



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:59 AM UTC

PDB ID : 8UAT / pdb_00008uat
Title : Thermus scotoductus SA-01 Ene-reductase Compound 3b Complex
Authors : Wilson, L.A.; Guddat, L.W.; Schenk, G.; Scott, C.
Deposited on : 2023-09-22
Resolution : 2.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

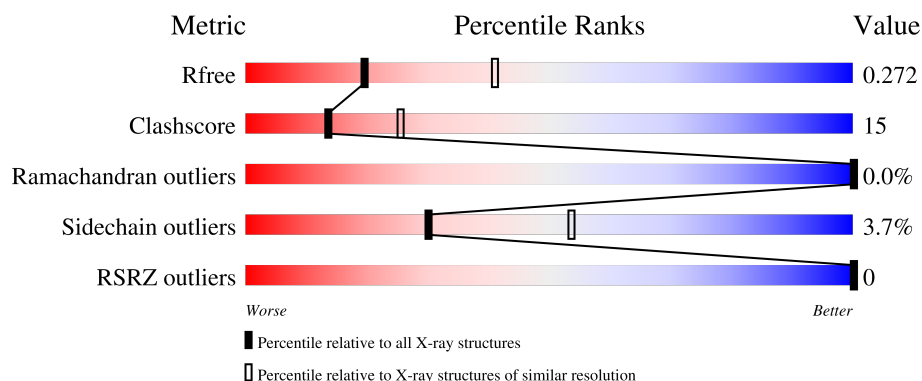
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

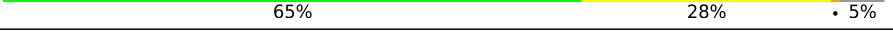
The reported resolution of this entry is 2.76 Å.

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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	369	 62% 32% • 5%
1	B	369	 68% 24% • 5%
1	C	369	 66% 27% • 5%
1	D	369	 65% 28% • 5%
1	E	369	 64% 29% • 5%

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Mol	Chain	Length	Quality of chain
1	F	369	 61%31%• 5%
1	G	369	 68%25%• 5%
1	H	369	 68%25%• 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 43906 atoms, of which 21814 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 NADPH dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	349	Total	C	H	N	O	S	0	1	0
			5425	1723	2732	486	476	8			
1	C	349	Total	C	H	N	O	S	0	1	0
			5425	1723	2732	486	476	8			
1	D	349	Total	C	H	N	O	S	0	0	0
			5386	1717	2704	482	475	8			
1	E	349	Total	C	H	N	O	S	0	1	0
			5418	1723	2725	486	476	8			
1	F	351	Total	C	H	N	O	S	0	2	0
			5465	1738	2745	494	480	8			
1	G	349	Total	C	H	N	O	S	0	1	0
			5402	1723	2709	486	476	8			
1	H	349	Total	C	H	N	O	S	0	0	0
			5401	1717	2719	482	475	8			
1	A	349	Total	C	H	N	O	S	0	1	0
			5425	1723	2732	486	476	8			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP E8PRF1
B	-18	GLY	-	expression tag	UNP E8PRF1
B	-17	SER	-	expression tag	UNP E8PRF1
B	-16	SER	-	expression tag	UNP E8PRF1
B	-15	HIS	-	expression tag	UNP E8PRF1
B	-14	HIS	-	expression tag	UNP E8PRF1
B	-13	HIS	-	expression tag	UNP E8PRF1
B	-12	HIS	-	expression tag	UNP E8PRF1
B	-11	HIS	-	expression tag	UNP E8PRF1
B	-10	HIS	-	expression tag	UNP E8PRF1
B	-9	SER	-	expression tag	UNP E8PRF1
B	-8	SER	-	expression tag	UNP E8PRF1
B	-7	GLY	-	expression tag	UNP E8PRF1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	LEU	-	expression tag	UNP E8PRF1
B	-5	VAL	-	expression tag	UNP E8PRF1
B	-4	PRO	-	expression tag	UNP E8PRF1
B	-3	ARG	-	expression tag	UNP E8PRF1
B	-2	GLY	-	expression tag	UNP E8PRF1
B	-1	SER	-	expression tag	UNP E8PRF1
B	0	HIS	-	expression tag	UNP E8PRF1
B	1	MET	-	expression tag	UNP E8PRF1
B	2	ALA	-	expression tag	UNP E8PRF1
B	3	LEU	-	expression tag	UNP E8PRF1
C	-19	MET	-	initiating methionine	UNP E8PRF1
C	-18	GLY	-	expression tag	UNP E8PRF1
C	-17	SER	-	expression tag	UNP E8PRF1
C	-16	SER	-	expression tag	UNP E8PRF1
C	-15	HIS	-	expression tag	UNP E8PRF1
C	-14	HIS	-	expression tag	UNP E8PRF1
C	-13	HIS	-	expression tag	UNP E8PRF1
C	-12	HIS	-	expression tag	UNP E8PRF1
C	-11	HIS	-	expression tag	UNP E8PRF1
C	-10	HIS	-	expression tag	UNP E8PRF1
C	-9	SER	-	expression tag	UNP E8PRF1
C	-8	SER	-	expression tag	UNP E8PRF1
C	-7	GLY	-	expression tag	UNP E8PRF1
C	-6	LEU	-	expression tag	UNP E8PRF1
C	-5	VAL	-	expression tag	UNP E8PRF1
C	-4	PRO	-	expression tag	UNP E8PRF1
C	-3	ARG	-	expression tag	UNP E8PRF1
C	-2	GLY	-	expression tag	UNP E8PRF1
C	-1	SER	-	expression tag	UNP E8PRF1
C	0	HIS	-	expression tag	UNP E8PRF1
C	1	MET	-	expression tag	UNP E8PRF1
C	2	ALA	-	expression tag	UNP E8PRF1
C	3	LEU	-	expression tag	UNP E8PRF1
D	-19	MET	-	initiating methionine	UNP E8PRF1
D	-18	GLY	-	expression tag	UNP E8PRF1
D	-17	SER	-	expression tag	UNP E8PRF1
D	-16	SER	-	expression tag	UNP E8PRF1
D	-15	HIS	-	expression tag	UNP E8PRF1
D	-14	HIS	-	expression tag	UNP E8PRF1
D	-13	HIS	-	expression tag	UNP E8PRF1
D	-12	HIS	-	expression tag	UNP E8PRF1
D	-11	HIS	-	expression tag	UNP E8PRF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	HIS	-	expression tag	UNP E8PRF1
D	-9	SER	-	expression tag	UNP E8PRF1
D	-8	SER	-	expression tag	UNP E8PRF1
D	-7	GLY	-	expression tag	UNP E8PRF1
D	-6	LEU	-	expression tag	UNP E8PRF1
D	-5	VAL	-	expression tag	UNP E8PRF1
D	-4	PRO	-	expression tag	UNP E8PRF1
D	-3	ARG	-	expression tag	UNP E8PRF1
D	-2	GLY	-	expression tag	UNP E8PRF1
D	-1	SER	-	expression tag	UNP E8PRF1
D	0	HIS	-	expression tag	UNP E8PRF1
D	1	MET	-	expression tag	UNP E8PRF1
D	2	ALA	-	expression tag	UNP E8PRF1
D	3	LEU	-	expression tag	UNP E8PRF1
E	-19	MET	-	initiating methionine	UNP E8PRF1
E	-18	GLY	-	expression tag	UNP E8PRF1
E	-17	SER	-	expression tag	UNP E8PRF1
E	-16	SER	-	expression tag	UNP E8PRF1
E	-15	HIS	-	expression tag	UNP E8PRF1
E	-14	HIS	-	expression tag	UNP E8PRF1
E	-13	HIS	-	expression tag	UNP E8PRF1
E	-12	HIS	-	expression tag	UNP E8PRF1
E	-11	HIS	-	expression tag	UNP E8PRF1
E	-10	HIS	-	expression tag	UNP E8PRF1
E	-9	SER	-	expression tag	UNP E8PRF1
E	-8	SER	-	expression tag	UNP E8PRF1
E	-7	GLY	-	expression tag	UNP E8PRF1
E	-6	LEU	-	expression tag	UNP E8PRF1
E	-5	VAL	-	expression tag	UNP E8PRF1
E	-4	PRO	-	expression tag	UNP E8PRF1
E	-3	ARG	-	expression tag	UNP E8PRF1
E	-2	GLY	-	expression tag	UNP E8PRF1
E	-1	SER	-	expression tag	UNP E8PRF1
E	0	HIS	-	expression tag	UNP E8PRF1
E	1	MET	-	expression tag	UNP E8PRF1
E	2	ALA	-	expression tag	UNP E8PRF1
E	3	LEU	-	expression tag	UNP E8PRF1
F	-19	MET	-	initiating methionine	UNP E8PRF1
F	-18	GLY	-	expression tag	UNP E8PRF1
F	-17	SER	-	expression tag	UNP E8PRF1
F	-16	SER	-	expression tag	UNP E8PRF1
F	-15	HIS	-	expression tag	UNP E8PRF1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	HIS	-	expression tag	UNP E8PRF1
F	-13	HIS	-	expression tag	UNP E8PRF1
F	-12	HIS	-	expression tag	UNP E8PRF1
F	-11	HIS	-	expression tag	UNP E8PRF1
F	-10	HIS	-	expression tag	UNP E8PRF1
F	-9	SER	-	expression tag	UNP E8PRF1
F	-8	SER	-	expression tag	UNP E8PRF1
F	-7	GLY	-	expression tag	UNP E8PRF1
F	-6	LEU	-	expression tag	UNP E8PRF1
F	-5	VAL	-	expression tag	UNP E8PRF1
F	-4	PRO	-	expression tag	UNP E8PRF1
F	-3	ARG	-	expression tag	UNP E8PRF1
F	-2	GLY	-	expression tag	UNP E8PRF1
F	-1	SER	-	expression tag	UNP E8PRF1
F	0	HIS	-	expression tag	UNP E8PRF1
F	1	MET	-	expression tag	UNP E8PRF1
F	2	ALA	-	expression tag	UNP E8PRF1
F	3	LEU	-	expression tag	UNP E8PRF1
G	-19	MET	-	initiating methionine	UNP E8PRF1
G	-18	GLY	-	expression tag	UNP E8PRF1
G	-17	SER	-	expression tag	UNP E8PRF1
G	-16	SER	-	expression tag	UNP E8PRF1
G	-15	HIS	-	expression tag	UNP E8PRF1
G	-14	HIS	-	expression tag	UNP E8PRF1
G	-13	HIS	-	expression tag	UNP E8PRF1
G	-12	HIS	-	expression tag	UNP E8PRF1
G	-11	HIS	-	expression tag	UNP E8PRF1
G	-10	HIS	-	expression tag	UNP E8PRF1
G	-9	SER	-	expression tag	UNP E8PRF1
G	-8	SER	-	expression tag	UNP E8PRF1
G	-7	GLY	-	expression tag	UNP E8PRF1
G	-6	LEU	-	expression tag	UNP E8PRF1
G	-5	VAL	-	expression tag	UNP E8PRF1
G	-4	PRO	-	expression tag	UNP E8PRF1
G	-3	ARG	-	expression tag	UNP E8PRF1
G	-2	GLY	-	expression tag	UNP E8PRF1
G	-1	SER	-	expression tag	UNP E8PRF1
G	0	HIS	-	expression tag	UNP E8PRF1
G	1	MET	-	expression tag	UNP E8PRF1
G	2	ALA	-	expression tag	UNP E8PRF1
G	3	LEU	-	expression tag	UNP E8PRF1
H	-19	MET	-	initiating methionine	UNP E8PRF1

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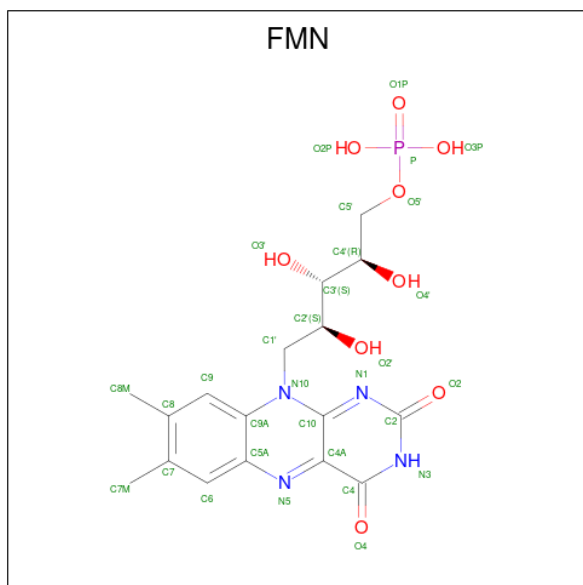
Chain	Residue	Modelled	Actual	Comment	Reference
H	-18	GLY	-	expression tag	UNP E8PRF1
H	-17	SER	-	expression tag	UNP E8PRF1
H	-16	SER	-	expression tag	UNP E8PRF1
H	-15	HIS	-	expression tag	UNP E8PRF1
H	-14	HIS	-	expression tag	UNP E8PRF1
H	-13	HIS	-	expression tag	UNP E8PRF1
H	-12	HIS	-	expression tag	UNP E8PRF1
H	-11	HIS	-	expression tag	UNP E8PRF1
H	-10	HIS	-	expression tag	UNP E8PRF1
H	-9	SER	-	expression tag	UNP E8PRF1
H	-8	SER	-	expression tag	UNP E8PRF1
H	-7	GLY	-	expression tag	UNP E8PRF1
H	-6	LEU	-	expression tag	UNP E8PRF1
H	-5	VAL	-	expression tag	UNP E8PRF1
H	-4	PRO	-	expression tag	UNP E8PRF1
H	-3	ARG	-	expression tag	UNP E8PRF1
H	-2	GLY	-	expression tag	UNP E8PRF1
H	-1	SER	-	expression tag	UNP E8PRF1
H	0	HIS	-	expression tag	UNP E8PRF1
H	1	MET	-	expression tag	UNP E8PRF1
H	2	ALA	-	expression tag	UNP E8PRF1
H	3	LEU	-	expression tag	UNP E8PRF1
A	-19	MET	-	initiating methionine	UNP E8PRF1
A	-18	GLY	-	expression tag	UNP E8PRF1
A	-17	SER	-	expression tag	UNP E8PRF1
A	-16	SER	-	expression tag	UNP E8PRF1
A	-15	HIS	-	expression tag	UNP E8PRF1
A	-14	HIS	-	expression tag	UNP E8PRF1
A	-13	HIS	-	expression tag	UNP E8PRF1
A	-12	HIS	-	expression tag	UNP E8PRF1
A	-11	HIS	-	expression tag	UNP E8PRF1
A	-10	HIS	-	expression tag	UNP E8PRF1
A	-9	SER	-	expression tag	UNP E8PRF1
A	-8	SER	-	expression tag	UNP E8PRF1
A	-7	GLY	-	expression tag	UNP E8PRF1
A	-6	LEU	-	expression tag	UNP E8PRF1
A	-5	VAL	-	expression tag	UNP E8PRF1
A	-4	PRO	-	expression tag	UNP E8PRF1
A	-3	ARG	-	expression tag	UNP E8PRF1
A	-2	GLY	-	expression tag	UNP E8PRF1
A	-1	SER	-	expression tag	UNP E8PRF1
A	0	HIS	-	expression tag	UNP E8PRF1

