



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2025 – 11:26 pm BST

PDB ID : 9GJX / pdb_00009gjx
Title : Bacillus licheniformis nitroreductase
Authors : Crennell, S.J.; Danson, M.J.; Emptage, C.
Deposited on : 2024-08-23
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

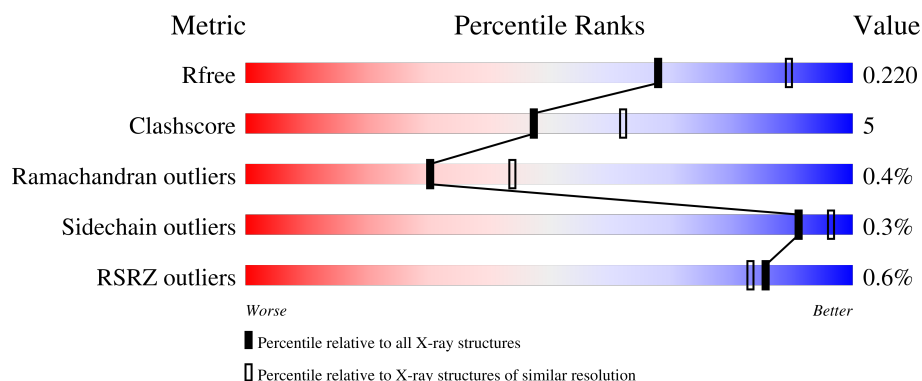
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.40 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	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	248	 82% 9% 9%
1	B	248	 81% 11% 8%
1	C	248	 79% 12% 8%
1	D	248	 83% 9% 8%
1	E	248	 79% 12% 8%

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Mol	Chain	Length	Quality of chain
1	F	248	<div> <div>%</div> <div> </div> <div>81%10%8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	E	306[A]	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23376 atoms, of which 11353 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 NADH-dependent nitro/flavin oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	226	Total	C	H	N	O	S	0	1	0
			3657	1169	1813	318	349	8			
1	B	228	Total	C	H	N	O	S	0	4	0
			3734	1193	1848	326	358	9			
1	C	228	Total	C	H	N	O	S	0	2	0
			3690	1181	1825	320	355	9			
1	D	229	Total	C	H	N	O	S	0	3	0
			3728	1191	1845	328	355	9			
1	E	228	Total	C	H	N	O	S	0	1	0
			3678	1177	1821	319	352	9			
1	F	227	Total	C	H	N	O	S	0	2	0
			3672	1176	1815	319	354	8			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q65MG6
A	-19	GLY	-	expression tag	UNP Q65MG6
A	-18	SER	-	expression tag	UNP Q65MG6
A	-17	SER	-	expression tag	UNP Q65MG6
A	-16	HIS	-	expression tag	UNP Q65MG6
A	-15	HIS	-	expression tag	UNP Q65MG6
A	-14	HIS	-	expression tag	UNP Q65MG6
A	-13	HIS	-	expression tag	UNP Q65MG6
A	-12	HIS	-	expression tag	UNP Q65MG6
A	-11	HIS	-	expression tag	UNP Q65MG6
A	-10	SER	-	expression tag	UNP Q65MG6
A	-9	SER	-	expression tag	UNP Q65MG6
A	-8	GLY	-	expression tag	UNP Q65MG6
A	-7	LEU	-	expression tag	UNP Q65MG6
A	-6	VAL	-	expression tag	UNP Q65MG6
A	-5	PRO	-	expression tag	UNP Q65MG6
A	-4	ARG	-	expression tag	UNP Q65MG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q65MG6
A	-2	SER	-	expression tag	UNP Q65MG6
A	-1	HIS	-	expression tag	UNP Q65MG6
A	0	MET	-	expression tag	UNP Q65MG6
B	-20	MET	-	initiating methionine	UNP Q65MG6
B	-19	GLY	-	expression tag	UNP Q65MG6
B	-18	SER	-	expression tag	UNP Q65MG6
B	-17	SER	-	expression tag	UNP Q65MG6
B	-16	HIS	-	expression tag	UNP Q65MG6
B	-15	HIS	-	expression tag	UNP Q65MG6
B	-14	HIS	-	expression tag	UNP Q65MG6
B	-13	HIS	-	expression tag	UNP Q65MG6
B	-12	HIS	-	expression tag	UNP Q65MG6
B	-11	HIS	-	expression tag	UNP Q65MG6
B	-10	SER	-	expression tag	UNP Q65MG6
B	-9	SER	-	expression tag	UNP Q65MG6
B	-8	GLY	-	expression tag	UNP Q65MG6
B	-7	LEU	-	expression tag	UNP Q65MG6
B	-6	VAL	-	expression tag	UNP Q65MG6
B	-5	PRO	-	expression tag	UNP Q65MG6
B	-4	ARG	-	expression tag	UNP Q65MG6
B	-3	GLY	-	expression tag	UNP Q65MG6
B	-2	SER	-	expression tag	UNP Q65MG6
B	-1	HIS	-	expression tag	UNP Q65MG6
B	0	MET	-	expression tag	UNP Q65MG6
C	-20	MET	-	initiating methionine	UNP Q65MG6
C	-19	GLY	-	expression tag	UNP Q65MG6
C	-18	SER	-	expression tag	UNP Q65MG6
C	-17	SER	-	expression tag	UNP Q65MG6
C	-16	HIS	-	expression tag	UNP Q65MG6
C	-15	HIS	-	expression tag	UNP Q65MG6
C	-14	HIS	-	expression tag	UNP Q65MG6
C	-13	HIS	-	expression tag	UNP Q65MG6
C	-12	HIS	-	expression tag	UNP Q65MG6
C	-11	HIS	-	expression tag	UNP Q65MG6
C	-10	SER	-	expression tag	UNP Q65MG6
C	-9	SER	-	expression tag	UNP Q65MG6
C	-8	GLY	-	expression tag	UNP Q65MG6
C	-7	LEU	-	expression tag	UNP Q65MG6
C	-6	VAL	-	expression tag	UNP Q65MG6
C	-5	PRO	-	expression tag	UNP Q65MG6
C	-4	ARG	-	expression tag	UNP Q65MG6

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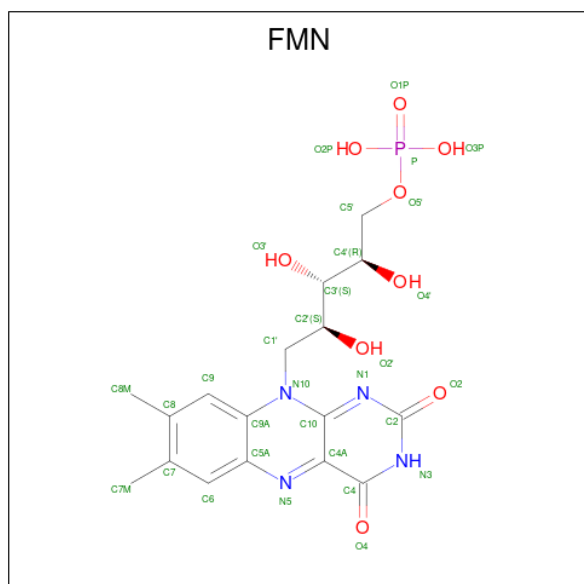
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q65MG6
C	-2	SER	-	expression tag	UNP Q65MG6
C	-1	HIS	-	expression tag	UNP Q65MG6
C	0	MET	-	expression tag	UNP Q65MG6
D	-20	MET	-	initiating methionine	UNP Q65MG6
D	-19	GLY	-	expression tag	UNP Q65MG6
D	-18	SER	-	expression tag	UNP Q65MG6
D	-17	SER	-	expression tag	UNP Q65MG6
D	-16	HIS	-	expression tag	UNP Q65MG6
D	-15	HIS	-	expression tag	UNP Q65MG6
D	-14	HIS	-	expression tag	UNP Q65MG6
D	-13	HIS	-	expression tag	UNP Q65MG6
D	-12	HIS	-	expression tag	UNP Q65MG6
D	-11	HIS	-	expression tag	UNP Q65MG6
D	-10	SER	-	expression tag	UNP Q65MG6
D	-9	SER	-	expression tag	UNP Q65MG6
D	-8	GLY	-	expression tag	UNP Q65MG6
D	-7	LEU	-	expression tag	UNP Q65MG6
D	-6	VAL	-	expression tag	UNP Q65MG6
D	-5	PRO	-	expression tag	UNP Q65MG6
D	-4	ARG	-	expression tag	UNP Q65MG6
D	-3	GLY	-	expression tag	UNP Q65MG6
D	-2	SER	-	expression tag	UNP Q65MG6
D	-1	HIS	-	expression tag	UNP Q65MG6
D	0	MET	-	expression tag	UNP Q65MG6
E	-20	MET	-	initiating methionine	UNP Q65MG6
E	-19	GLY	-	expression tag	UNP Q65MG6
E	-18	SER	-	expression tag	UNP Q65MG6
E	-17	SER	-	expression tag	UNP Q65MG6
E	-16	HIS	-	expression tag	UNP Q65MG6
E	-15	HIS	-	expression tag	UNP Q65MG6
E	-14	HIS	-	expression tag	UNP Q65MG6
E	-13	HIS	-	expression tag	UNP Q65MG6
E	-12	HIS	-	expression tag	UNP Q65MG6
E	-11	HIS	-	expression tag	UNP Q65MG6
E	-10	SER	-	expression tag	UNP Q65MG6
E	-9	SER	-	expression tag	UNP Q65MG6
E	-8	GLY	-	expression tag	UNP Q65MG6
E	-7	LEU	-	expression tag	UNP Q65MG6
E	-6	VAL	-	expression tag	UNP Q65MG6
E	-5	PRO	-	expression tag	UNP Q65MG6
E	-4	ARG	-	expression tag	UNP Q65MG6

