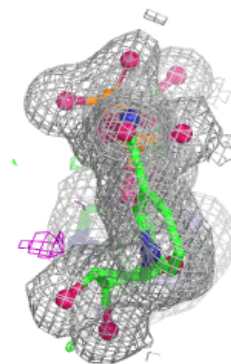
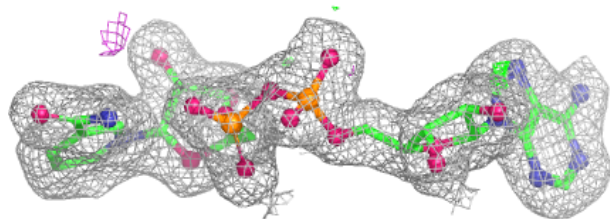
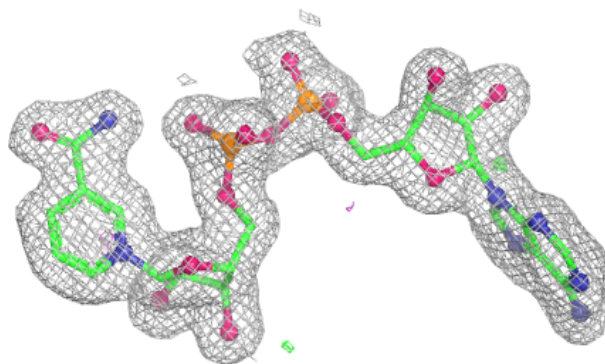
**Electron density around NAD F 403:**

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

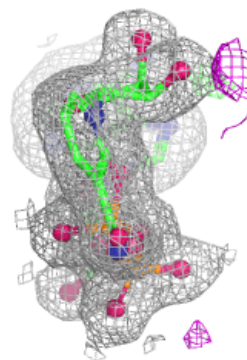
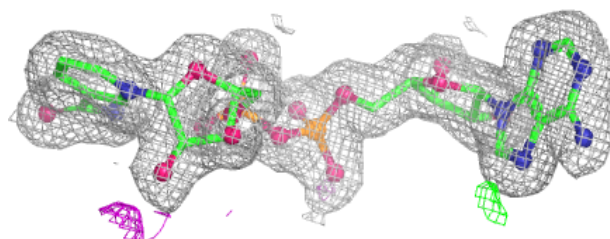
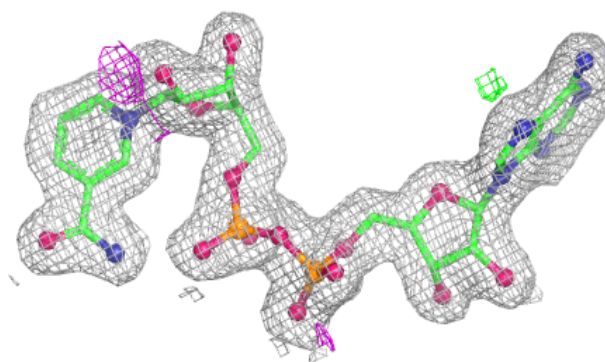


Electron density around NAD G 403:

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

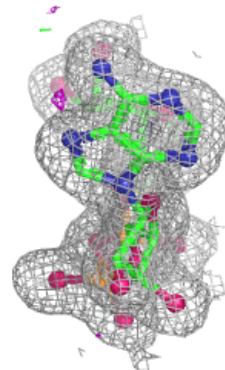
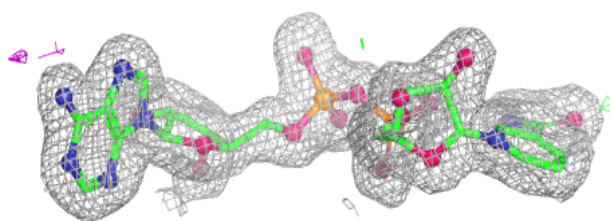
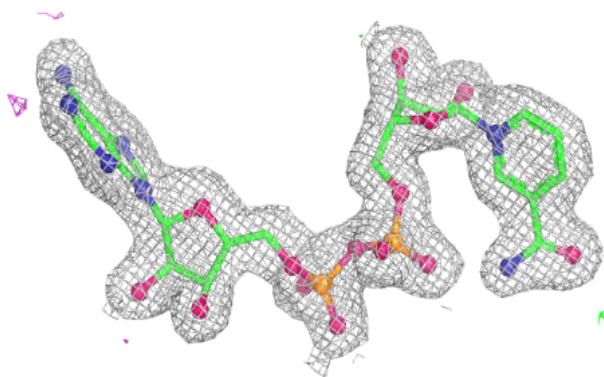
**Electron density around NAD H 403:**

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

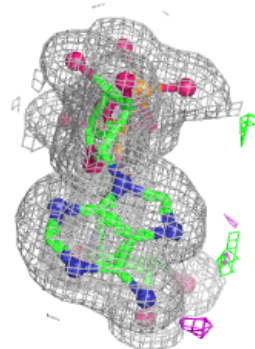
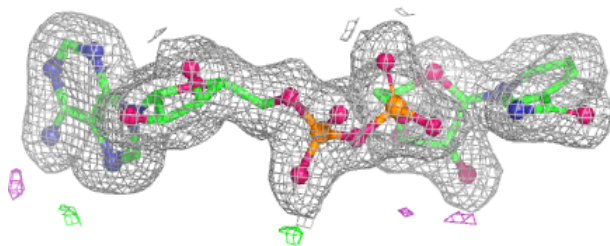
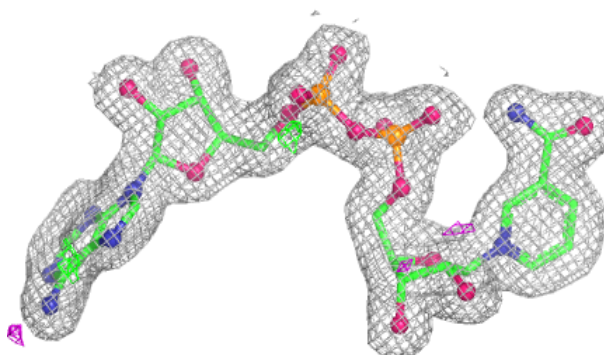


Electron density around NAD A 404:

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

**Electron density around NAD B 403:**

$2mF_o-DF_c$ (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.