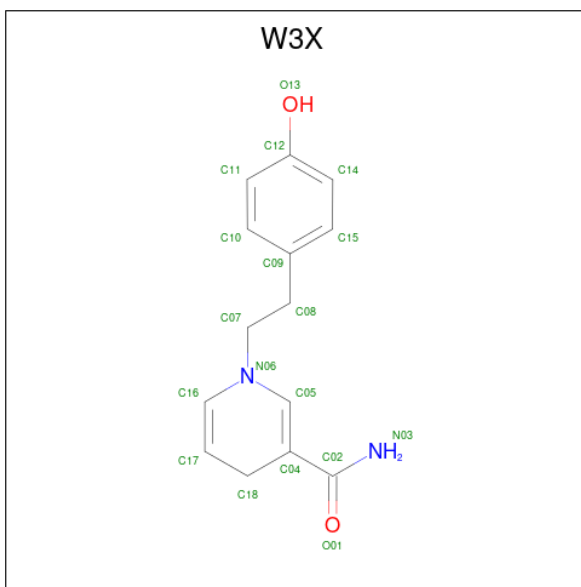
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP E8PRF1
A	2	ALA	-	expression tag	UNP E8PRF1
A	3	LEU	-	expression tag	UNP E8PRF1

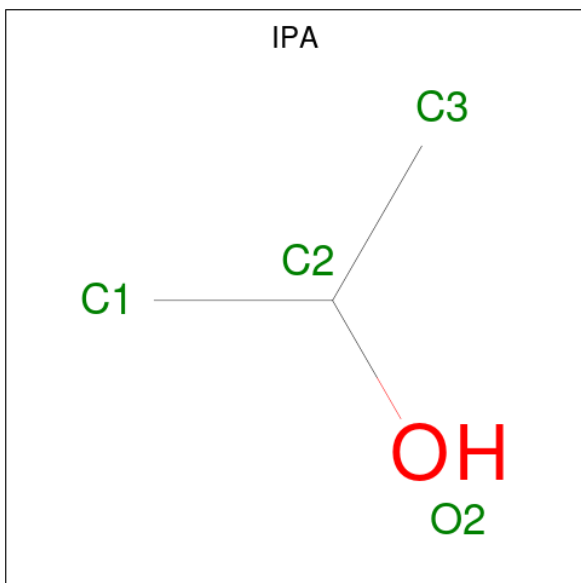
- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			18	14	2	2		
3	E	1	Total	C	N	O	0	0
			9	6	2	1		
3	F	1	Total	C	N	O	0	0
			9	6	2	1		
3	A	1	Total	C	N	O	0	0
			18	14	2	2		

- Molecule 4 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C H O 12 3 8 1	0	0
4	H	1	Total C H O 12 3 8 1	0	0

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

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Cl 1 1	0	0

- Molecule 7 is water.

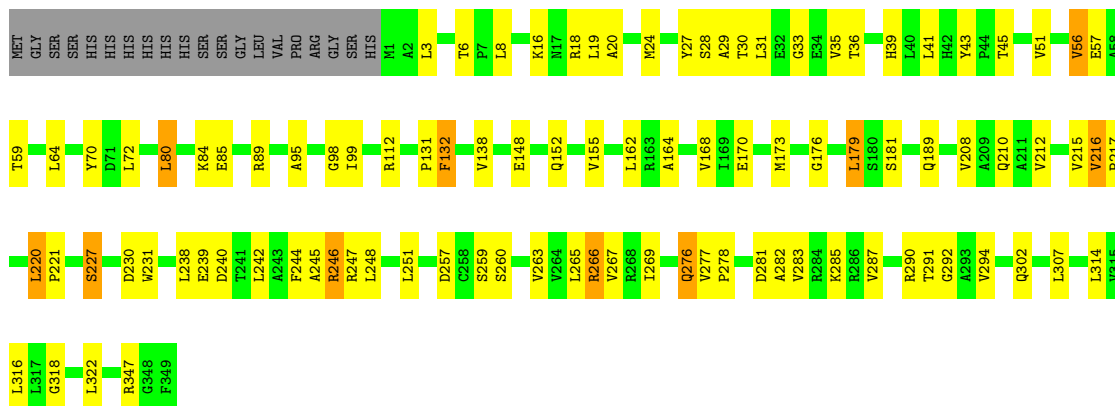
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	28	Total O 28 28	0	0
7	C	31	Total O 31 31	0	0
7	D	18	Total O 18 18	0	0
7	E	25	Total O 25 25	0	0
7	F	37	Total O 37 37	0	0
7	G	30	Total O 30 30	0	0
7	H	28	Total O 28 28	0	0
7	A	34	Total O 34 34	0	0

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.

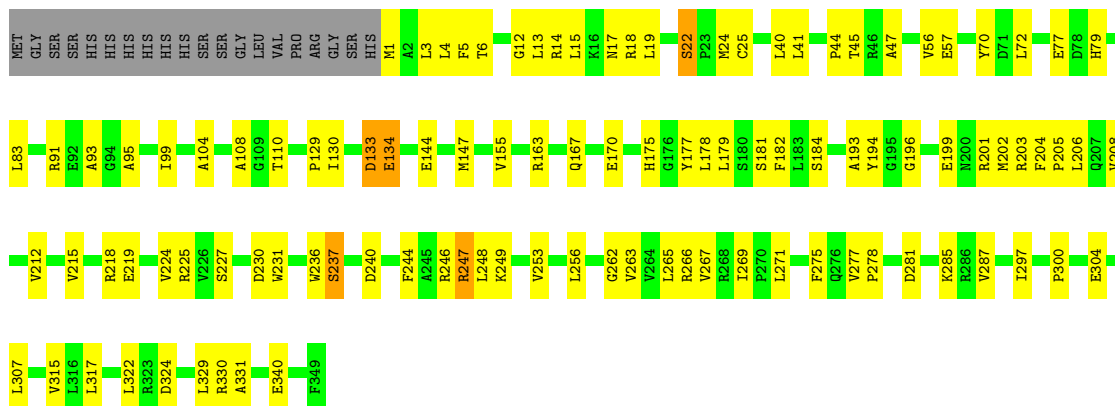
- Molecule 1: NADPH dehydrogenase

Chain B: 



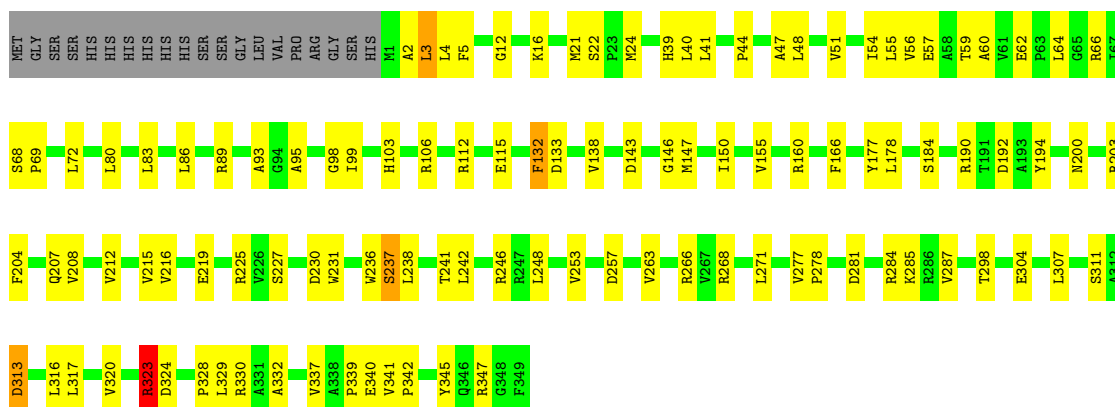
- Molecule 1: NADPH dehydrogenase

Chain C: 

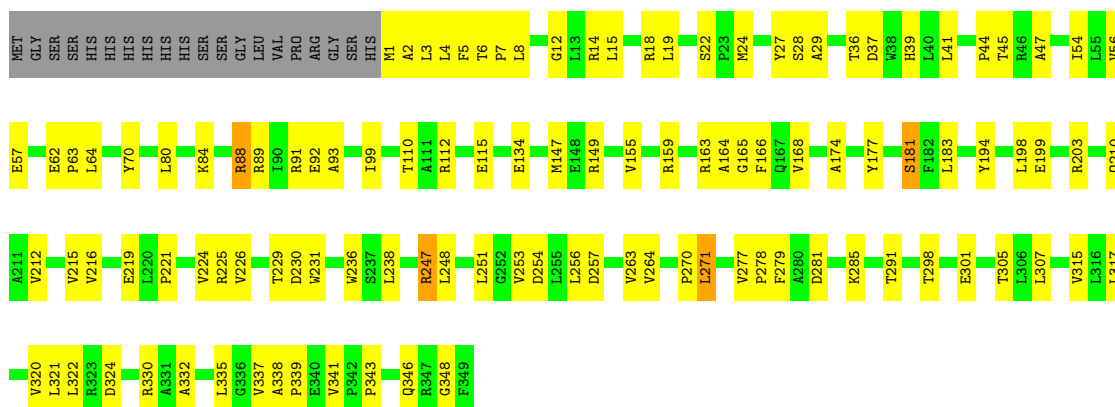


- Molecule 1: NADPH dehydrogenase

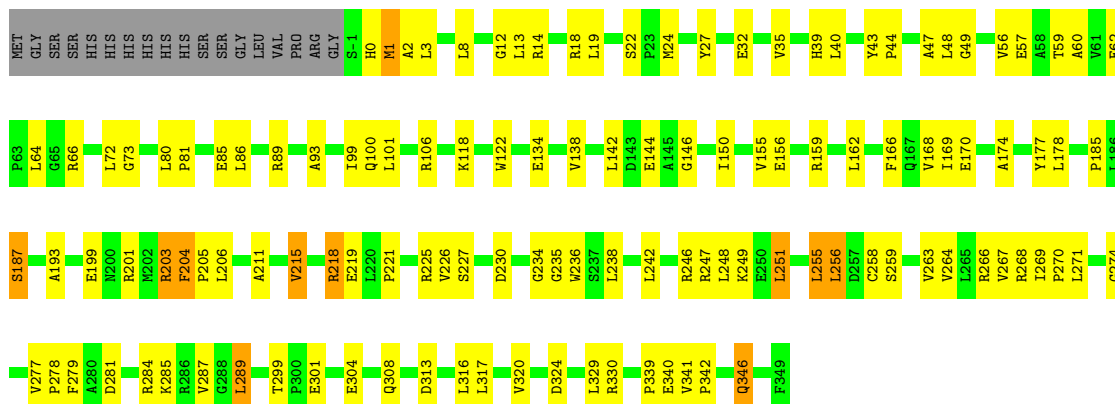
Chain D: 