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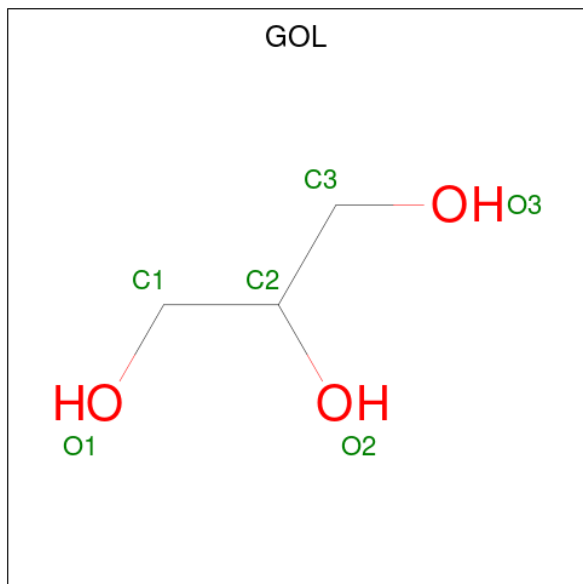
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP Q65MG6
E	-2	SER	-	expression tag	UNP Q65MG6
E	-1	HIS	-	expression tag	UNP Q65MG6
E	0	MET	-	expression tag	UNP Q65MG6
F	-20	MET	-	initiating methionine	UNP Q65MG6
F	-19	GLY	-	expression tag	UNP Q65MG6
F	-18	SER	-	expression tag	UNP Q65MG6
F	-17	SER	-	expression tag	UNP Q65MG6
F	-16	HIS	-	expression tag	UNP Q65MG6
F	-15	HIS	-	expression tag	UNP Q65MG6
F	-14	HIS	-	expression tag	UNP Q65MG6
F	-13	HIS	-	expression tag	UNP Q65MG6
F	-12	HIS	-	expression tag	UNP Q65MG6
F	-11	HIS	-	expression tag	UNP Q65MG6
F	-10	SER	-	expression tag	UNP Q65MG6
F	-9	SER	-	expression tag	UNP Q65MG6
F	-8	GLY	-	expression tag	UNP Q65MG6
F	-7	LEU	-	expression tag	UNP Q65MG6
F	-6	VAL	-	expression tag	UNP Q65MG6
F	-5	PRO	-	expression tag	UNP Q65MG6
F	-4	ARG	-	expression tag	UNP Q65MG6
F	-3	GLY	-	expression tag	UNP Q65MG6
F	-2	SER	-	expression tag	UNP Q65MG6
F	-1	HIS	-	expression tag	UNP Q65MG6
F	0	MET	-	expression tag	UNP Q65MG6

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	
			50	17	19	4	9	1	0
2	B	1	Total	C	H	N	O	P	
			50	17	19	4	9	1	0
2	C	1	Total	C	H	N	O	P	
			50	17	19	4	9	1	0
2	D	1	Total	C	H	N	O	P	
			50	17	19	4	9	1	0
2	E	1	Total	C	H	N	O	P	
			50	17	19	4	9	1	0
2	F	1	Total	C	H	N	O	P	
			50	17	19	4	9	1	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



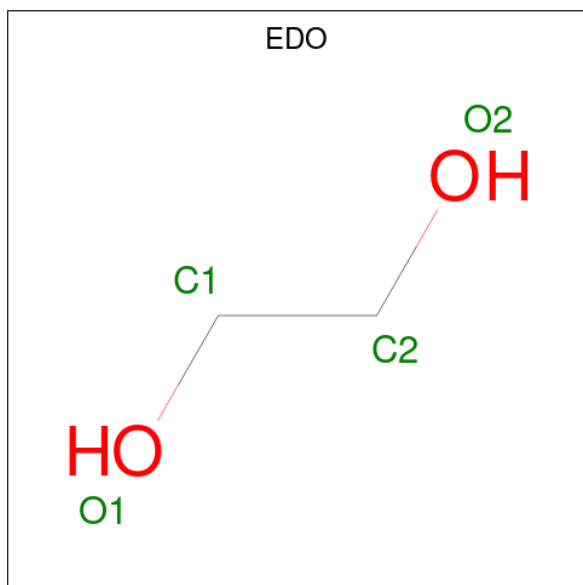
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O		
			14	3	8	3	0	0
3	A	1	Total	C	H	O		
			14	3	8	3	0	1
3	B	1	Total	C	H	O		
			14	3	8	3	14	1
3	B	1	Total	C	H	O		
			14	3	8	3	0	0
3	C	1	Total	C	H	O		
			14	3	8	3	0	1
3	D	1	Total	C	H	O		
			14	3	8	3	14	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	1
			14	3	8	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



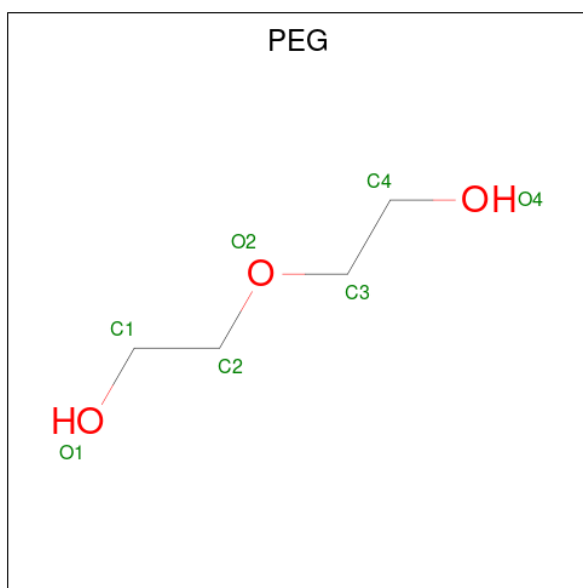
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

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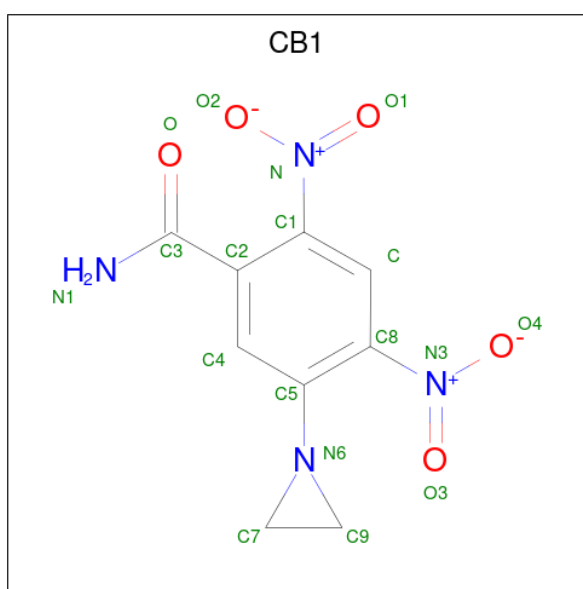
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	E	1	Total	C	H	O	0	0
			10	2	6	2		
4	E	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	E	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is 5-(AZIRIDIN-1-YL)-2,4-DINITROBENZAMIDE (CCD ID: CB1) (formula: $C_9H_8N_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	1
			26	9	8	4	5		
6	B	1	Total	C	H	N	O	0	1
			26	9	8	4	5		
6	C	1	Total	C	H	N	O	0	1
			26	9	8	4	5		
6	D	1	Total	C	H	N	O	0	1
			26	9	8	4	5		
6	E	1	Total	C	H	N	O	0	1
			26	9	8	4	5		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

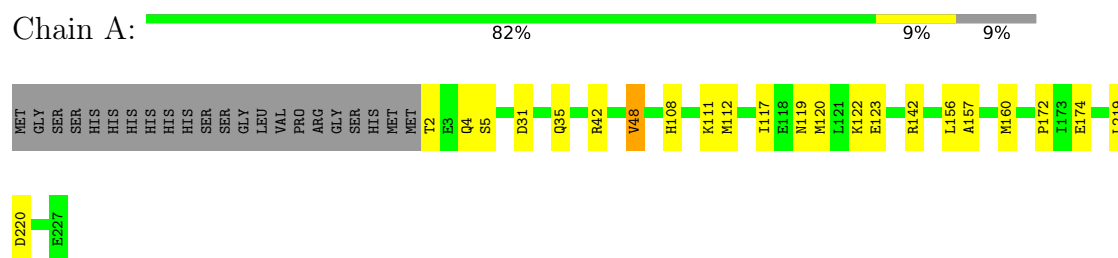
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	66	Total	O	0	0
			66	66		
8	B	76	Total	O	0	0
			76	76		
8	C	64	Total	O	0	0
			64	64		
8	D	65	Total	O	0	0
			65	65		
8	E	53	Total	O	0	0
			53	53		
8	F	49	Total	O	0	0
			49	49		

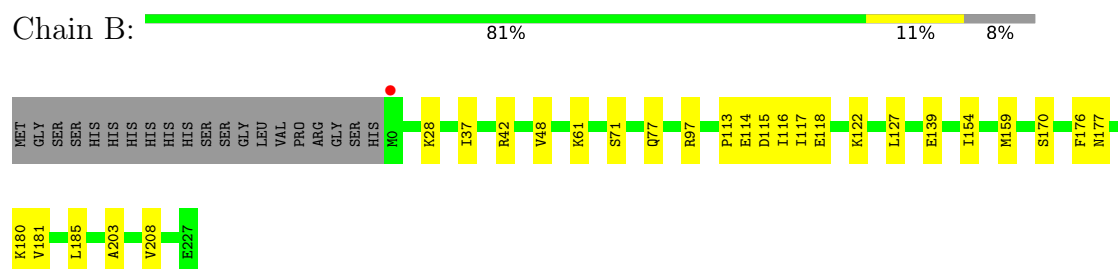
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

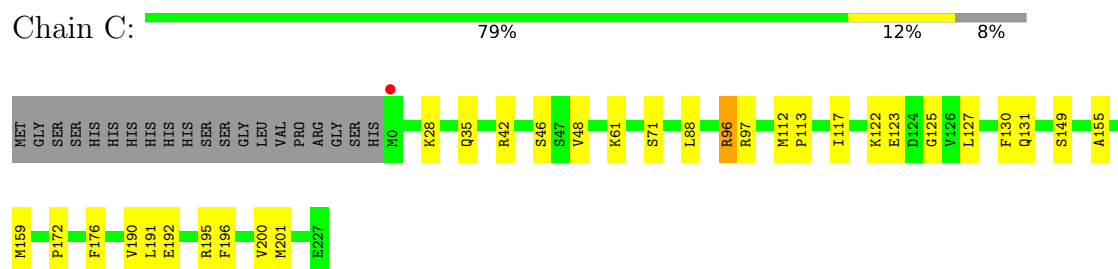
- Molecule 1: NADH-dependent nitro/flavin oxidoreductase



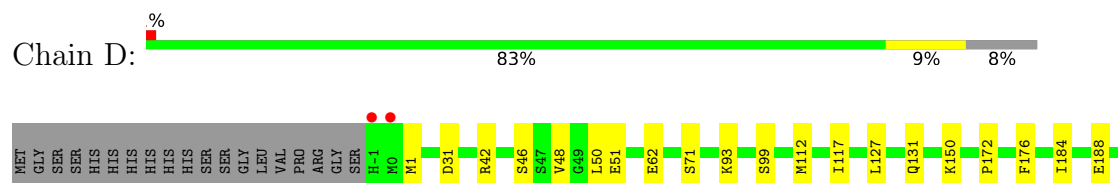
- Molecule 1: NADH-dependent nitro/flavin oxidoreductase



- Molecule 1: NADH-dependent nitro/flavin oxidoreductase

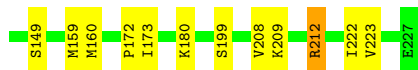
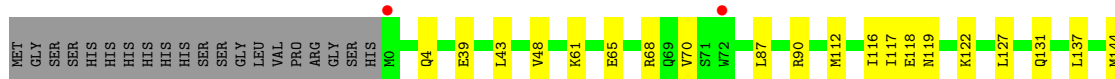
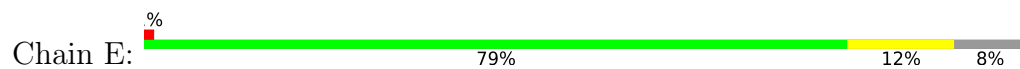


- Molecule 1: NADH-dependent nitro/flavin oxidoreductase

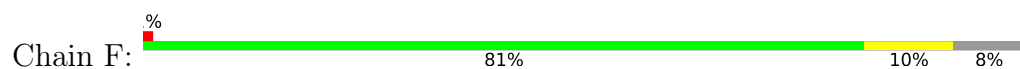




- Molecule 1: NADH-dependent nitro/flavin oxidoreductase



- Molecule 1: NADH-dependent nitro/flavin oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.78Å 115.81Å 103.81Å 90.00° 110.29° 90.00°	Depositor
Resolution (Å)	19.86 – 2.40 19.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.86-2.40) 99.6 (19.86-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.41Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.161 , 0.219 0.161 , 0.220	Depositor DCC
R_{free} test set	3261 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23376	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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: SO4, PEG, GOL, FMN, EDO, CB1

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	0.44	0/1882	0.59	0/2532
1	B	0.43	0/1924	0.57	0/2587
1	C	0.40	0/1903	0.54	0/2560
1	D	0.39	0/1921	0.54	0/2584
1	E	0.42	1/1895 (0.1%)	0.53	0/2549
1	F	0.38	0/1895	0.54	0/2550
All	All	0.41	1/11420 (0.0%)	0.55	0/15362

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	A	0	1
1	C	0	1
1	E	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	199	SER	C-N	5.07	1.36	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	ARG	Sidechain
1	C	42	ARG	Sidechain
1	E	212	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	1844	1813	1812	17	0
1	B	1886	1848	1848	18	0
1	C	1865	1825	1827	23	0
1	D	1883	1845	1849	17	1
1	E	1857	1821	1824	27	0
1	F	1857	1815	1818	21	0
2	A	31	19	19	2	0
2	B	31	19	19	0	0
2	C	31	19	19	2	0
2	D	31	19	19	2	0
2	E	31	19	19	3	0
2	F	31	19	19	0	0
3	A	12	16	16	0	0
3	B	12	16	16	0	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
3	E	18	24	24	1	0
4	A	12	18	18	0	0
4	B	20	30	30	1	1
4	C	8	12	12	0	0
4	D	16	24	24	1	0
4	E	8	12	12	0	0
4	F	16	24	24	0	0
5	A	7	10	10	0	0
5	B	7	10	10	0	0
5	D	7	10	10	0	0
5	E	7	10	10	1	0
6	A	18	8	8	3	0
6	B	18	8	8	2	0
6	C	18	8	8	4	0
6	D	18	8	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	18	8	8	2	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
8	A	66	0	0	1	0
8	B	76	0	0	3	0
8	C	64	0	0	2	0
8	D	65	0	0	2	0
8	E	53	0	0	3	0
8	F	49	0	0	1	0
All	All	12023	11353	11364	126	1

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 5.