- Molecule 1: NADPH dehydrogenase

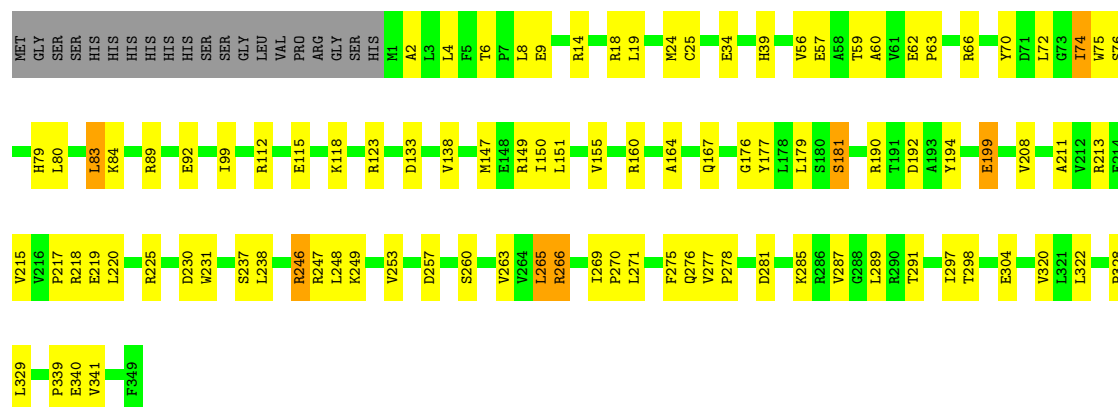


- Molecule 1: NADPH dehydrogenase



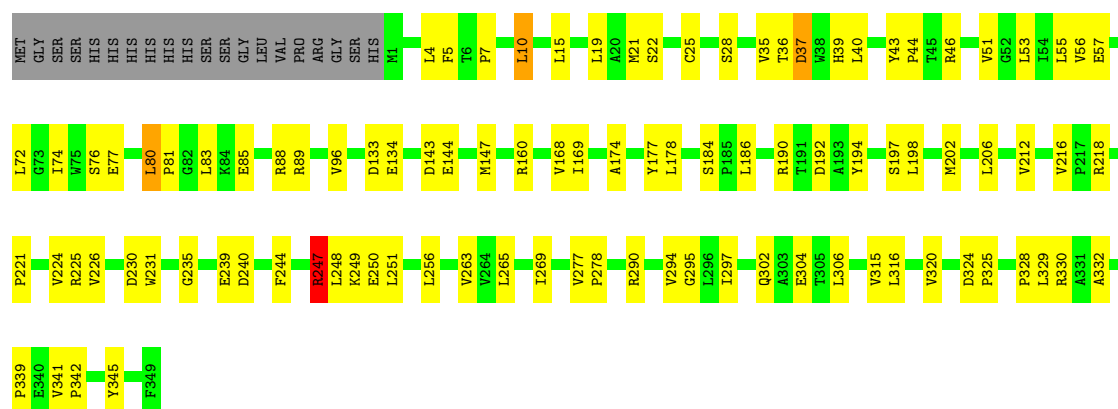
- Molecule 1: NADPH dehydrogenase





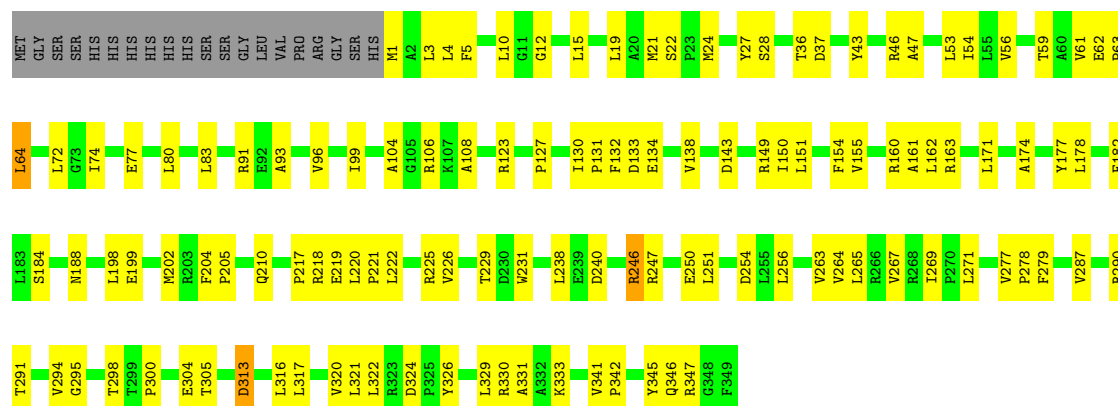
• Molecule 1: NADPH dehydrogenase

Chain H: 68% 25% • 5%



• Molecule 1: NADPH dehydrogenase

Chain A: 62% 32% • 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.85Å 100.47Å 100.41Å 89.80° 65.75° 89.92°	Depositor
Resolution (Å)	48.75 – 2.76 48.75 – 2.76	Depositor EDS
% Data completeness (in resolution range)	92.9 (48.75-2.76) 92.5 (48.75-2.76)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.233 , 0.271 0.233 , 0.272	Depositor DCC
R_{free} test set	2007 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.377 for -h,k,-l 0.016 for l,-k,h 0.023 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	43906	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, W3X, NA, FMN, IPA

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	0.41	0/2758	0.49	0/3749
1	B	0.49	0/2758	0.56	6/3749 (0.2%)
1	C	0.35	0/2758	0.51	3/3749 (0.1%)
1	D	0.37	0/2747	0.49	1/3735 (0.0%)
1	E	0.34	0/2758	0.52	4/3749 (0.1%)
1	F	0.45	0/2786	0.55	4/3786 (0.1%)
1	G	0.54	1/2758 (0.0%)	0.63	2/3749 (0.1%)
1	H	0.40	0/2747	0.51	1/3735 (0.0%)
All	All	0.42	1/22070 (0.0%)	0.54	21/30001 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	83	LEU	CG-CD1	5.24	1.69	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	134	GLU	CA-CB-CG	-10.75	92.60	114.10
1	B	132	PHE	N-CA-C	-9.23	101.29	111.36
1	D	132	PHE	N-CA-C	-7.22	103.35	111.07
1	G	265	LEU	N-CA-C	-6.96	99.01	109.94
1	E	271	LEU	CA-CB-CG	6.67	139.65	116.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	245	ALA	Mainchain
1	D	323	ARG	Sidechain
1	E	247	ARG	Sidechain
1	H	247	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	2693	2732	2743	95	0
1	B	2693	2732	2743	77	0
1	C	2693	2732	2743	69	2
1	D	2682	2704	2731	82	0
1	E	2693	2725	2743	77	2
1	F	2720	2745	2767	94	1
1	G	2693	2709	2743	81	0
1	H	2682	2719	2731	73	1
2	A	31	0	19	6	0
2	B	31	0	19	3	0
2	C	31	0	19	2	0
2	D	31	0	19	5	0
2	E	31	0	19	2	0
2	F	31	0	19	3	0
2	G	31	0	19	3	0
2	H	31	0	19	4	0
3	A	18	0	0	3	0
3	B	18	0	0	1	0
3	E	9	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	9	0	0	1	0
4	E	4	8	8	2	0
4	H	4	8	8	0	0
5	F	1	0	0	0	0
6	F	1	0	0	0	0
7	A	34	0	0	3	0
7	B	28	0	0	7	0
7	C	31	0	0	1	0
7	D	18	0	0	2	0
7	E	25	0	0	2	0
7	F	37	0	0	6	0
7	G	30	0	0	3	0
7	H	28	0	0	0	0
All	All	22092	21814	22112	642	3

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 15.

The worst 5 of 642 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:D:284:ARG:NH1	1:D:313:ASP:OD1	2.01	0.93
1:E:62:GLU:OE2	1:E:149:ARG:NH1	2.06	0.88
1:A:218:ARG:O	7:A:501:HOH:O	1.96	0.83
1:G:24:MET:CE	1:G:322:LEU:HD21	2.09	0.82
1:H:169:ILE:HD11	1:H:216:VAL:HG21	1.63	0.81

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ARG:NH1	1:E:199:GLU:OE2[1_456]	1.60	0.60
1:C:203:ARG:HH12	1:E:199:GLU:OE2[1_456]	1.14	0.46
1:F:218:ARG:HH12	1:H:143:ASP:OD2[1_554]	1.45	0.15

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	348/369 (94%)	326 (94%)	21 (6%)	1 (0%)	36	56
1	B	348/369 (94%)	333 (96%)	15 (4%)	0	100	100
1	C	348/369 (94%)	332 (95%)	16 (5%)	0	100	100
1	D	347/369 (94%)	328 (94%)	19 (6%)	0	100	100
1	E	348/369 (94%)	331 (95%)	17 (5%)	0	100	100
1	F	351/369 (95%)	330 (94%)	21 (6%)	0	100	100
1	G	348/369 (94%)	332 (95%)	16 (5%)	0	100	100
1	H	347/369 (94%)	329 (95%)	18 (5%)	0	100	100
All	All	2785/2952 (94%)	2641 (95%)	143 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	PRO

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	276/292 (94%)	269 (98%)	7 (2%)	42	64
1	B	276/292 (94%)	263 (95%)	13 (5%)	23	45
1	C	276/292 (94%)	268 (97%)	8 (3%)	37	61
1	D	275/292 (94%)	263 (96%)	12 (4%)	25	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	276/292 (94%)	269 (98%)	7 (2%)	42 64
1	F	279/292 (96%)	261 (94%)	18 (6%)	15 29
1	G	276/292 (94%)	264 (96%)	12 (4%)	26 47
1	H	275/292 (94%)	266 (97%)	9 (3%)	33 57
All	All	2209/2336 (95%)	2123 (96%)	86 (4%)	30 51

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	346	GLN
1	H	37	ASP
1	G	74	ILE
1	G	199	GLU
1	H	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	42	HIS
1	A	39	HIS
1	G	152	GLN
1	A	276	GLN
1	H	39	HIS

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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	W3X	B	402	-	19,19,19	2.86	7 (36%)	18,25,25	1.18	1 (5%)
2	FMN	C	401	-	33,33,33	2.75	10 (30%)	48,50,50	2.10	14 (29%)
3	W3X	A	402	-	19,19,19	2.87	8 (42%)	18,25,25	0.98	1 (5%)
3	W3X	E	403	-	8,9,19	5.53	6 (75%)	6,11,25	1.35	0
2	FMN	H	401	-	33,33,33	2.78	10 (30%)	48,50,50	2.04	13 (27%)
4	IPA	E	402	-	3,3,3	0.50	0	3,3,3	0.47	0
4	IPA	H	402	-	3,3,3	0.51	0	3,3,3	0.46	0
2	FMN	F	401	-	33,33,33	2.76	11 (33%)	48,50,50	2.07	12 (25%)
2	FMN	A	401	-	33,33,33	2.75	10 (30%)	48,50,50	2.07	13 (27%)
3	W3X	F	404	-	8,9,19	5.51	6 (75%)	6,11,25	1.67	2 (33%)
2	FMN	D	401	-	33,33,33	2.74	10 (30%)	48,50,50	2.08	14 (29%)
2	FMN	G	401	-	33,33,33	2.78	10 (30%)	48,50,50	2.03	12 (25%)
2	FMN	B	401	-	33,33,33	2.78	10 (30%)	48,50,50	2.09	12 (25%)
2	FMN	E	401	-	33,33,33	2.78	10 (30%)	48,50,50	2.10	12 (25%)

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	W3X	B	402	-	-	4/8/19/19	0/2/2/2
2	FMN	C	401	-	-	5/18/18/18	0/3/3/3
3	W3X	A	402	-	-	5/8/19/19	0/2/2/2
3	W3X	E	403	-	-	0/3/12/19	0/1/1/2
2	FMN	H	401	-	-	4/18/18/18	0/3/3/3
2	FMN	F	401	-	-	1/18/18/18	0/3/3/3
2	FMN	A	401	-	-	8/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	W3X	F	404	-	-	1/3/12/19	0/1/1/2
2	FMN	D	401	-	-	1/18/18/18	0/3/3/3
2	FMN	G	401	-	-	1/18/18/18	0/3/3/3
2	FMN	B	401	-	-	2/18/18/18	0/3/3/3
2	FMN	E	401	-	-	8/18/18/18	0/3/3/3

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	403	W3X	C05-C04	11.68	1.53	1.36
3	F	404	W3X	C05-C04	11.60	1.53	1.36
3	F	404	W3X	C05-N06	7.95	1.45	1.35
3	E	403	W3X	C05-N06	7.95	1.45	1.35
2	H	401	FMN	C4A-N5	6.84	1.45	1.30

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FMN	C7M-C7-C6	-7.95	105.57	119.57
2	E	401	FMN	C7M-C7-C6	-7.91	105.63	119.57
2	B	401	FMN	C7M-C7-C6	-7.88	105.69	119.57
2	A	401	FMN	C7M-C7-C6	-7.88	105.69	119.57
2	D	401	FMN	C7M-C7-C6	-7.86	105.72	119.57

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	FMN	C5'-O5'-P-O2P
2	E	401	FMN	C5'-O5'-P-O3P
2	H	401	FMN	C5'-O5'-P-O3P
2	A	401	FMN	C5'-O5'-P-O2P
2	A	401	FMN	C5'-O5'-P-O3P

There are no ring outliers.