All (126) 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:B:61:LYS:NZ	8:B:401:HOH:O	1.83	1.09
1:C:28:LYS:NZ	8:C:401:HOH:O	1.96	0.98
1:E:137:LEU:HB3	1:E:144:MET:HE2	1.64	0.80
1:E:61:LYS:NZ	8:E:401:HOH:O	2.09	0.79
1:F:113:PRO:HG2	1:F:116:ILE:HD13	1.65	0.79
1:D:93:LYS:O	1:D:99:SER:OG	2.07	0.73
1:C:112:MET:HG2	1:C:117:ILE:HG12	1.70	0.72
1:A:123:GLU:OE2	1:A:123:GLU:N	2.18	0.72
1:C:97:ARG:NH2	1:C:123:GLU:OE1	2.22	0.71
1:E:119:ASN:HA	1:E:122:LYS:HE2	1.73	0.71
1:E:212:ARG:NH2	8:E:402:HOH:O	2.23	0.70
1:D:31:ASP:OD1	8:D:401:HOH:O	2.09	0.69
1:F:113:PRO:HB2	1:F:115:ASP:OD1	1.94	0.68
1:F:115:ASP:OD2	1:F:116:ILE:HD12	1.96	0.65
6:A:306[B]:CB1:O1	8:A:401:HOH:O	2.14	0.62
1:A:142:ARG:NH1	1:B:139:GLU:OE1	2.32	0.61
1:F:115:ASP:CG	1:F:116:ILE:HD12	2.26	0.60
1:D:176:PHE:CD2	1:D:201:MET:HE3	2.38	0.59
1:F:189:GLY:HA2	8:F:415:HOH:O	2.03	0.59
1:A:112:MET:HG2	1:A:117:ILE:HG12	1.87	0.57
1:C:130:PHE:CD1	6:C:304[B]:CB1:H91	2.40	0.57
6:C:304[B]:CB1:H71	6:C:304[B]:CB1:O4	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:LEU:HG	1:F:160:MET:HE2	1.86	0.56
1:E:208:VAL:HG23	1:E:209:LYS:HD2	1.88	0.56
6:A:306[B]:CB1:O4	6:A:306[B]:CB1:N6	2.39	0.55
1:E:116:ILE:H	1:E:116:ILE:HD12	1.72	0.55
1:D:62:GLU:HA	1:D:62:GLU:OE1	2.06	0.54
1:A:48:VAL:HG12	1:A:48:VAL:O	2.08	0.53
1:B:115:ASP:OD2	8:B:402:HOH:O	2.18	0.53
1:E:90:ARG:HH12	5:E:305:PEG:H22	1.73	0.53
1:B:177:ASN:OD1	1:B:180:LYS:HG3	2.10	0.52
1:D:1:MET:HE2	1:E:223:VAL:HG11	1.91	0.52
1:F:127:LEU:O	1:F:131:GLN:HG3	2.10	0.52
1:C:155:ALA:O	1:C:159:MET:HG3	2.10	0.52
1:D:93:LYS:HB3	4:D:304:EDO:H21	1.92	0.52
1:E:172:PRO:HG2	2:E:301:FMN:C9	2.40	0.52
1:C:71:SER:HA	1:C:176:PHE:HA	1.92	0.51
1:E:116:ILE:HD12	1:E:116:ILE:N	2.26	0.50
1:F:113:PRO:HG2	1:F:116:ILE:CD1	2.39	0.50
1:E:68:ARG:HD3	8:E:404:HOH:O	2.10	0.50
1:F:119:ASN:HA	1:F:122:LYS:HD3	1.94	0.50
6:B:302[B]:CB1:O4	6:B:302[B]:CB1:N6	2.45	0.50
1:B:115:ASP:OD2	1:B:115:ASP:N	2.45	0.49
1:C:192:GLU:HB3	1:C:195:ARG:HD2	1.94	0.49
1:D:184:ILE:O	1:D:188:GLU:HG2	2.12	0.49
6:D:302[B]:CB1:O4	6:D:302[B]:CB1:N6	2.45	0.49
1:D:127:LEU:O	1:D:131:GLN:HG3	2.13	0.49
1:A:172:PRO:HG2	2:A:301:FMN:C9	2.42	0.49
1:C:35:GLN:NE2	1:E:4:GLN:OE1	2.47	0.48
1:B:113:PRO:HG2	1:B:116:ILE:HG13	1.94	0.48
1:A:156:LEU:HG	1:A:160:MET:HE2	1.95	0.48
1:C:130:PHE:CD1	6:C:304[B]:CB1:C9	2.97	0.48
1:E:160:MET:SD	1:E:172:PRO:HD3	2.54	0.48
1:B:118:GLU:O	1:B:122:LYS:HB3	2.13	0.48
1:A:31:ASP:O	1:A:35:GLN:HG2	2.14	0.47
6:B:302[B]:CB1:O4	6:B:302[B]:CB1:C7	2.63	0.47
1:E:118:GLU:O	1:E:122:LYS:HG2	2.14	0.47
1:F:128:GLU:HG3	1:F:138:TYR:OH	2.15	0.47
1:C:192:GLU:O	1:C:195:ARG:HD2	2.15	0.46
1:A:119:ASN:OD1	1:A:122:LYS:NZ	2.49	0.46
1:A:219:LEU:CD1	1:B:42:ARG:HD3	2.45	0.46
1:C:113:PRO:O	1:C:117:ILE:HG13	2.16	0.46
2:E:301:FMN:C4A	3:E:302:GOL:H2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LEU:O	1:C:131:GLN:HG3	2.16	0.46
1:C:149:SER:HB3	1:D:150:LYS:HE2	1.98	0.46
1:B:77:GLN:OE1	4:B:306:EDO:H21	2.16	0.45
1:D:112:MET:HG2	1:D:117:ILE:CG1	2.46	0.45
1:F:71:SER:HA	1:F:176:PHE:HA	1.98	0.45
1:C:35:GLN:CD	1:E:4:GLN:OE1	2.60	0.45
1:C:200:VAL:HG22	1:C:201:MET:N	2.32	0.45
1:E:70:VAL:CG1	1:E:180:LYS:HD2	2.46	0.45
1:E:39:GLU:O	1:E:43:LEU:HG	2.17	0.45
6:D:302[B]:CB1:O4	6:D:302[B]:CB1:C7	2.64	0.45
1:F:115:ASP:OD2	1:F:116:ILE:CD1	2.64	0.45
6:A:306[B]:CB1:O4	6:A:306[B]:CB1:C7	2.65	0.45
1:B:37:ILE:HG22	1:B:159:MET:HG2	1.99	0.45
2:C:301:FMN:HM81	1:D:46:SER:N	2.32	0.45
1:E:70:VAL:HG12	1:E:180:LYS:HD2	1.99	0.45
1:A:2:THR:HG22	1:A:4:GLN:H	1.82	0.45
1:E:112:MET:HG2	1:E:117:ILE:HG12	1.99	0.44
1:F:180:LYS:O	1:F:184:ILE:HG13	2.17	0.44
1:C:192:GLU:O	1:C:195:ARG:HG3	2.17	0.44
1:E:137:LEU:CB	1:E:144:MET:HE2	2.39	0.44
1:B:71:SER:HA	1:B:176:PHE:HA	2.00	0.44
6:E:307[B]:CB1:N6	6:E:307[B]:CB1:O4	2.51	0.44
1:C:88:LEU:HD11	1:C:190:VAL:HG12	2.00	0.43
1:C:96:ARG:NH2	8:C:402:HOH:O	2.29	0.43
1:C:172:PRO:HG2	2:C:301:FMN:C9	2.48	0.43
1:F:155:ALA:O	1:F:159:MET:HG3	2.19	0.43
1:E:127:LEU:O	1:E:131:GLN:HG3	2.19	0.43
6:E:307[B]:CB1:O4	6:E:307[B]:CB1:C7	2.66	0.43
1:B:170:SER:HA	1:B:203:ALA:O	2.19	0.43
1:B:181:VAL:O	1:B:185:LEU:HG	2.18	0.43
1:D:1:MET:HE2	1:E:223:VAL:CG1	2.48	0.43
1:E:172:PRO:C	1:E:173:ILE:HG13	2.44	0.43
1:E:222:ILE:HG13	1:E:223:VAL:HG23	2.01	0.43
2:E:301:FMN:O1P	2:E:301:FMN:O3'	2.19	0.43
1:E:87:LEU:HD21	1:E:159:MET:CE	2.49	0.43
1:A:174:GLU:HG3	2:A:301:FMN:H6	2.02	0.42
1:F:113:PRO:CG	1:F:116:ILE:HD13	2.42	0.42
1:C:46:SER:N	2:D:303:FMN:HM81	2.34	0.42
1:C:122:LYS:O	1:C:125:GLY:N	2.51	0.42
1:A:220:ASP:OD1	1:A:220:ASP:N	2.53	0.42
1:D:93:LYS:HE2	1:D:194:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:VAL:HB	1:F:50:LEU:HG	2.01	0.42
1:B:114:GLU:HA	1:B:117:ILE:HG22	2.01	0.42
1:C:61:LYS:HB3	1:C:61:LYS:HE2	1.82	0.41
1:F:77:GLN:OE1	1:F:77:GLN:N	2.53	0.41
1:B:28:LYS:NZ	8:B:411:HOH:O	2.52	0.41
1:F:50:LEU:HD13	1:F:95:MET:CE	2.50	0.41
1:A:157:ALA:HB2	1:B:154:ILE:HG23	2.02	0.41
1:E:149:SER:HB3	1:F:150:LYS:HE2	2.03	0.41
1:F:200:VAL:HG22	1:F:201:MET:N	2.36	0.41
1:A:108:HIS:O	1:A:111:LYS:HE2	2.21	0.41
1:A:120:MET:HE2	1:A:120:MET:HB2	1.91	0.41
1:A:219:LEU:HD13	1:B:42:ARG:HD3	2.03	0.41
1:D:50:LEU:O	1:D:51:GLU:C	2.64	0.41
1:E:212:ARG:NH2	1:E:212:ARG:H	2.18	0.41
1:D:71:SER:HA	1:D:176:PHE:HA	2.02	0.41
1:F:93:LYS:O	1:F:99:SER:OG	2.36	0.41
6:C:304[B]:CB1:O4	6:C:304[B]:CB1:C7	2.67	0.40
1:D:150:LYS:NZ	8:D:413:HOH:O	2.54	0.40
1:A:2:THR:HB	1:A:5:SER:OG	2.22	0.40
1:B:97:ARG:HA	1:B:127:LEU:HD23	2.02	0.40
1:C:191:LEU:HB3	1:C:196:PHE:O	2.22	0.40
1:D:172:PRO:HG2	2:D:303:FMN:C9	2.51	0.40

All (1) 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:D:42:ARG:HH22	4:B:304:EDO:O2[1_455]	1.58	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/248 (91%)	218 (97%)	6 (3%)	1 (0%)	30	44
1	B	230/248 (93%)	226 (98%)	3 (1%)	1 (0%)	30	44
1	C	228/248 (92%)	219 (96%)	8 (4%)	1 (0%)	30	44
1	D	230/248 (93%)	223 (97%)	6 (3%)	1 (0%)	30	44
1	E	227/248 (92%)	219 (96%)	7 (3%)	1 (0%)	30	44
1	F	227/248 (92%)	219 (96%)	7 (3%)	1 (0%)	30	44
All	All	1367/1488 (92%)	1324 (97%)	37 (3%)	6 (0%)	30	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	VAL
1	E	48	VAL
1	A	48	VAL
1	B	48	VAL
1	F	48	VAL
1	D	48	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/216 (92%)	198 (100%)	0	100	100
1	B	202/216 (94%)	201 (100%)	1 (0%)	86	94
1	C	200/216 (93%)	199 (100%)	1 (0%)	86	94
1	D	201/216 (93%)	201 (100%)	0	100	100
1	E	199/216 (92%)	198 (100%)	1 (0%)	86	94
1	F	199/216 (92%)	198 (100%)	1 (0%)	86	94
All	All	1199/1296 (92%)	1195 (100%)	4 (0%)	91	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	208	VAL
1	C	96	ARG
1	E	65	GLU
1	F	48	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	136	HIS
1	C	15	GLN
1	C	35	GLN
1	C	54	GLN
1	C	131	GLN
1	D	54	GLN
1	D	119	ASN
1	F	18	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