13 monomers are involved in 35 short contacts:

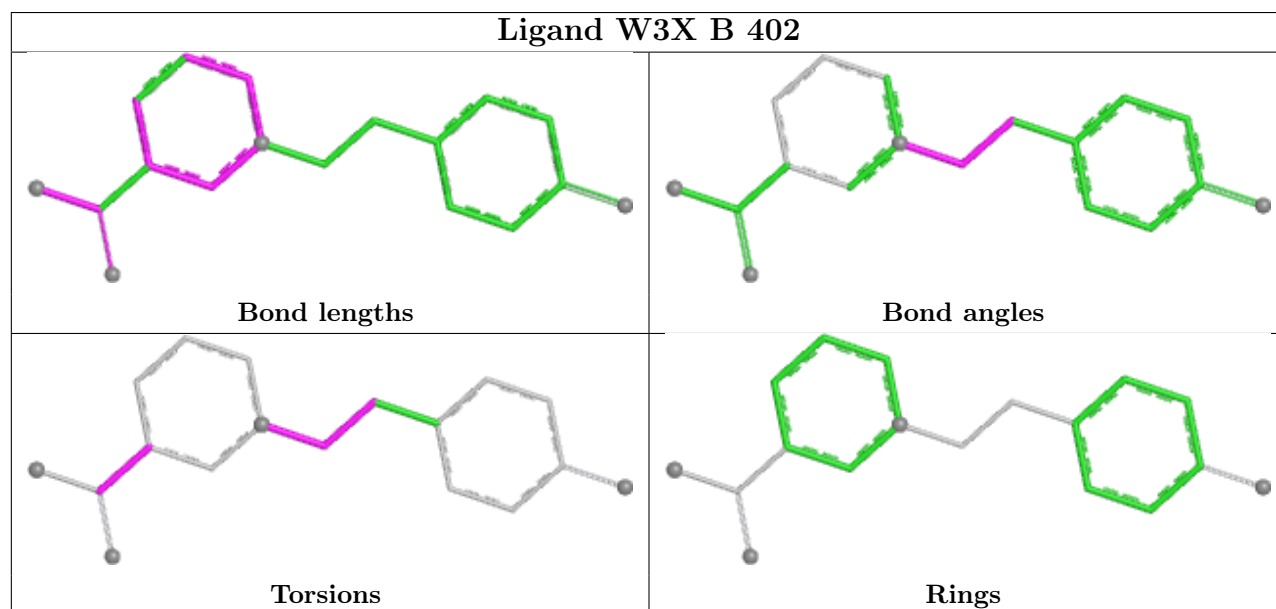
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	W3X	1	0
2	C	401	FMN	2	0

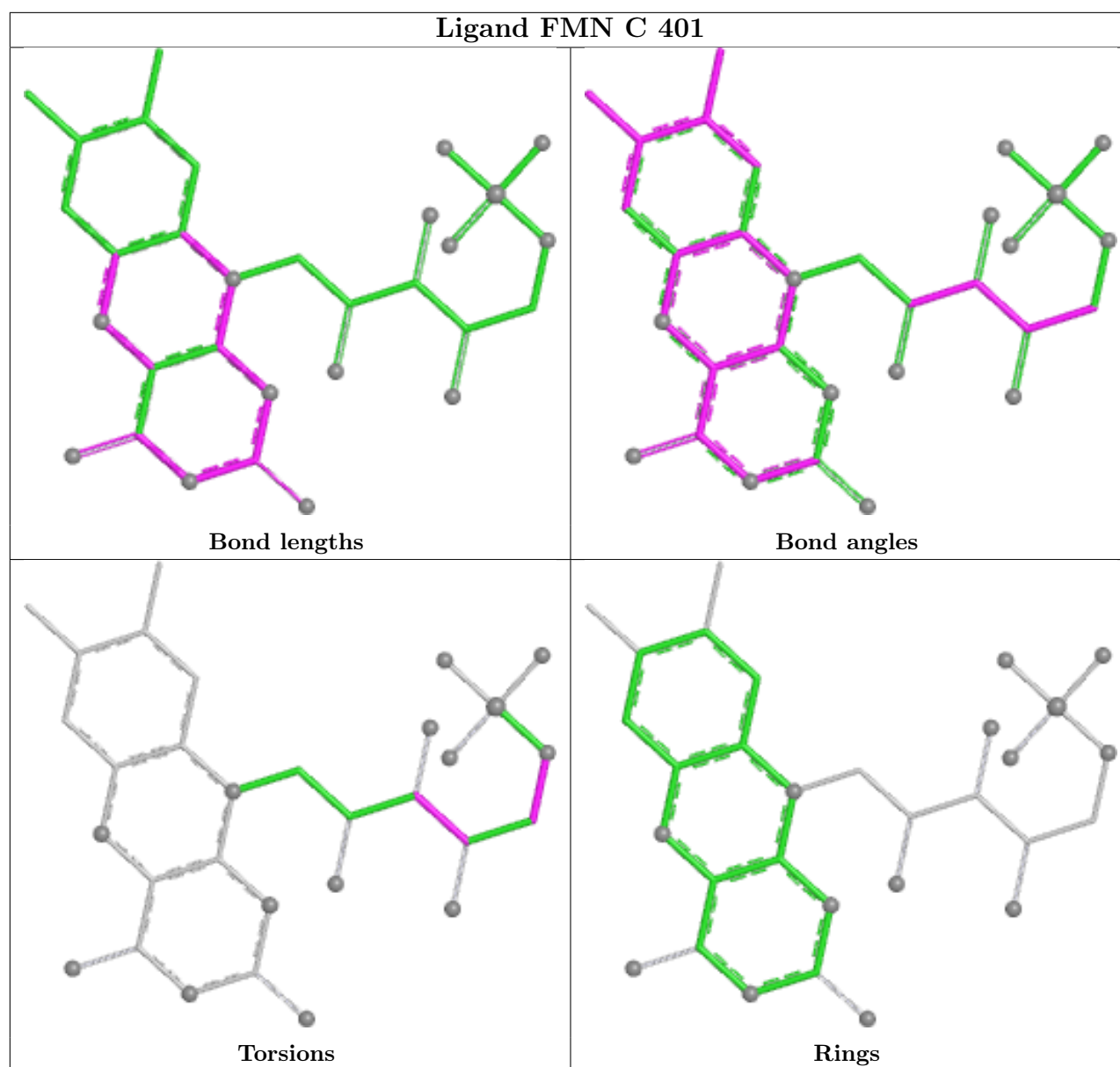
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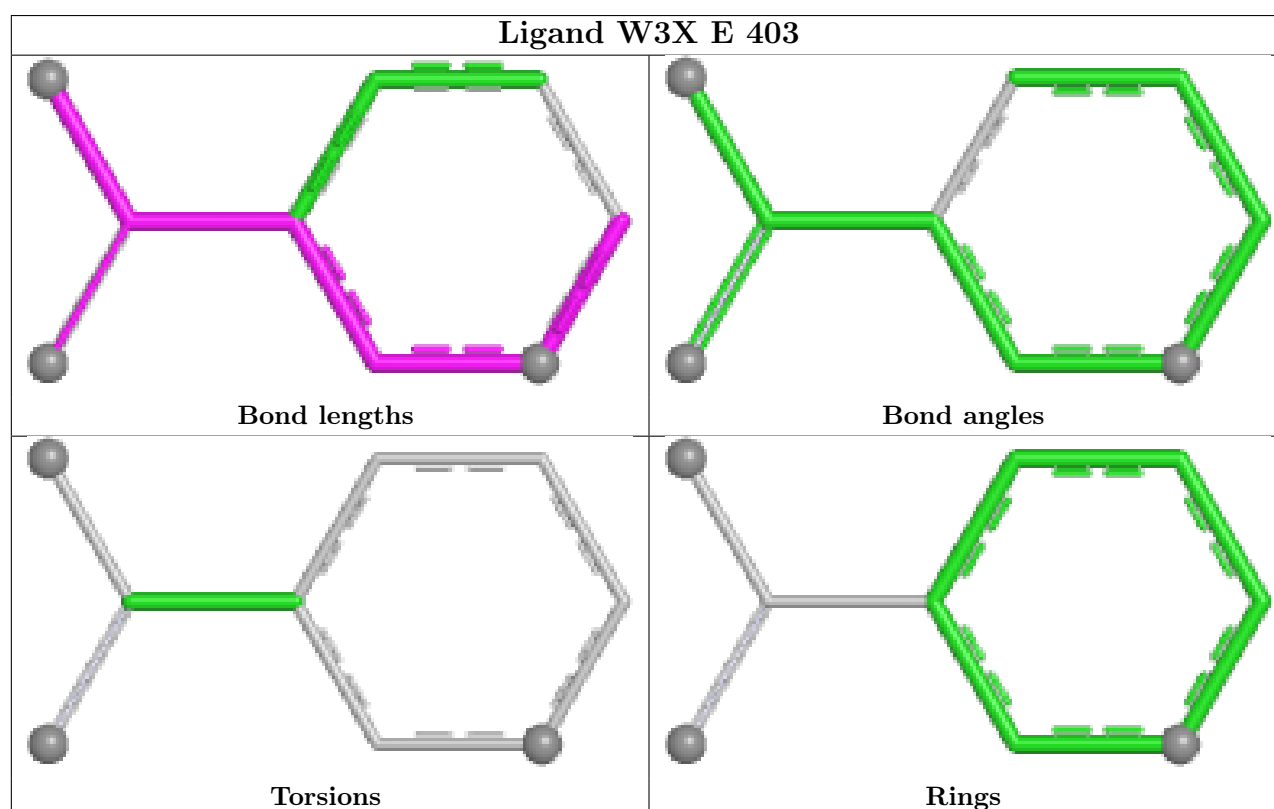
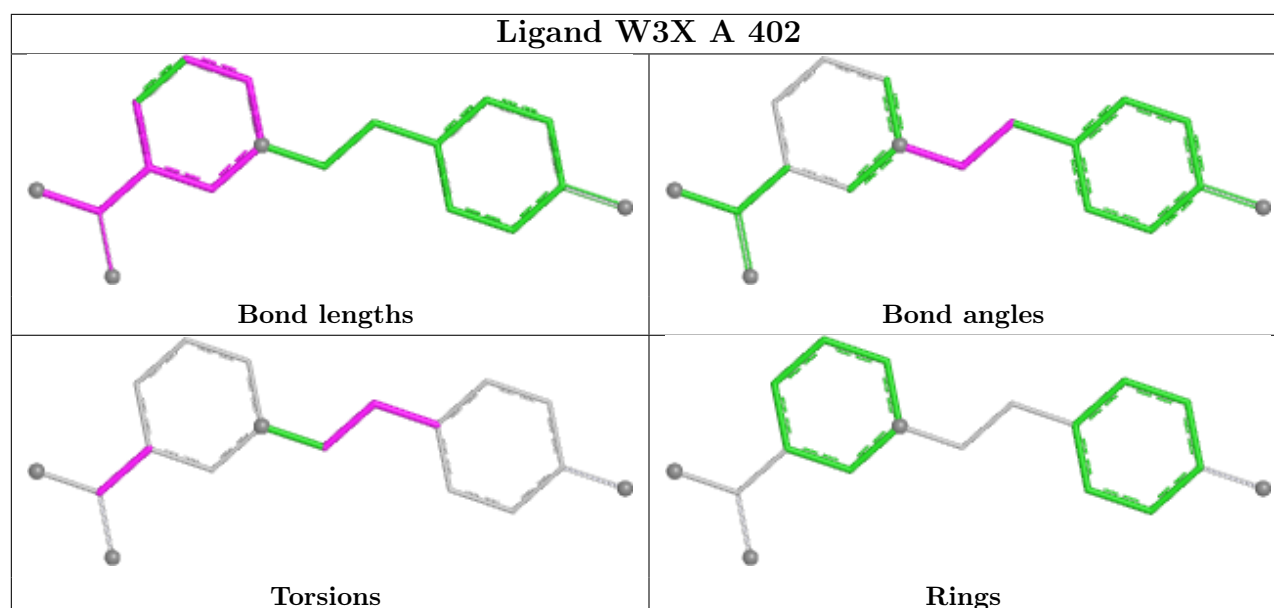
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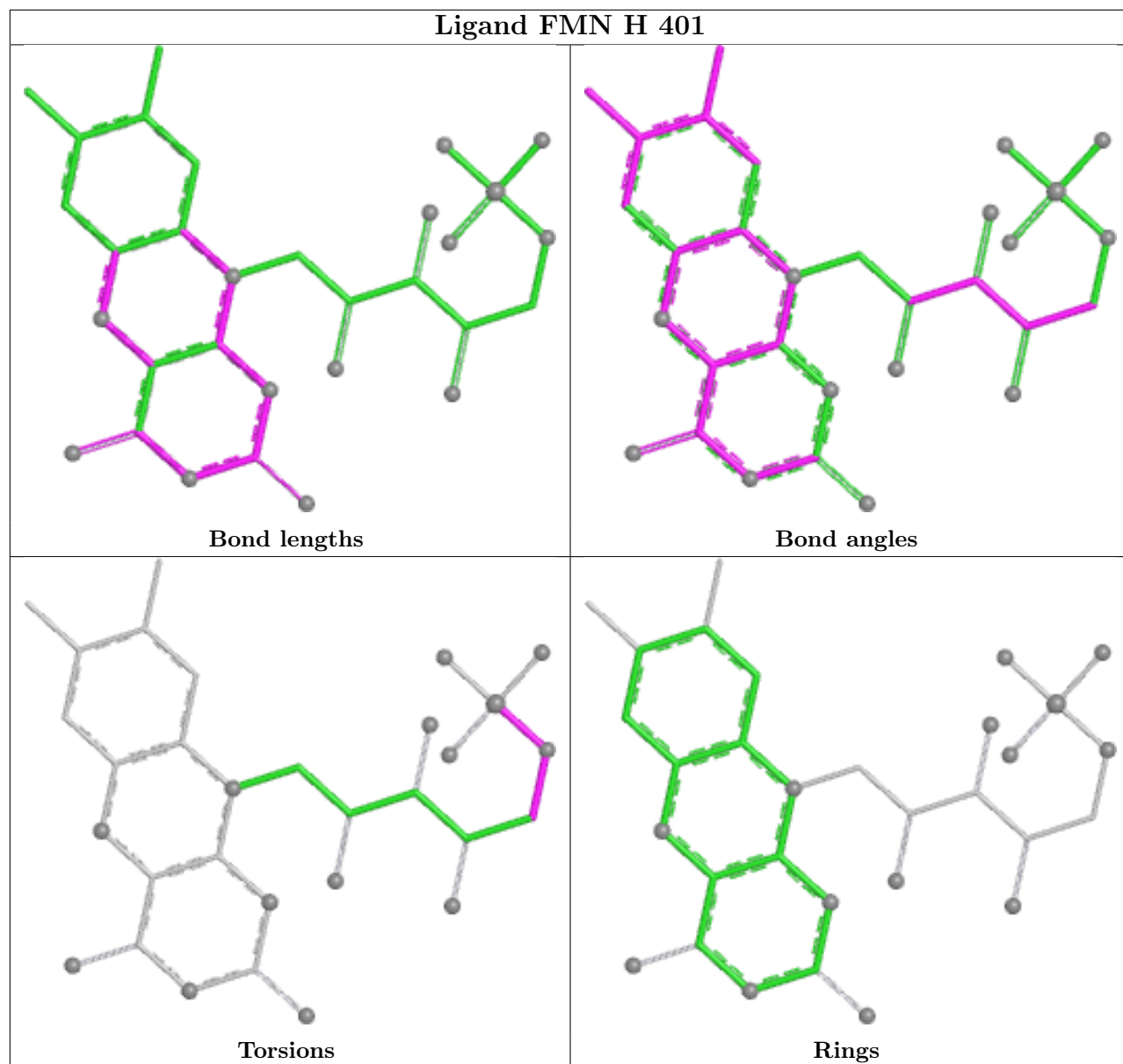
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	W3X	3	0
3	E	403	W3X	2	0
2	H	401	FMN	4	0
4	E	402	IPA	2	0
2	F	401	FMN	3	0
2	A	401	FMN	6	0
3	F	404	W3X	1	0
2	D	401	FMN	5	0
2	G	401	FMN	3	0
2	B	401	FMN	3	0
2	E	401	FMN	2	0

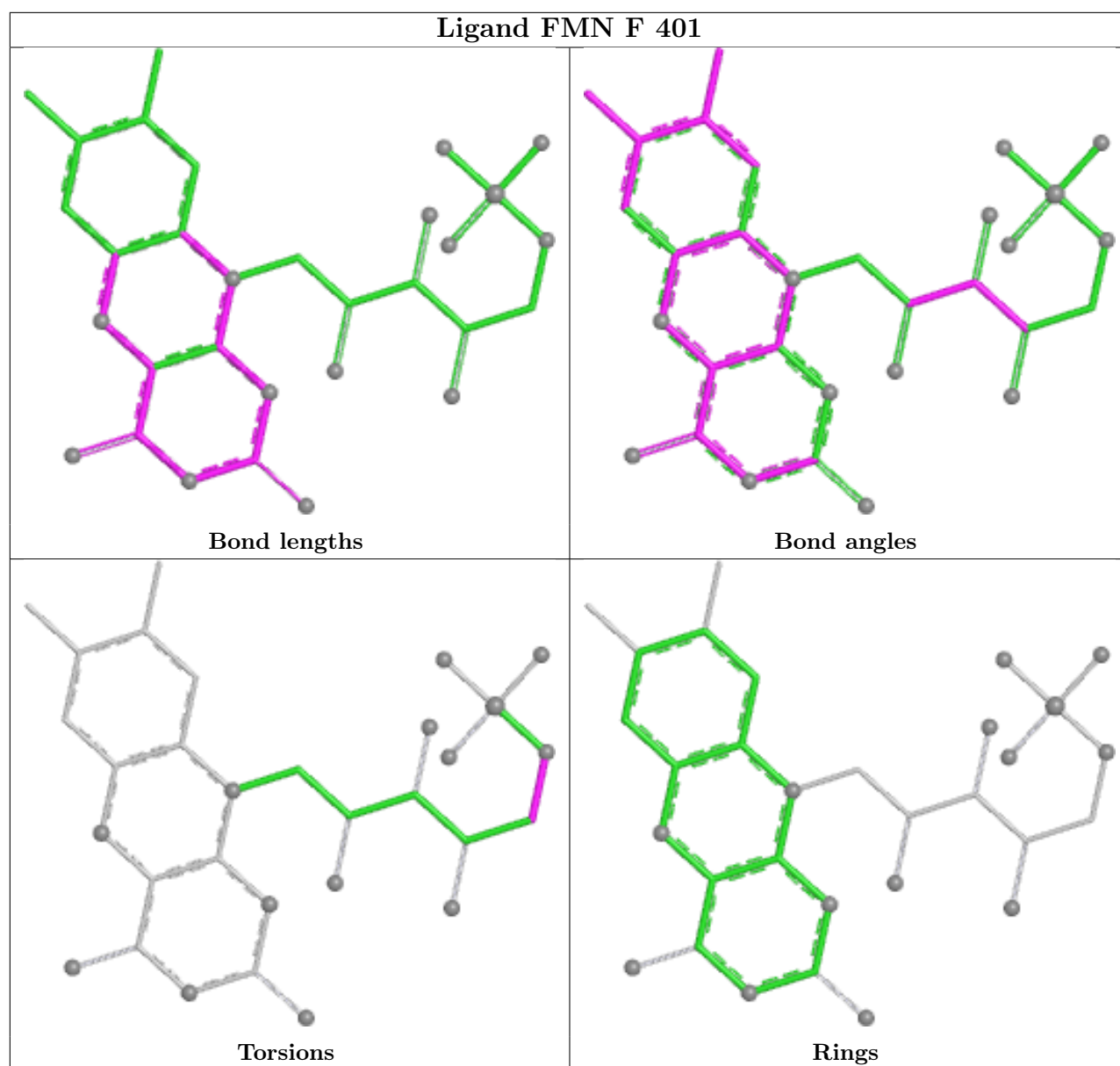
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