48 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	F	305	-	3,3,3	0.49	0	2,2,2	0.36	0
3	GOL	B	305	-	5,5,5	0.74	0	5,5,5	1.17	0
3	GOL	E	306[A]	-	5,5,5	0.79	0	5,5,5	0.71	0
5	PEG	B	309	-	6,6,6	0.21	0	5,5,5	0.18	0
4	EDO	E	304	-	3,3,3	0.58	0	2,2,2	0.36	0
4	EDO	E	308	-	3,3,3	0.60	0	2,2,2	0.20	0
3	GOL	E	302	-	5,5,5	0.68	0	5,5,5	1.24	1 (20%)
5	PEG	A	304	-	6,6,6	0.41	0	5,5,5	0.22	0
4	EDO	C	305	-	3,3,3	0.48	0	2,2,2	0.78	0
4	EDO	C	302	-	3,3,3	0.49	0	2,2,2	0.99	0
4	EDO	D	306	-	3,3,3	0.42	0	2,2,2	0.94	0
7	SO4	C	306	-	4,4,4	0.18	0	6,6,6	0.21	0
7	SO4	A	309	-	4,4,4	0.18	0	6,6,6	0.47	0
4	EDO	B	308	-	3,3,3	0.57	0	2,2,2	0.18	0
4	EDO	D	304	-	3,3,3	0.39	0	2,2,2	1.01	0
6	CB1	C	304[B]	-	17,19,19	2.38	6 (35%)	18,28,28	2.83	2 (11%)
3	GOL	E	303	-	5,5,5	0.81	0	5,5,5	0.84	0
4	EDO	A	308	-	3,3,3	0.50	0	2,2,2	0.81	0
2	FMN	D	303	-	33,33,33	1.56	6 (18%)	48,50,50	1.51	10 (20%)
2	FMN	B	303	-	33,33,33	1.43	4 (12%)	48,50,50	1.57	12 (25%)
2	FMN	A	301	-	33,33,33	1.42	3 (9%)	48,50,50	1.34	8 (16%)
6	CB1	A	306[B]	-	17,19,19	2.50	8 (47%)	18,28,28	1.41	3 (16%)
6	CB1	D	302[B]	-	17,19,19	2.52	8 (47%)	18,28,28	1.32	4 (22%)
4	EDO	F	304	-	3,3,3	0.61	0	2,2,2	0.43	0
5	PEG	E	305	-	6,6,6	0.22	0	5,5,5	0.20	0
4	EDO	B	310	-	3,3,3	0.60	0	2,2,2	0.04	0
2	FMN	C	301	-	33,33,33	1.39	4 (12%)	48,50,50	1.45	8 (16%)
6	CB1	B	302[B]	-	17,19,19	2.44	7 (41%)	18,28,28	1.31	2 (11%)
3	GOL	A	302	-	5,5,5	0.98	0	5,5,5	0.82	0
3	GOL	A	305[A]	-	5,5,5	1.03	0	5,5,5	1.03	0
4	EDO	F	301	-	3,3,3	0.55	0	2,2,2	0.21	0
6	CB1	E	307[B]	-	17,19,19	2.59	8 (47%)	18,28,28	1.42	4 (22%)
4	EDO	B	307	-	3,3,3	0.54	0	2,2,2	0.32	0
4	EDO	B	306	-	3,3,3	0.66	0	2,2,2	0.07	0
4	EDO	D	307	-	3,3,3	0.44	0	2,2,2	0.58	0
7	SO4	D	309	-	4,4,4	0.14	0	6,6,6	0.19	0
7	SO4	B	311	-	4,4,4	0.15	0	6,6,6	0.31	0
5	PEG	D	305	-	6,6,6	0.23	0	5,5,5	0.11	0
2	FMN	F	302	-	33,33,33	1.51	4 (12%)	48,50,50	1.48	9 (18%)
4	EDO	D	308	-	3,3,3	0.58	0	2,2,2	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	E	301	-	33,33,33	1.40	4 (12%)	48,50,50	1.41	10 (20%)
4	EDO	A	303	-	3,3,3	0.60	0	2,2,2	0.31	0
3	GOL	C	303[A]	-	5,5,5	0.82	0	5,5,5	1.04	0
3	GOL	B	301[A]	-	5,5,5	0.82	0	5,5,5	1.03	0
3	GOL	D	301[A]	-	5,5,5	0.84	0	5,5,5	0.93	0
4	EDO	F	303	-	3,3,3	0.40	0	2,2,2	0.87	0
4	EDO	B	304	-	3,3,3	0.66	0	2,2,2	0.32	0
4	EDO	A	307	-	3,3,3	0.69	0	2,2,2	0.41	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
4	EDO	F	305	-	-	0/1/1/1	-
3	GOL	B	305	-	-	0/4/4/4	-
3	GOL	E	306[A]	-	-	4/4/4/4	-
5	PEG	B	309	-	-	2/4/4/4	-
4	EDO	E	304	-	-	0/1/1/1	-
4	EDO	E	308	-	-	0/1/1/1	-
3	GOL	E	302	-	-	2/4/4/4	-
5	PEG	A	304	-	-	3/4/4/4	-
4	EDO	C	305	-	-	1/1/1/1	-
4	EDO	C	302	-	-	0/1/1/1	-
4	EDO	D	306	-	-	1/1/1/1	-
4	EDO	B	308	-	-	0/1/1/1	-
4	EDO	D	304	-	-	1/1/1/1	-
6	CB1	C	304[B]	-	-	8/12/18/18	0/2/2/2
3	GOL	E	303	-	-	2/4/4/4	-
4	EDO	A	308	-	-	1/1/1/1	-
2	FMN	D	303	-	-	2/18/18/18	0/3/3/3
2	FMN	B	303	-	-	2/18/18/18	0/3/3/3
2	FMN	A	301	-	-	2/18/18/18	0/3/3/3
6	CB1	A	306[B]	-	-	2/12/18/18	0/2/2/2
6	CB1	D	302[B]	-	-	2/12/18/18	0/2/2/2
4	EDO	F	304	-	-	1/1/1/1	-
5	PEG	E	305	-	-	0/4/4/4	-
4	EDO	B	310	-	-	0/1/1/1	-
2	FMN	C	301	-	-	2/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CB1	B	302[B]	-	-	2/12/18/18	0/2/2/2
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	A	305[A]	-	-	2/4/4/4	-
4	EDO	F	301	-	-	0/1/1/1	-
6	CB1	E	307[B]	-	-	2/12/18/18	0/2/2/2
4	EDO	B	307	-	-	0/1/1/1	-
4	EDO	B	306	-	-	0/1/1/1	-
4	EDO	D	307	-	-	1/1/1/1	-
5	PEG	D	305	-	-	0/4/4/4	-
2	FMN	F	302	-	-	4/18/18/18	0/3/3/3
4	EDO	D	308	-	-	1/1/1/1	-
2	FMN	E	301	-	-	2/18/18/18	0/3/3/3
4	EDO	A	303	-	-	0/1/1/1	-
3	GOL	C	303[A]	-	-	0/4/4/4	-
3	GOL	B	301[A]	-	-	0/4/4/4	-
3	GOL	D	301[A]	-	-	0/4/4/4	-
4	EDO	F	303	-	-	1/1/1/1	-
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	A	307	-	-	0/1/1/1	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	306[B]	CB1	C3-N1	7.07	1.46	1.33
6	B	302[B]	CB1	C3-N1	7.07	1.46	1.33
6	D	302[B]	CB1	C3-N1	7.05	1.46	1.33
6	E	307[B]	CB1	C3-N1	6.99	1.46	1.33
6	C	304[B]	CB1	C3-N1	6.80	1.45	1.33
2	D	303	FMN	C9A-C5A	5.34	1.50	1.41
2	B	303	FMN	C9A-C5A	5.25	1.50	1.41
2	F	302	FMN	C9A-C5A	5.13	1.49	1.41
2	A	301	FMN	C9A-C5A	4.77	1.49	1.41
2	C	301	FMN	C9A-C5A	4.76	1.49	1.41
2	E	301	FMN	C9A-C5A	4.37	1.48	1.41
6	D	302[B]	CB1	C2-C3	3.54	1.54	1.50
6	C	304[B]	CB1	C5-N6	3.53	1.49	1.41
6	B	302[B]	CB1	C2-C3	3.45	1.54	1.50
6	E	307[B]	CB1	O3-N3	-3.39	1.17	1.22
2	D	303	FMN	C8-C7	3.31	1.49	1.40
6	E	307[B]	CB1	C2-C3	3.29	1.54	1.50
2	F	302	FMN	C8-C7	3.29	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	304[B]	CB1	C2-C3	3.28	1.54	1.50
2	A	301	FMN	C4-N3	-3.25	1.32	1.38
6	E	307[B]	CB1	C7-N6	3.08	1.48	1.46
6	E	307[B]	CB1	C5-N6	3.05	1.48	1.41
6	A	306[B]	CB1	C2-C3	3.04	1.54	1.50
2	E	301	FMN	C4A-N5	2.99	1.36	1.30
6	A	306[B]	CB1	O1-N	-2.93	1.17	1.22
2	D	303	FMN	C5'-C4'	2.92	1.55	1.51
2	C	301	FMN	C4-N3	-2.91	1.33	1.38
6	B	302[B]	CB1	C9-N6	2.89	1.48	1.46
2	C	301	FMN	C8-C7	2.88	1.48	1.40
6	A	306[B]	CB1	O-C3	-2.84	1.18	1.24
6	D	302[B]	CB1	C5-N6	2.82	1.47	1.41
6	D	302[B]	CB1	O1-N	-2.81	1.18	1.22
6	D	302[B]	CB1	C9-N6	2.81	1.48	1.46
2	B	303	FMN	C4-N3	-2.80	1.33	1.38
2	B	303	FMN	C8-C7	2.79	1.47	1.40
2	F	302	FMN	C4-N3	-2.78	1.33	1.38
2	D	303	FMN	C4-N3	-2.77	1.33	1.38
6	B	302[B]	CB1	O1-N	-2.76	1.18	1.22
6	E	307[B]	CB1	C9-N6	2.75	1.48	1.46
6	E	307[B]	CB1	O-C3	-2.74	1.18	1.24
6	A	306[B]	CB1	C9-N6	2.74	1.48	1.46
6	A	306[B]	CB1	C7-N6	2.73	1.48	1.46
6	D	302[B]	CB1	C7-N6	2.69	1.48	1.46
2	F	302	FMN	C5A-N5	-2.69	1.34	1.39
2	A	301	FMN	C8-C7	2.67	1.47	1.40
6	B	302[B]	CB1	O-C3	-2.66	1.19	1.24
6	E	307[B]	CB1	O1-N	-2.65	1.18	1.22
6	D	302[B]	CB1	O-C3	-2.61	1.19	1.24
2	E	301	FMN	C8-C7	2.59	1.47	1.40
6	C	304[B]	CB1	O-C3	-2.54	1.19	1.24
6	C	304[B]	CB1	O3-N3	-2.41	1.18	1.22
2	C	301	FMN	C5A-N5	-2.39	1.34	1.39
6	A	306[B]	CB1	C5-N6	2.38	1.46	1.41
6	D	302[B]	CB1	O3-N3	-2.36	1.18	1.22
6	A	306[B]	CB1	O3-N3	-2.33	1.18	1.22
6	B	302[B]	CB1	C7-N6	2.33	1.48	1.46
2	D	303	FMN	C5A-N5	-2.31	1.35	1.39
6	C	304[B]	CB1	O1-N	-2.30	1.18	1.22
2	B	303	FMN	C5A-N5	-2.19	1.35	1.39
2	E	301	FMN	C4-N3	-2.16	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	303	FMN	C2-N3	-2.16	1.34	1.39
6	B	302[B]	CB1	C5-N6	2.12	1.45	1.41

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	304[B]	CB1	C4-C5-N6	-10.29	107.30	122.52
6	C	304[B]	CB1	C8-C5-N6	4.93	132.62	123.79
2	D	303	FMN	C9A-C5A-N5	-3.39	118.75	122.43
2	B	303	FMN	C4-C4A-N5	3.30	122.92	118.23
2	B	303	FMN	O2P-P-O5'	-3.30	97.96	106.73
2	C	301	FMN	C9A-C5A-N5	-3.09	119.07	122.43
6	B	302[B]	CB1	C8-C5-N6	-3.08	118.28	123.79
6	A	306[B]	CB1	C8-C5-N6	-3.04	118.35	123.79
2	B	303	FMN	C4A-C10-N1	-2.98	117.81	124.73
2	D	303	FMN	C9A-N10-C10	-2.95	116.17	120.77
2	D	303	FMN	C4A-C10-N1	-2.93	117.92	124.73
2	F	302	FMN	O4'-C4'-C5'	2.88	116.40	109.92
2	B	303	FMN	C9A-N10-C10	-2.87	116.29	120.77
2	B	303	FMN	C10-N1-C2	2.86	122.61	116.90
2	B	303	FMN	C4A-C10-N10	2.83	120.62	116.48
2	C	301	FMN	C1'-N10-C9A	2.79	125.16	120.51
2	F	302	FMN	O4-C4-C4A	-2.74	119.33	126.60
2	E	301	FMN	O5'-P-O1P	-2.74	98.79	106.47
2	F	302	FMN	C5A-C9A-N10	2.74	120.78	117.95
6	E	307[B]	CB1	C-C8-C5	2.74	121.76	118.69
6	E	307[B]	CB1	C8-C5-N6	-2.71	118.94	123.79
2	F	302	FMN	C9A-N10-C10	-2.70	116.56	120.77
2	B	303	FMN	O3P-P-O2P	2.69	117.91	107.64
2	A	301	FMN	C4A-C10-N1	-2.67	118.53	124.73
2	C	301	FMN	C4A-C10-N1	-2.63	118.63	124.73
2	E	301	FMN	C4-C4A-N5	2.62	121.96	118.23
6	A	306[B]	CB1	C9-N6-C7	-2.62	59.63	60.53
2	F	302	FMN	C1'-N10-C9A	2.61	124.86	120.51
2	D	303	FMN	C4'-C3'-C2'	2.59	118.74	113.36
2	E	301	FMN	O2-C2-N1	-2.57	117.57	121.83
6	D	302[B]	CB1	C8-C5-N6	-2.57	119.19	123.79
2	A	301	FMN	C9A-C5A-N5	-2.56	119.65	122.43
2	A	301	FMN	C4-C4A-N5	2.55	121.86	118.23
2	B	303	FMN	O2-C2-N1	-2.54	117.62	121.83
2	C	301	FMN	O4-C4-C4A	-2.53	119.89	126.60
2	E	301	FMN	O4-C4-C4A	-2.49	120.00	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	303	FMN	N3-C2-N1	2.48	124.25	119.38
2	E	301	FMN	C9A-N10-C10	-2.47	116.92	120.77
2	C	301	FMN	C4A-C4-N3	2.47	119.45	113.19
2	D	303	FMN	C4-N3-C2	-2.45	121.12	125.64
2	F	302	FMN	C4A-C10-N1	-2.45	119.05	124.73
2	C	301	FMN	C9A-N10-C10	-2.40	117.03	120.77
2	A	301	FMN	C4A-C4-N3	2.38	119.25	113.19
2	B	303	FMN	C4-N3-C2	-2.38	121.24	125.64
2	B	303	FMN	C4A-C4-N3	2.36	119.19	113.19
2	E	301	FMN	C5A-C9A-N10	2.34	120.37	117.95
6	D	302[B]	CB1	C-C8-C5	2.31	121.28	118.69
2	E	301	FMN	C4A-C10-N1	-2.30	119.39	124.73
2	F	302	FMN	C9A-C5A-N5	-2.29	119.94	122.43
2	C	301	FMN	C4-N3-C2	-2.29	121.41	125.64
6	E	307[B]	CB1	O-C3-N1	-2.28	119.33	122.58
2	C	301	FMN	C10-N1-C2	2.24	121.39	116.90
2	F	302	FMN	C4A-C4-N3	2.23	118.86	113.19
2	D	303	FMN	C5A-C9A-N10	2.22	120.25	117.95
2	A	301	FMN	C9A-N10-C10	-2.21	117.32	120.77
6	A	306[B]	CB1	C-C8-C5	2.20	121.15	118.69
2	A	301	FMN	C4-N3-C2	-2.19	121.61	125.64
2	E	301	FMN	C4A-C4-N3	2.18	118.72	113.19
6	D	302[B]	CB1	O-C3-N1	-2.13	119.56	122.58
6	D	302[B]	CB1	C9-N6-C7	-2.12	59.80	60.53
2	A	301	FMN	C1'-N10-C9A	2.12	124.04	120.51
2	A	301	FMN	O4-C4-C4A	-2.11	121.00	126.60
2	B	303	FMN	C9A-C5A-N5	-2.08	120.17	122.43
6	B	302[B]	CB1	O-C3-N1	-2.07	119.64	122.58
2	D	303	FMN	O4-C4-C4A	-2.04	121.19	126.60
3	E	302	GOL	C3-C2-C1	-2.04	103.79	111.70
2	D	303	FMN	C4A-C4-N3	2.03	118.35	113.19
2	E	301	FMN	C10-N1-C2	2.03	120.97	116.90
2	E	301	FMN	O2P-P-O1P	2.03	118.63	110.68
2	D	303	FMN	C1'-N10-C9A	2.03	123.89	120.51
6	E	307[B]	CB1	C9-N6-C7	-2.02	59.84	60.53
2	B	303	FMN	C10-C4A-N5	-2.00	120.61	124.86
2	F	302	FMN	C4-N3-C2	-2.00	121.95	125.64

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	FMN	C2'-C1'-N10-C10
2	B	303	FMN	C2'-C1'-N10-C10
2	C	301	FMN	C2'-C1'-N10-C10
2	D	303	FMN	C2'-C1'-N10-C10
2	E	301	FMN	C2'-C1'-N10-C10
2	F	302	FMN	C5'-O5'-P-O2P
3	E	302	GOL	O1-C1-C2-C3
3	E	306[A]	GOL	C1-C2-C3-O3
6	C	304[B]	CB1	C8-C5-N6-C7
6	C	304[B]	CB1	C-C1-N-O1
3	E	303	GOL	C1-C2-C3-O3
3	E	306[A]	GOL	O1-C1-C2-C3
3	E	302	GOL	O1-C1-C2-O2
3	E	306[A]	GOL	O2-C2-C3-O3
4	D	308	EDO	O1-C1-C2-O2
4	F	304	EDO	O1-C1-C2-O2
6	C	304[B]	CB1	C1-C2-C3-O
5	A	304	PEG	O1-C1-C2-O2
5	B	309	PEG	O2-C3-C4-O4
6	A	306[B]	CB1	C-C1-N-O1
6	B	302[B]	CB1	C-C1-N-O1
6	D	302[B]	CB1	C-C1-N-O1
6	E	307[B]	CB1	C-C1-N-O1
3	A	305[A]	GOL	O1-C1-C2-O2
2	F	302	FMN	C5'-O5'-P-O3P
5	A	304	PEG	O2-C3-C4-O4
6	C	304[B]	CB1	C1-C2-C3-N1
3	A	302	GOL	O1-C1-C2-O2
3	A	305[A]	GOL	O1-C1-C2-C3
5	A	304	PEG	C1-C2-O2-C3
2	C	301	FMN	N10-C1'-C2'-O2'
3	E	306[A]	GOL	O1-C1-C2-O2
4	F	303	EDO	O1-C1-C2-O2
6	A	306[B]	CB1	C4-C5-N6-C7
6	B	302[B]	CB1	C4-C5-N6-C7
6	C	304[B]	CB1	C4-C5-N6-C9
6	D	302[B]	CB1	C4-C5-N6-C7
6	E	307[B]	CB1	C4-C5-N6-C7
6	C	304[B]	CB1	C2-C1-N-O1
2	F	302	FMN	C4'-C5'-O5'-P
4	D	304	EDO	O1-C1-C2-O2
3	A	302	GOL	C1-C2-C3-O3
5	B	309	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	B	304	EDO	O1-C1-C2-O2
4	C	305	EDO	O1-C1-C2-O2
4	D	307	EDO	O1-C1-C2-O2
6	C	304[B]	CB1	C4-C2-C3-O
3	E	303	GOL	O2-C2-C3-O3
6	C	304[B]	CB1	C4-C2-C3-N1
2	D	303	FMN	C4'-C5'-O5'-P
2	E	301	FMN	O3'-C3'-C4'-C5'
4	A	308	EDO	O1-C1-C2-O2
4	D	306	EDO	O1-C1-C2-O2
2	A	301	FMN	N10-C1'-C2'-O2'
2	B	303	FMN	N10-C1'-C2'-O2'
2	F	302	FMN	N10-C1'-C2'-O2'