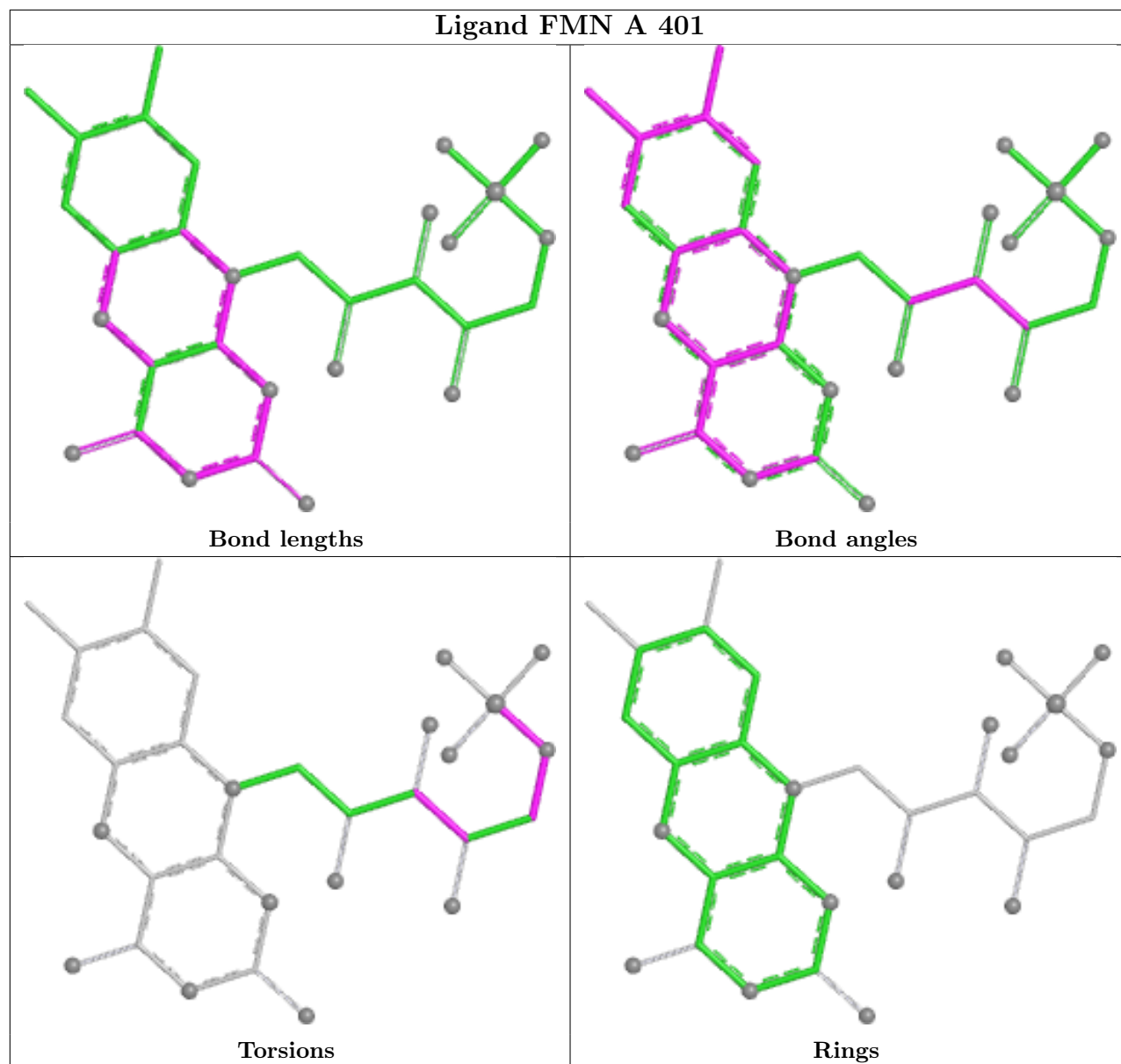


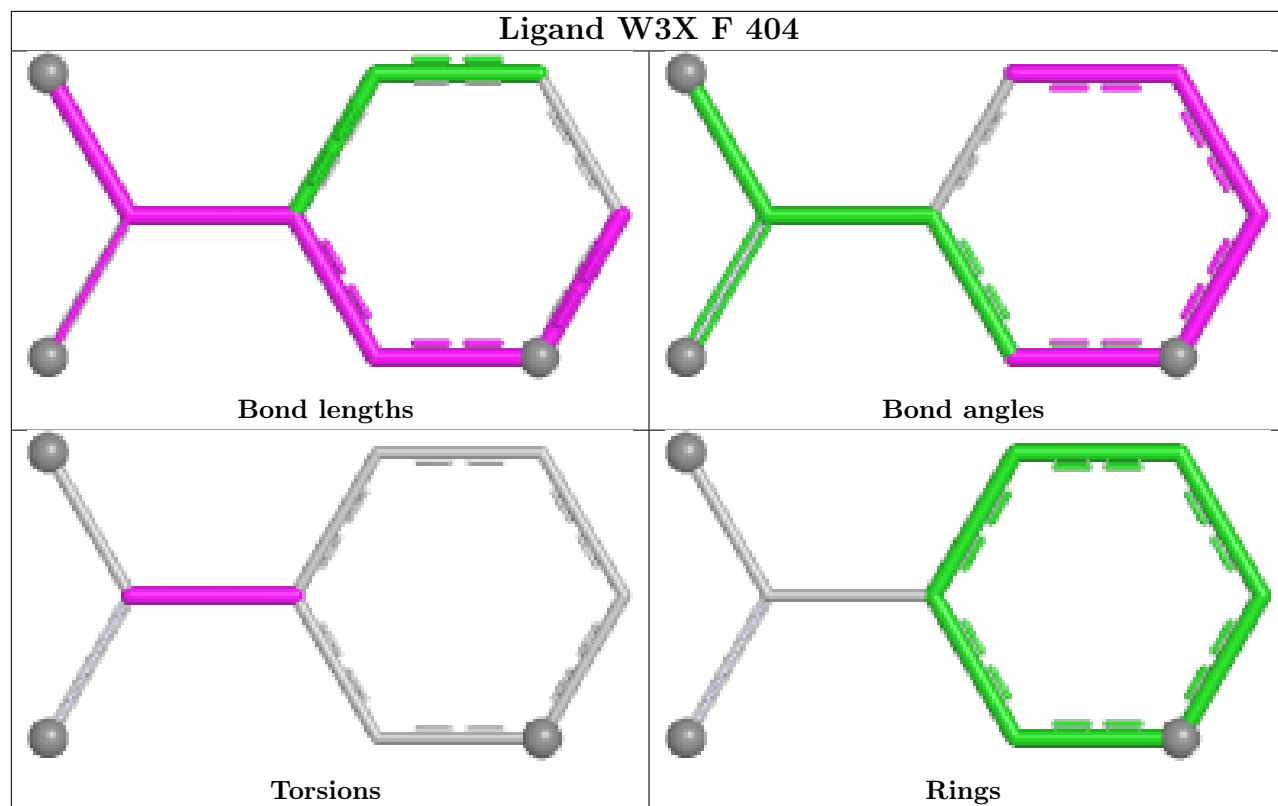


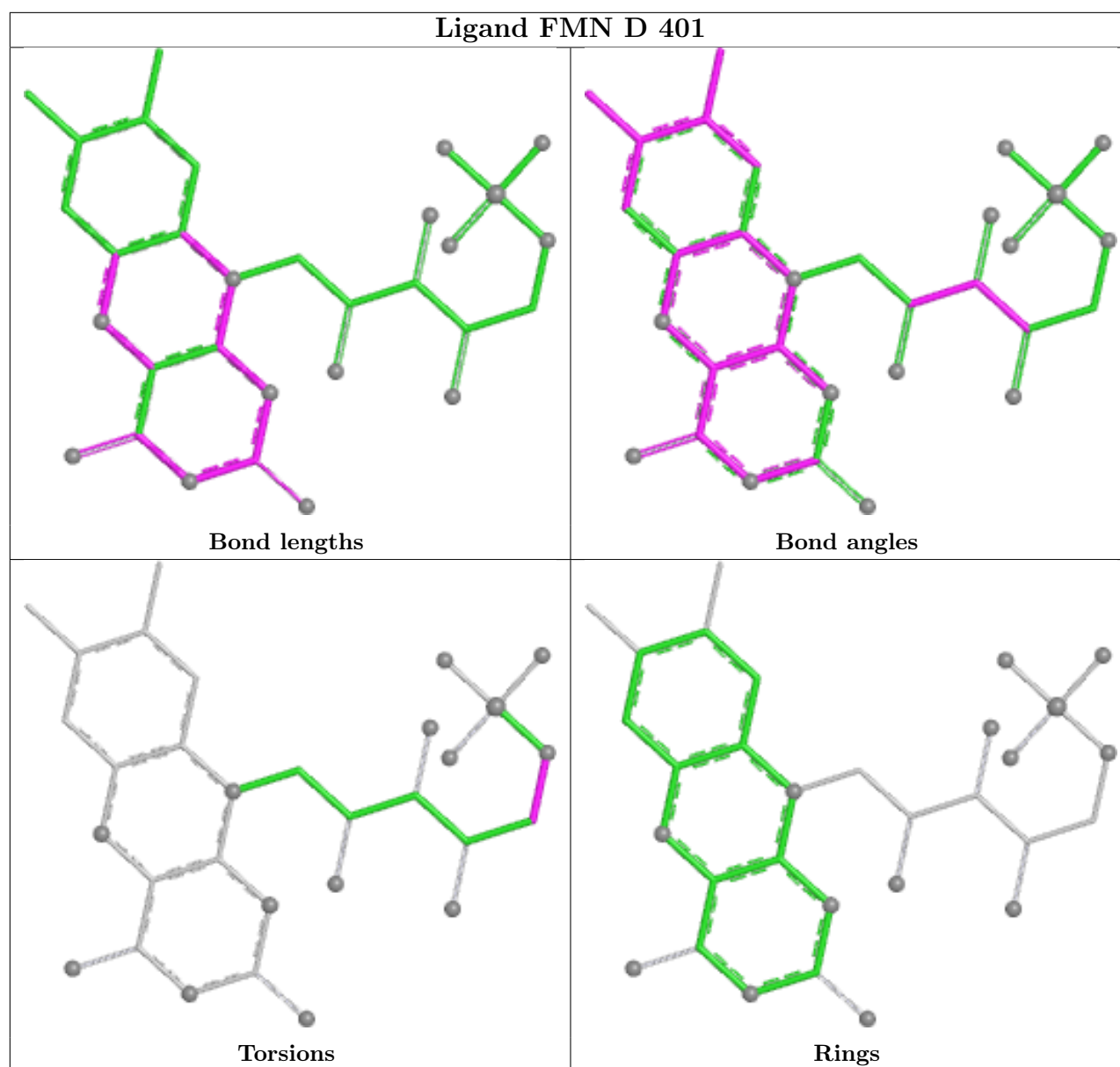


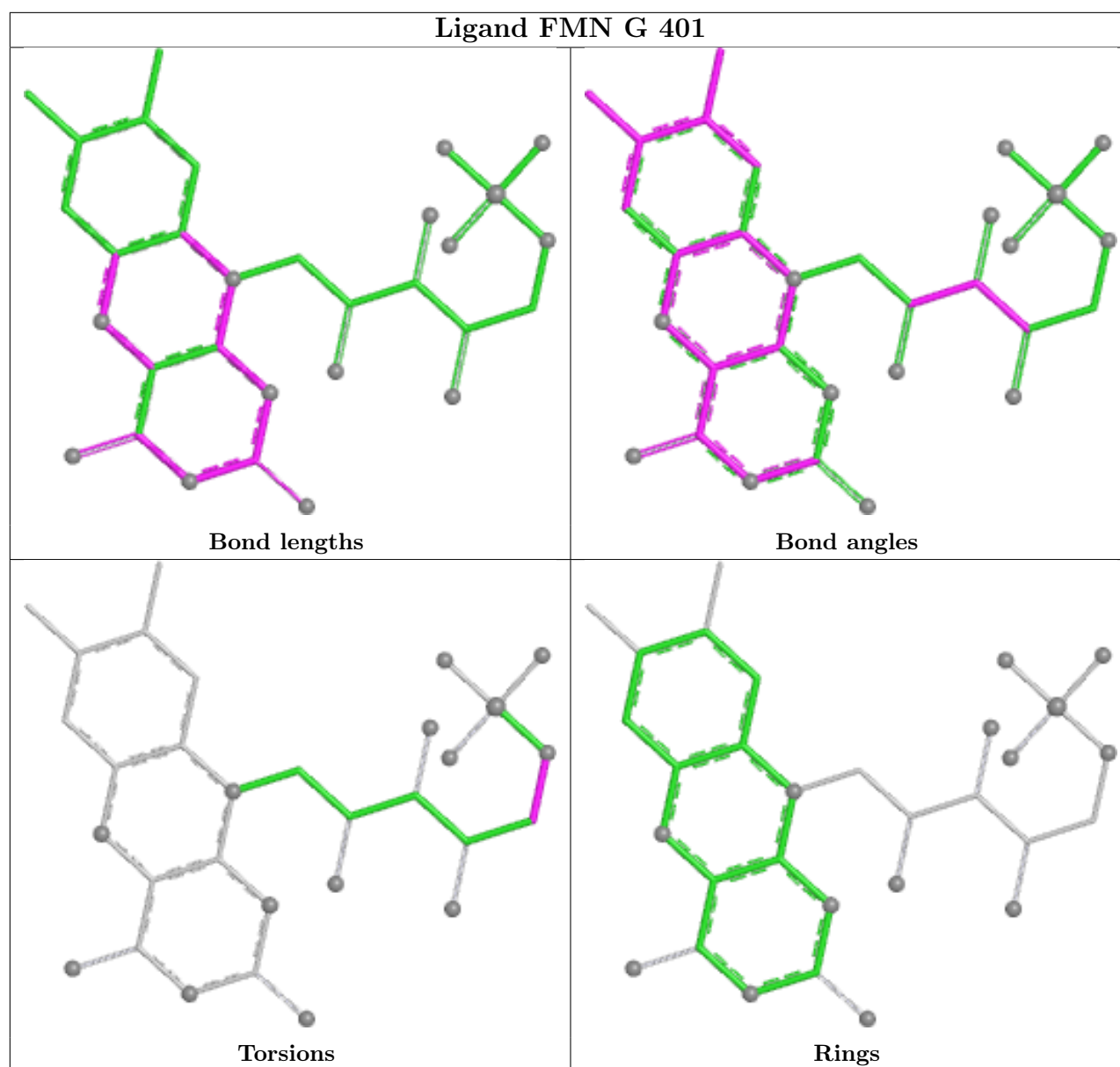


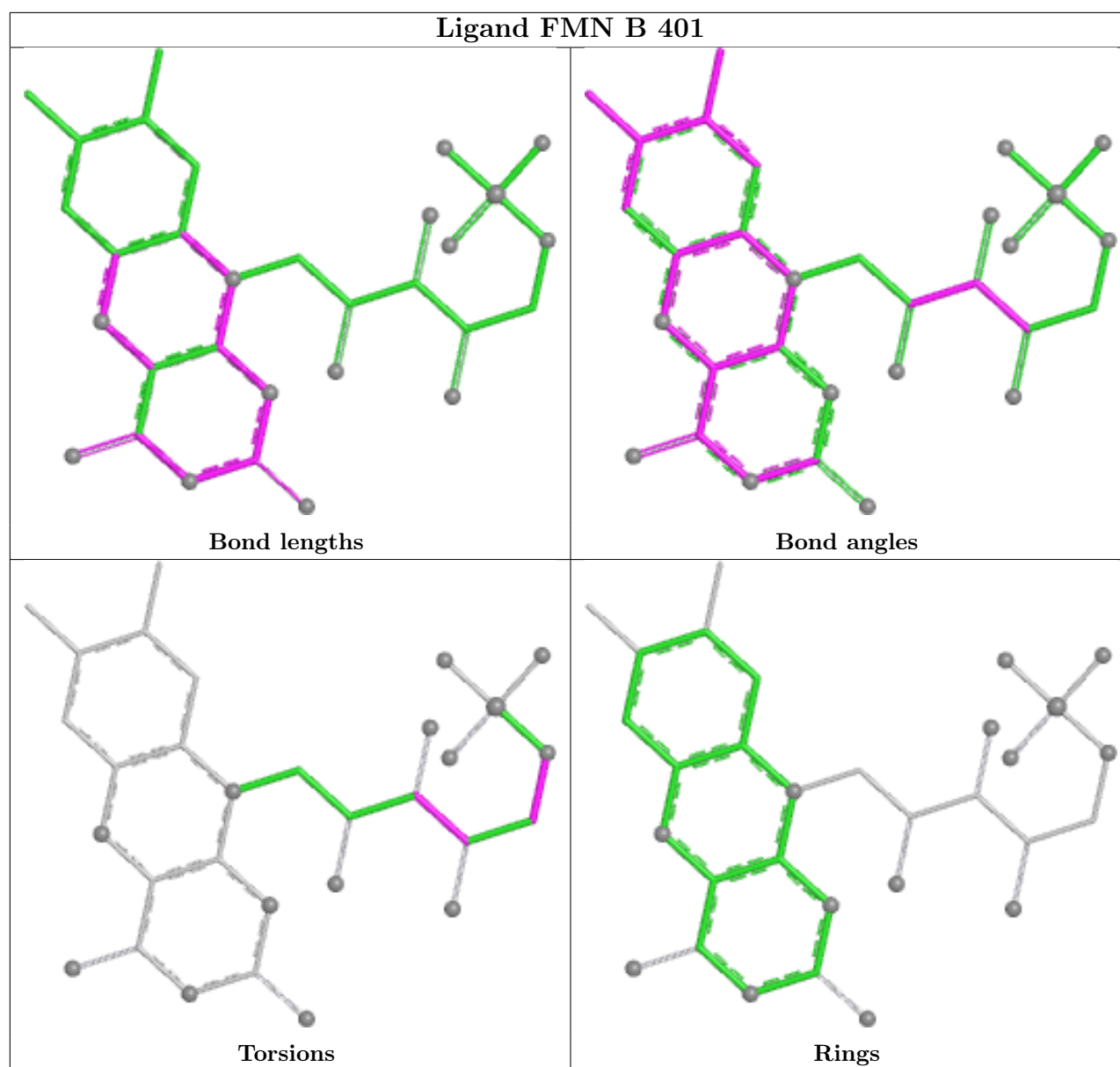


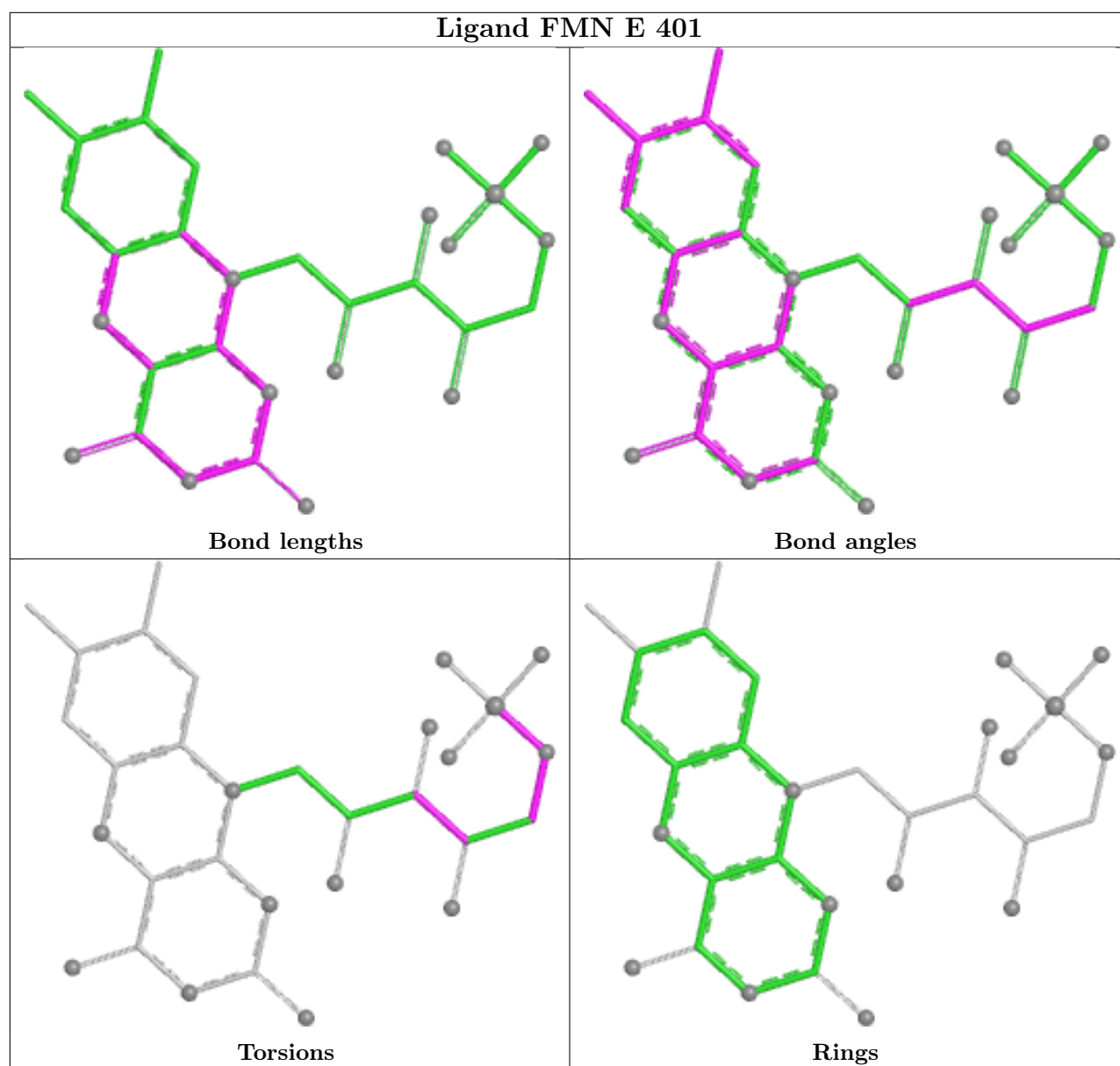












5.7 Other polymers [i](#)

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	349/369 (94%)	-1.38	0 100 100	32, 53, 66, 94	1 (0%)
1	B	349/369 (94%)	-1.37	0 100 100	28, 54, 73, 101	1 (0%)
1	C	349/369 (94%)	-1.36	0 100 100	32, 52, 66, 94	1 (0%)
1	D	349/369 (94%)	-1.37	0 100 100	40, 54, 70, 103	0
1	E	349/369 (94%)	-1.43	0 100 100	32, 51, 65, 86	1 (0%)
1	F	351/369 (95%)	-1.37	0 100 100	29, 55, 70, 108	2 (0%)
1	G	349/369 (94%)	-1.38	0 100 100	30, 55, 70, 91	1 (0%)
1	H	349/369 (94%)	-1.36	0 100 100	42, 53, 66, 83	0
All	All	2794/2952 (94%)	-1.38	0 100 100	28, 53, 69, 108	7 (0%)

There are no RSRZ outliers to report.