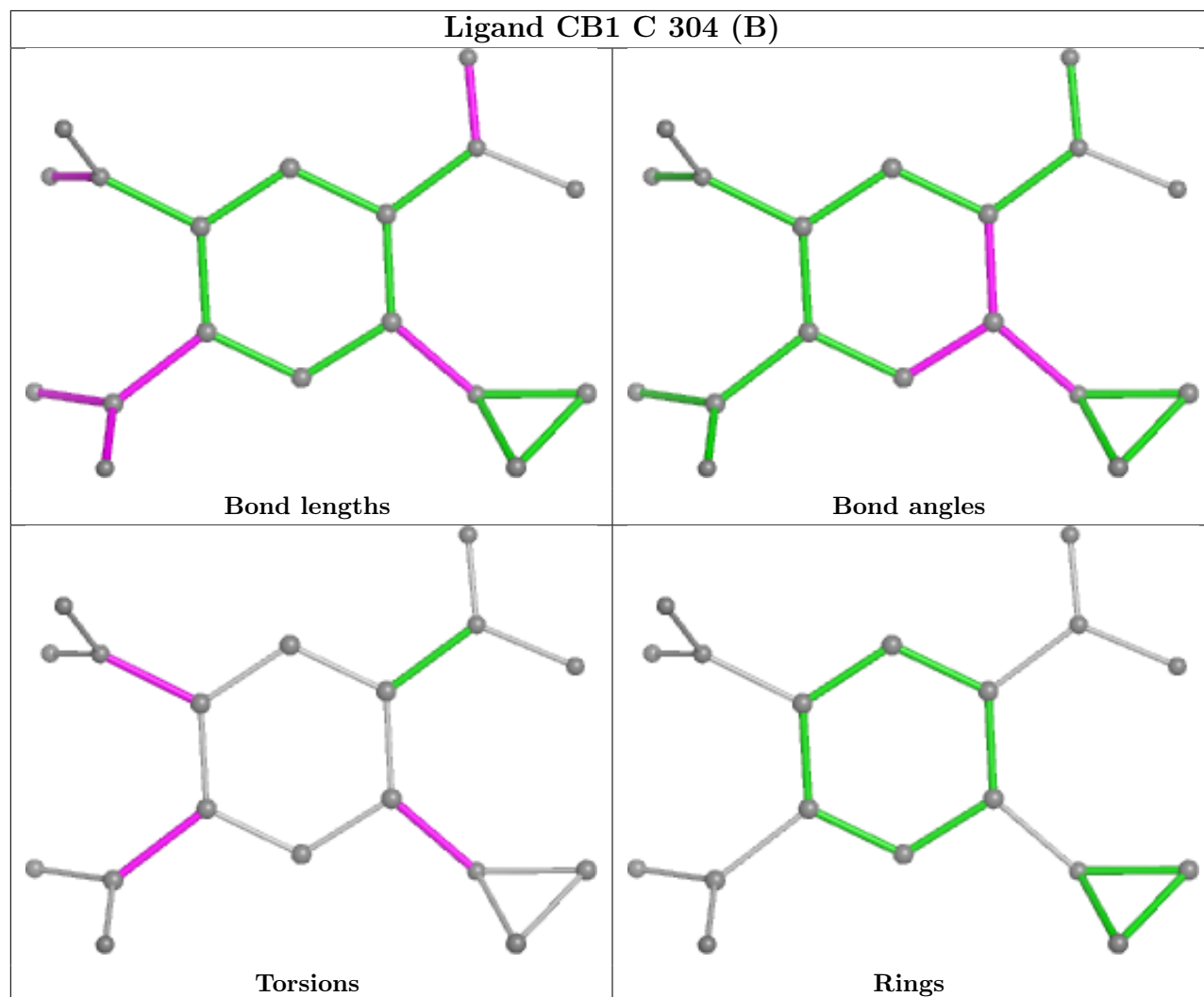
There are no ring outliers.

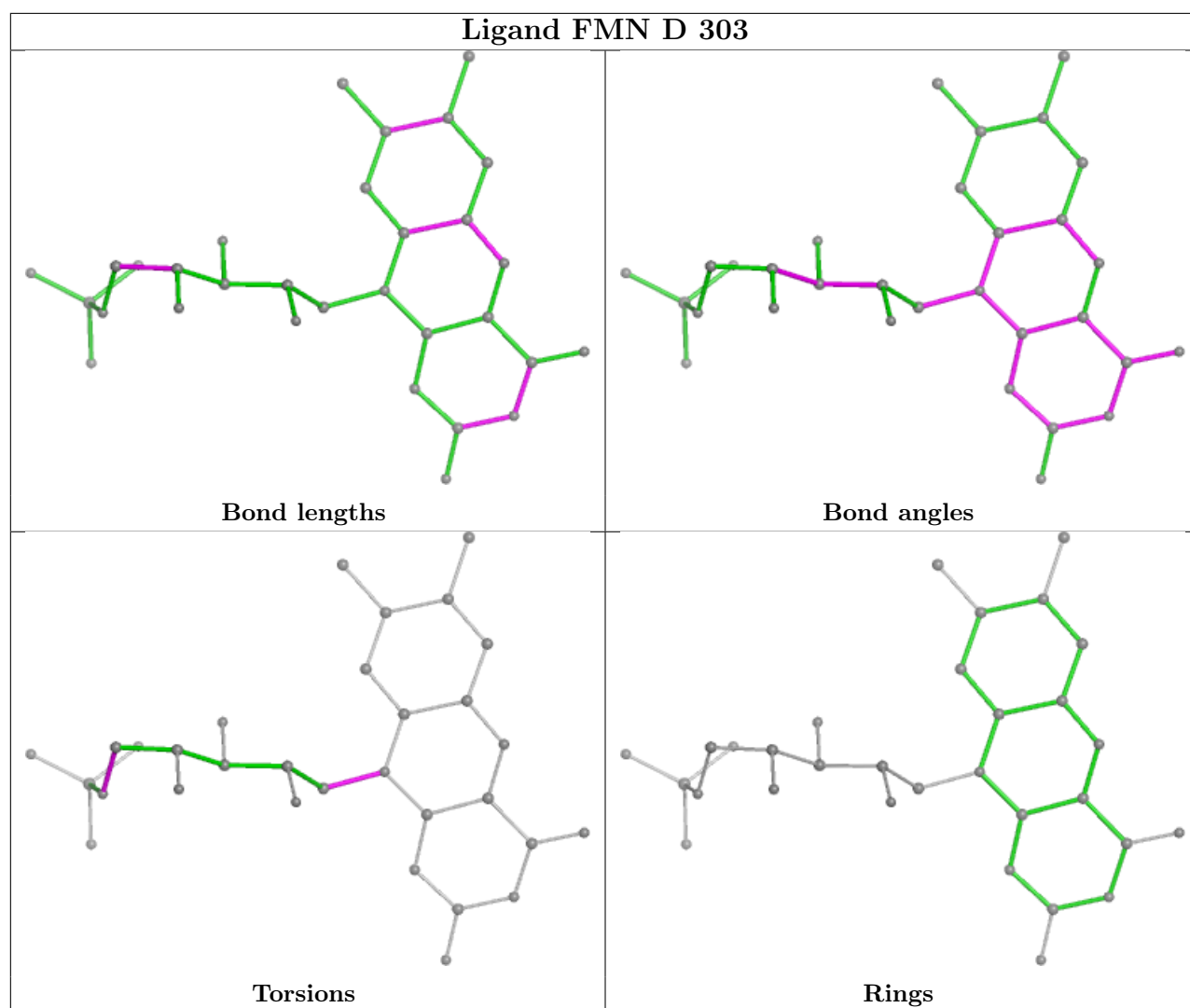
14 monomers are involved in 26 short contacts:

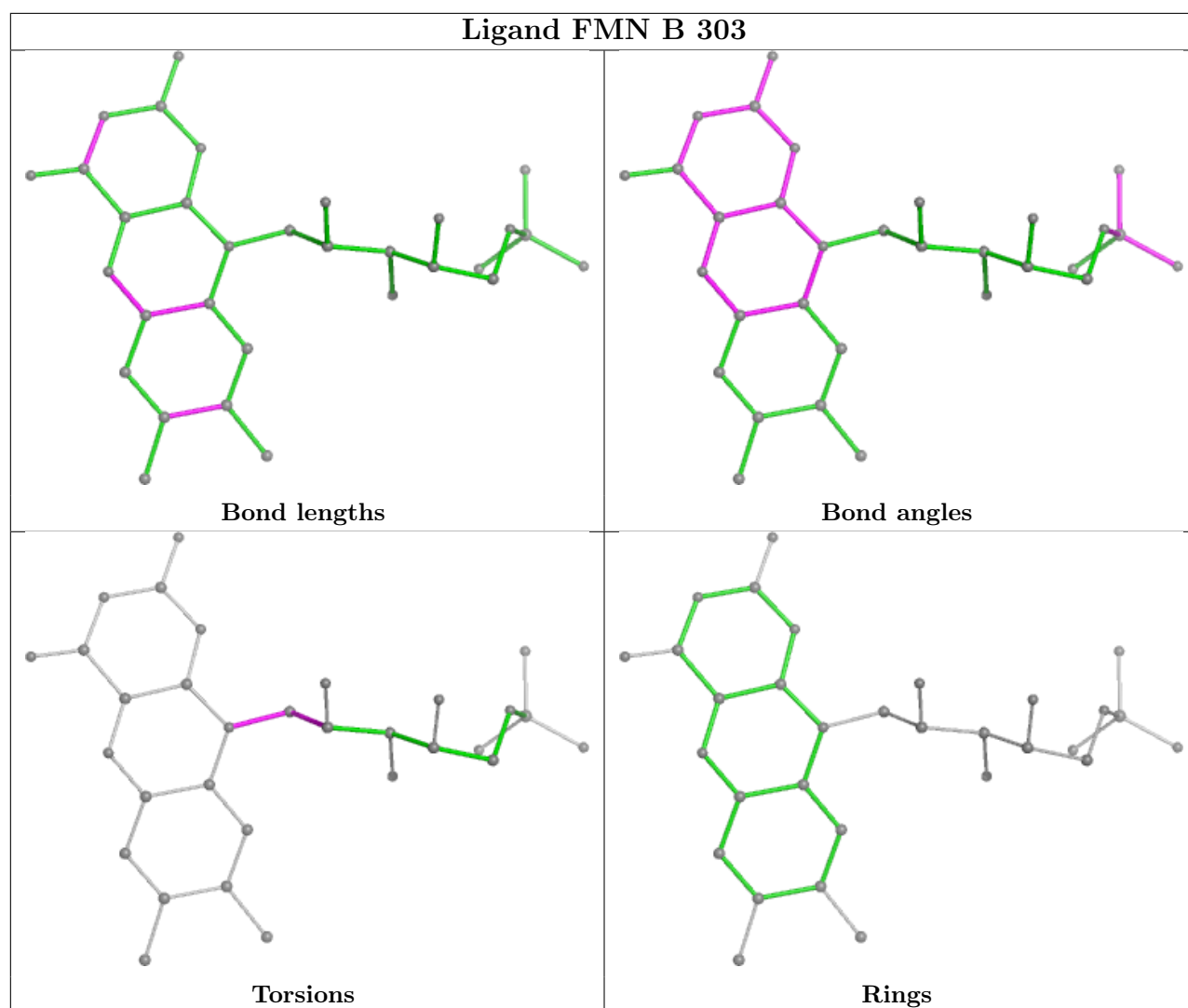
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	GOL	1	0
4	D	304	EDO	1	0
6	C	304[B]	CB1	4	0
2	D	303	FMN	2	0
2	A	301	FMN	2	0
6	A	306[B]	CB1	3	0
6	D	302[B]	CB1	2	0
5	E	305	PEG	1	0
2	C	301	FMN	2	0
6	B	302[B]	CB1	2	0
6	E	307[B]	CB1	2	0
4	B	306	EDO	1	0
2	E	301	FMN	3	0
4	B	304	EDO	0	1