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](#)

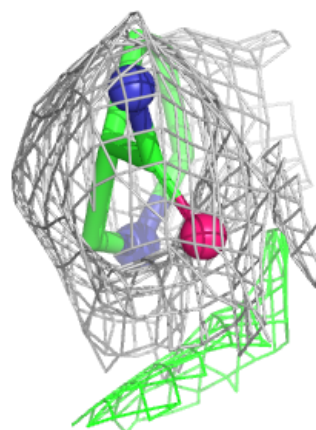
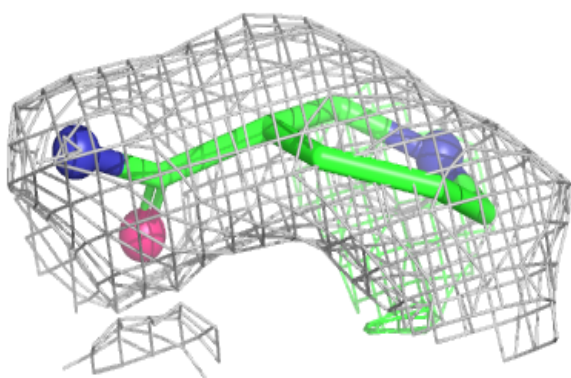
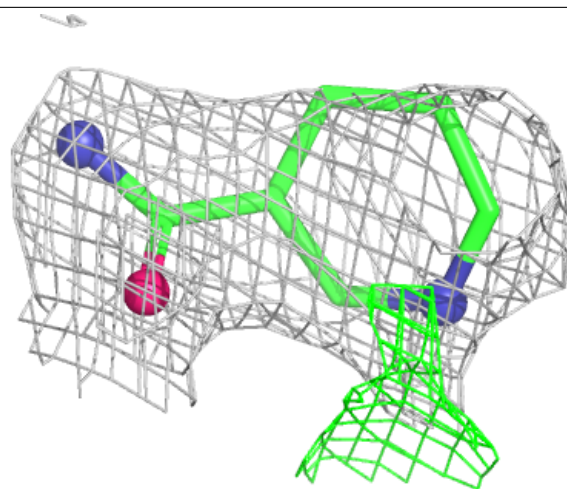
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	W3X	F	404	9/18	0.98	0.07	50,52,55,57	0
3	W3X	A	402	18/18	0.98	0.06	48,55,60,63	0
2	FMN	D	401	31/31	0.99	0.04	38,40,44,49	0
2	FMN	E	401	31/31	0.99	0.03	42,45,48,49	0
2	FMN	G	401	31/31	0.99	0.03	39,45,53,60	0
2	FMN	H	401	31/31	0.99	0.03	43,46,52,53	0
2	FMN	A	401	31/31	0.99	0.04	41,46,51,54	0
3	W3X	B	402	18/18	0.99	0.06	53,64,73,73	0
3	W3X	E	403	9/18	0.99	0.06	51,51,57,59	0
2	FMN	B	401	31/31	0.99	0.03	41,47,49,52	0
2	FMN	C	401	31/31	0.99	0.04	37,41,49,49	0
4	IPA	E	402	4/4	0.99	0.06	44,53,60,60	0
4	IPA	H	402	4/4	0.99	0.03	43,52,59,59	0
5	NA	F	402	1/1	0.99	0.08	49,49,49,49	0
2	FMN	F	401	31/31	1.00	0.03	39,47,50,54	0
6	CL	F	403	1/1	1.00	0.03	56,56,56,56	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.

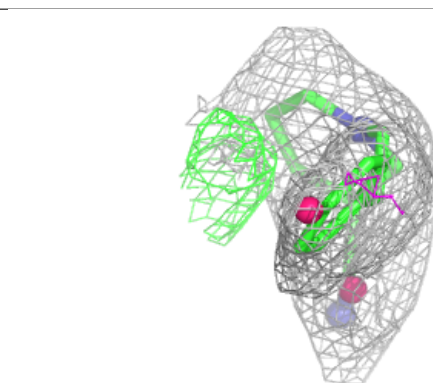
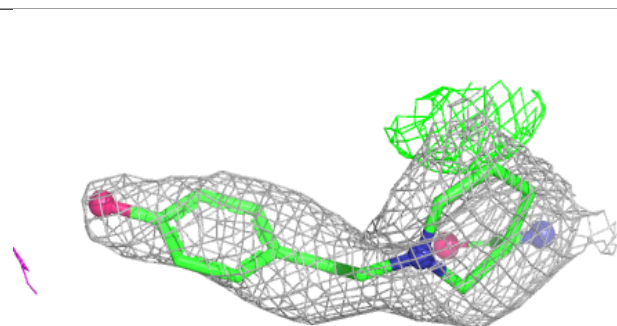
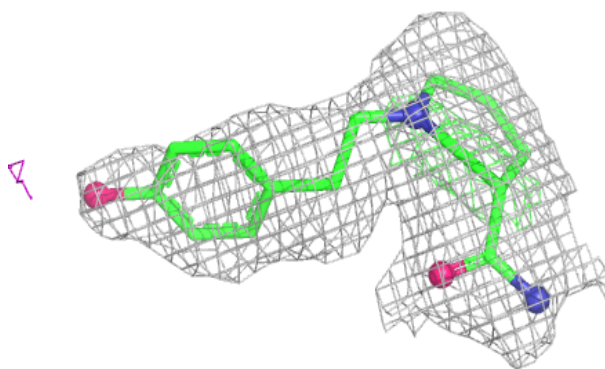
Electron density around W3X F 404:

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

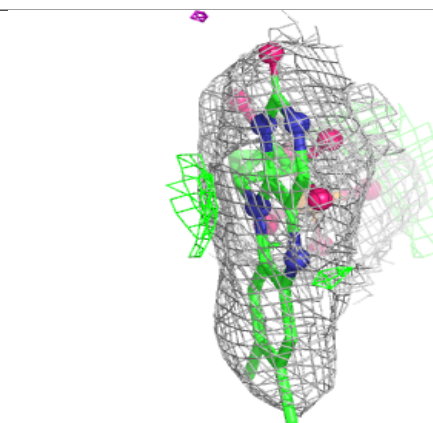
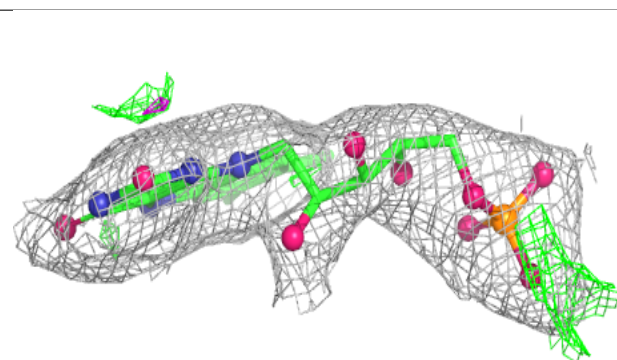
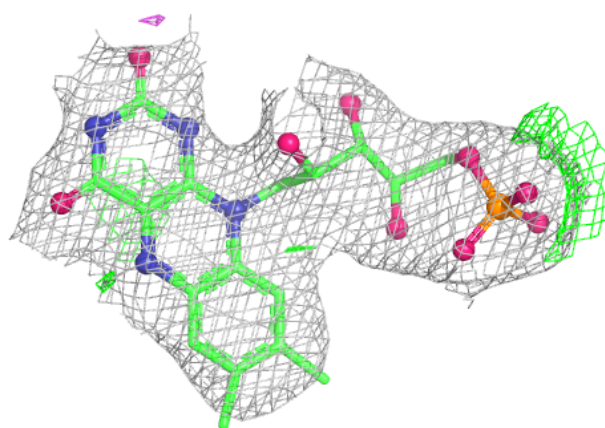


Electron density around W3X A 402:

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

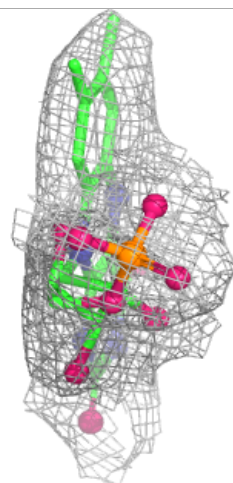
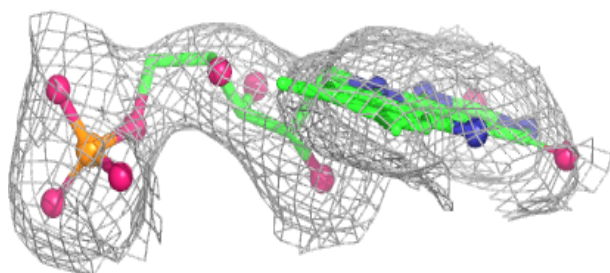
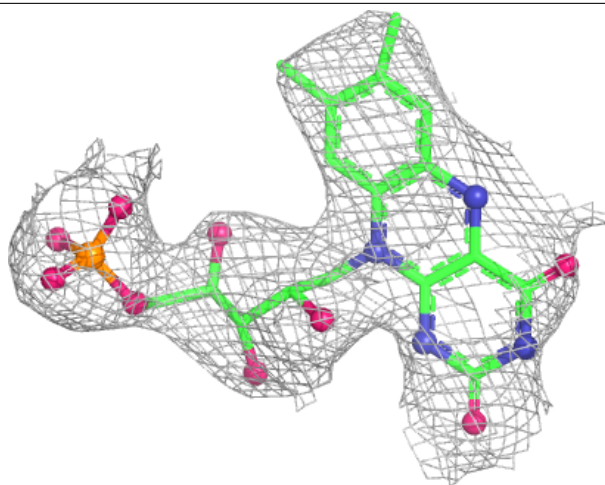
**Electron density around FMN D 401:**

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



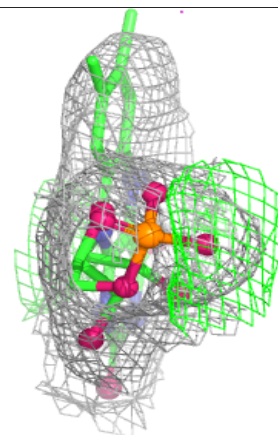
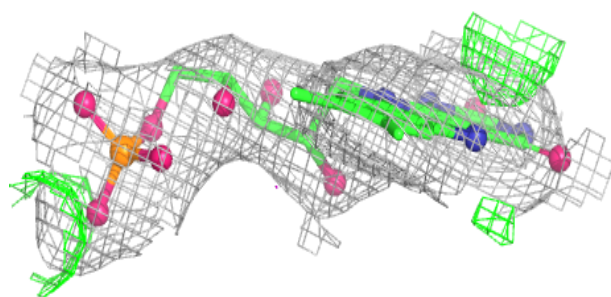
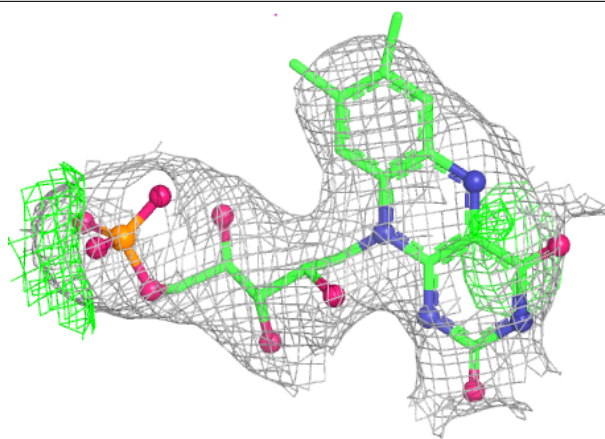
Electron density around FMN E 401:

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



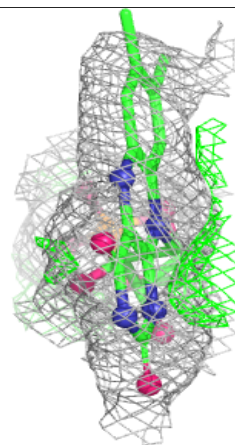
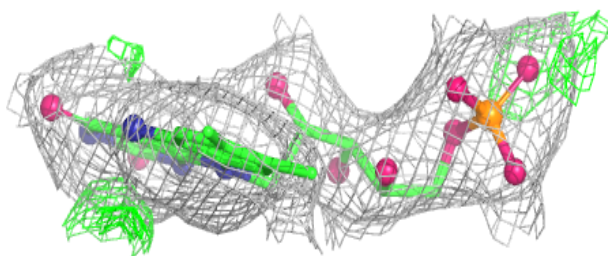
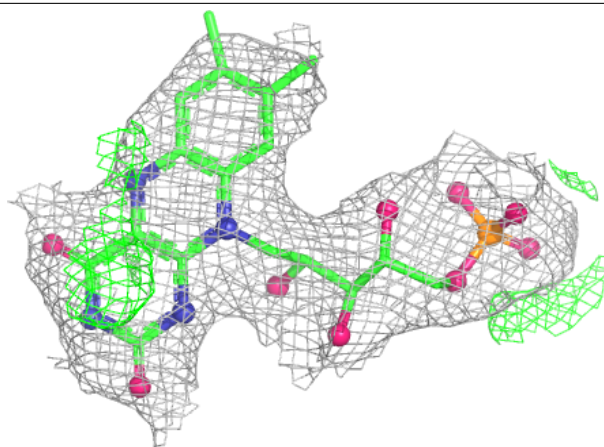
Electron density around FMN G 401:

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



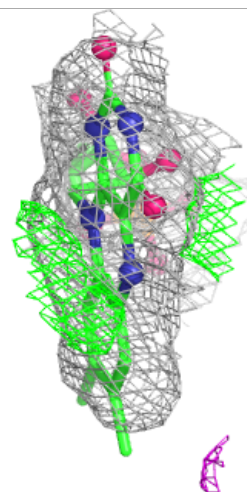
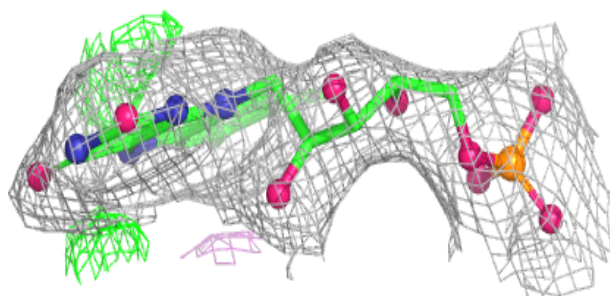
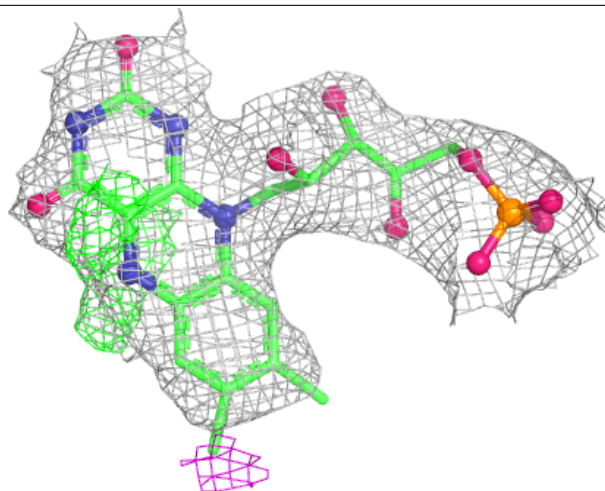
Electron density around FMN H 401:

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



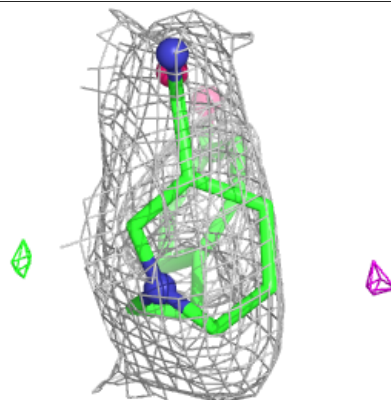
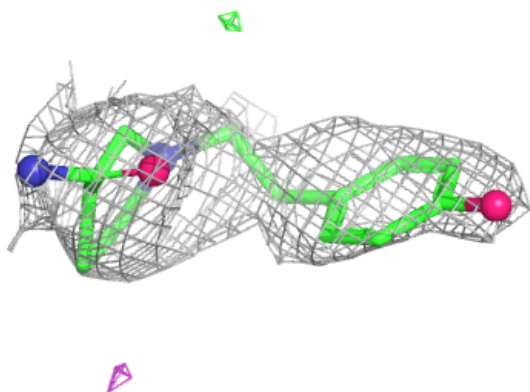
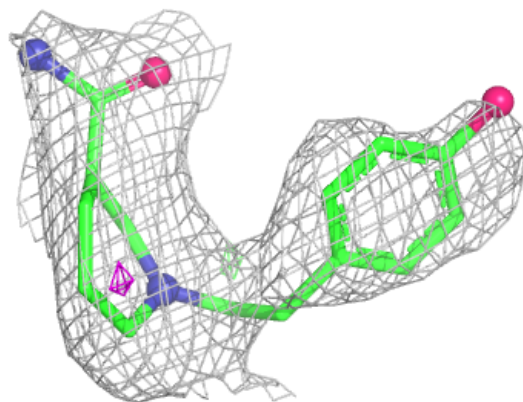
Electron density around FMN A 401:

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



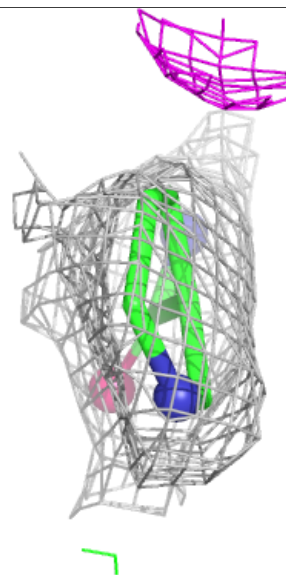
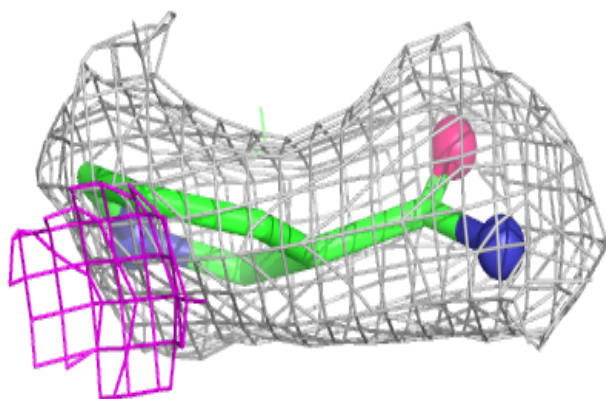
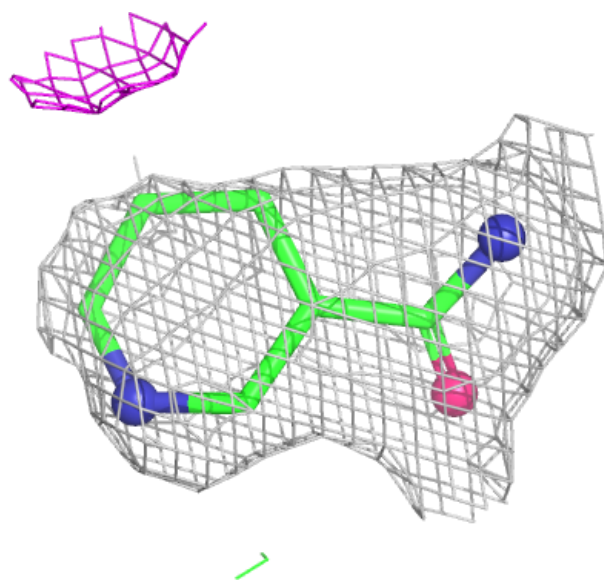
Electron density around W3X B 402:

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



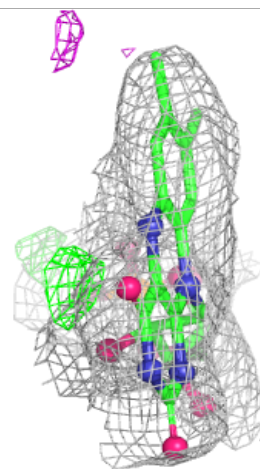
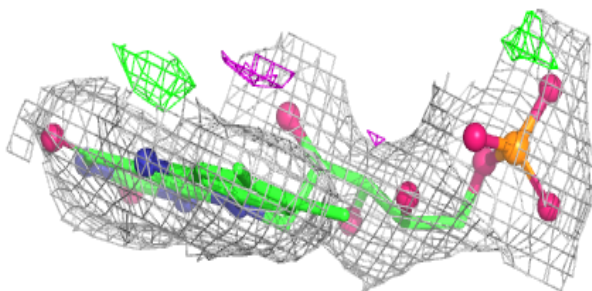
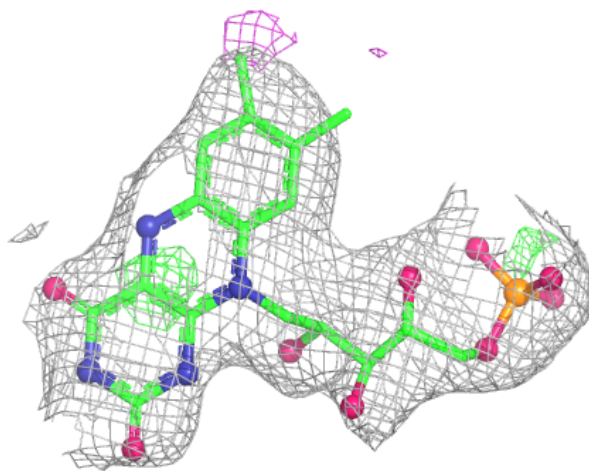
Electron density around W3X E 403:

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



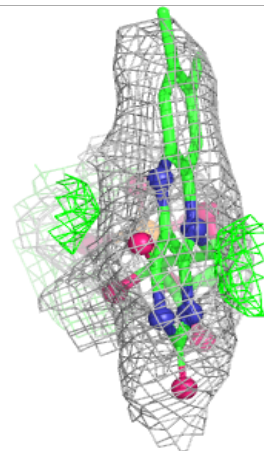
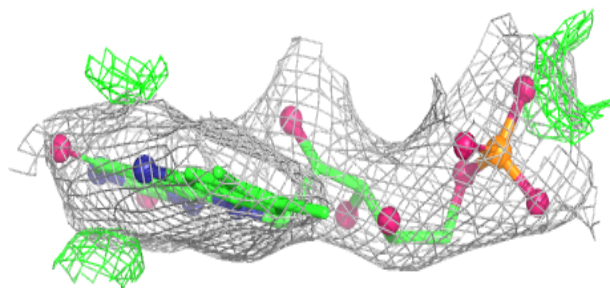
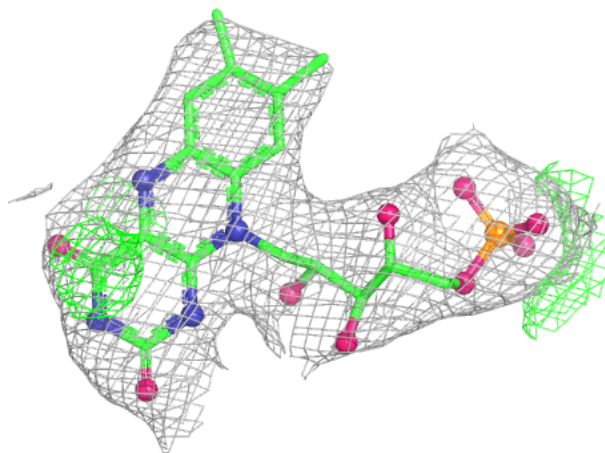
Electron density around FMN B 401:

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



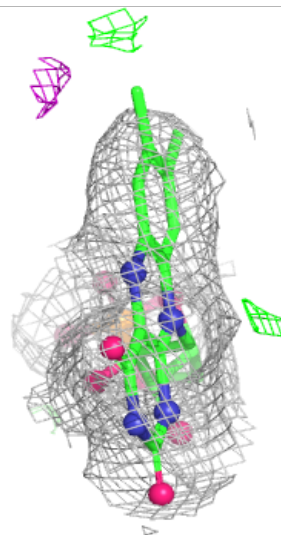
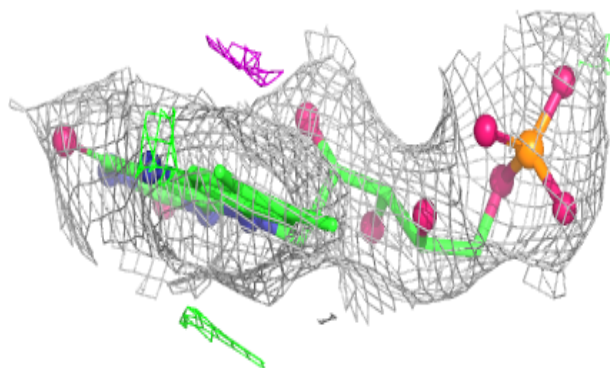
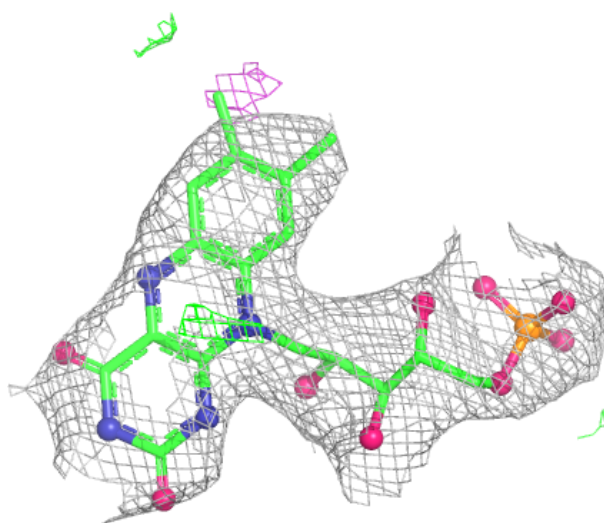
Electron density around FMN C 401:

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



Electron density around FMN 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.