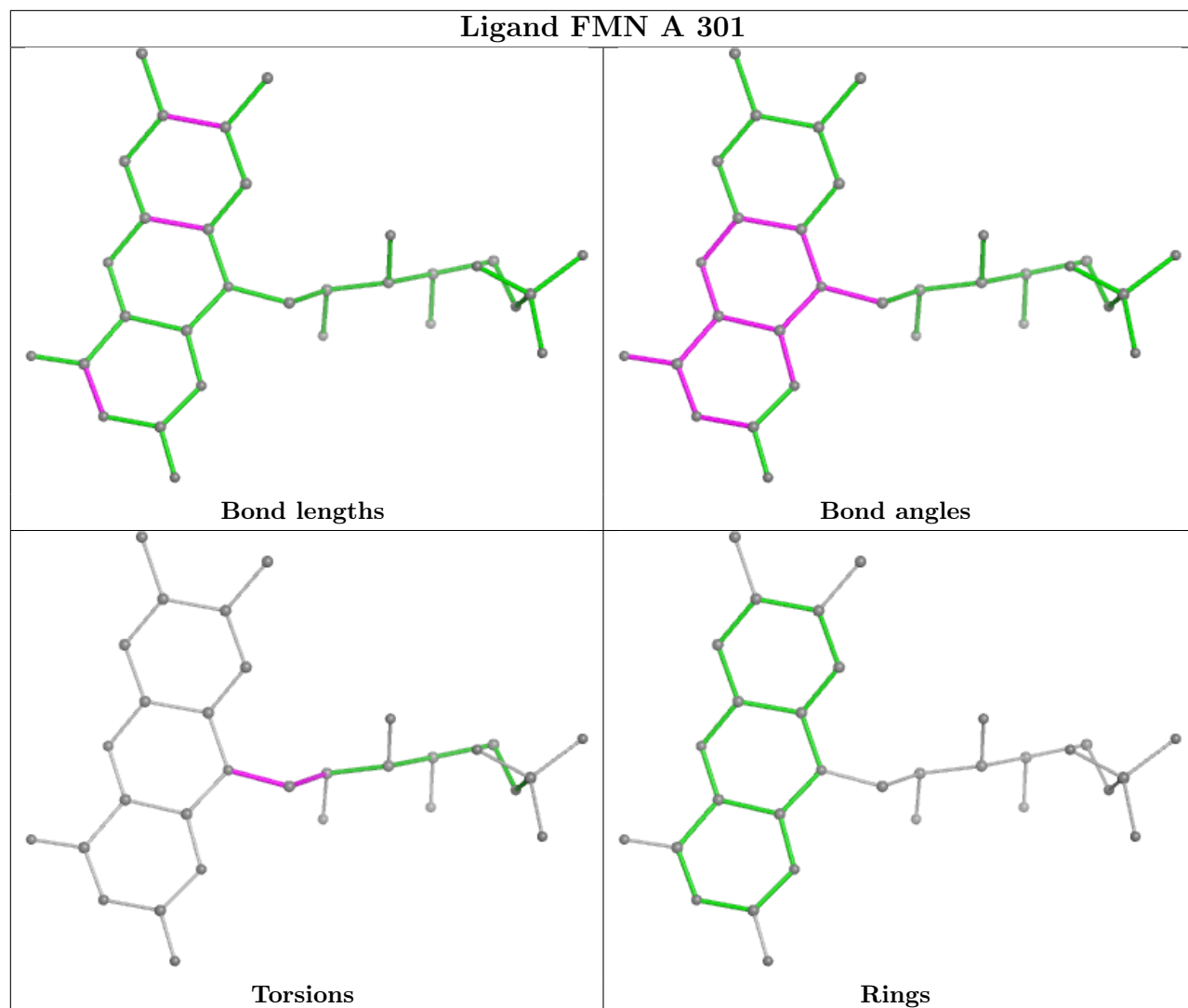
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

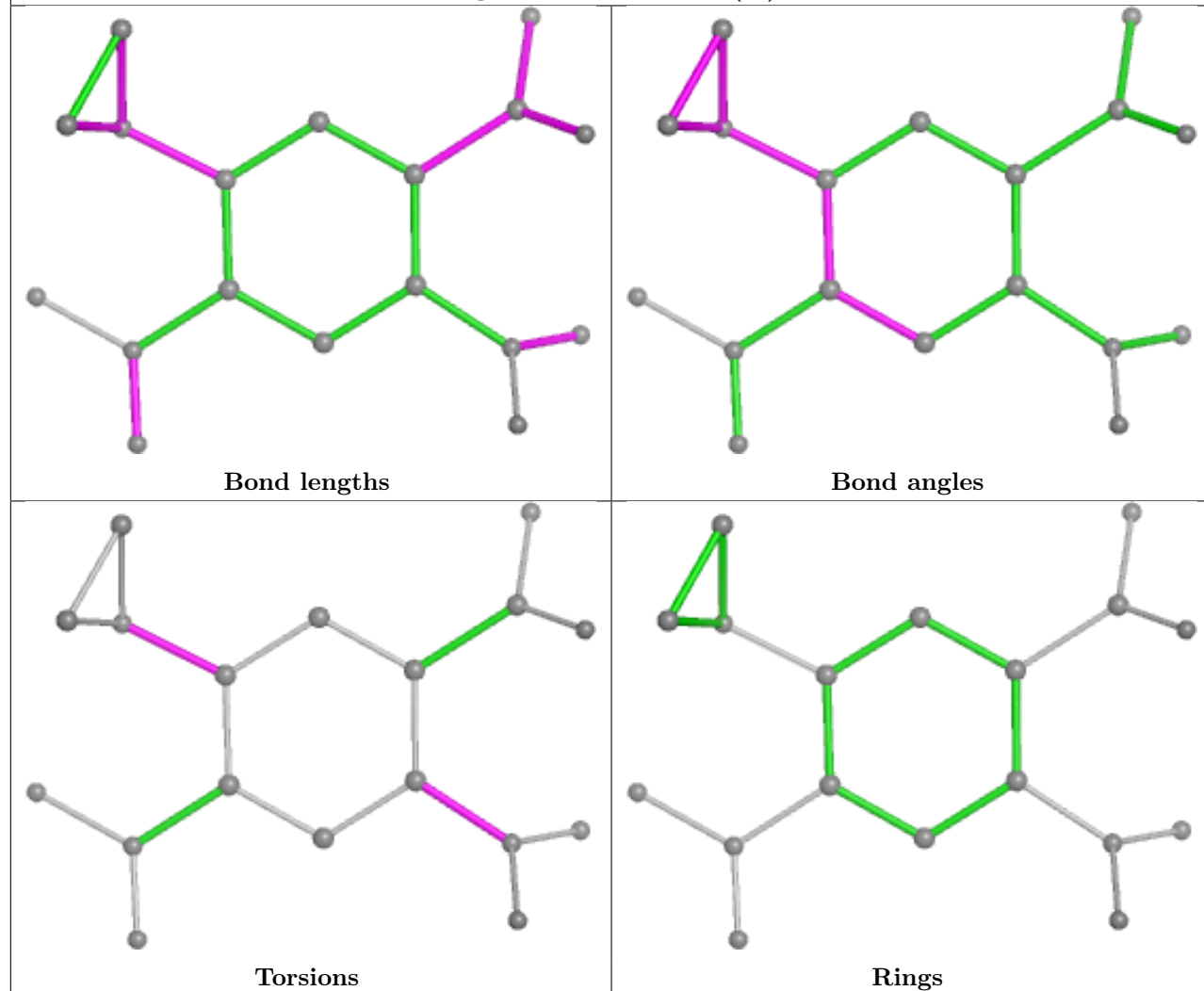




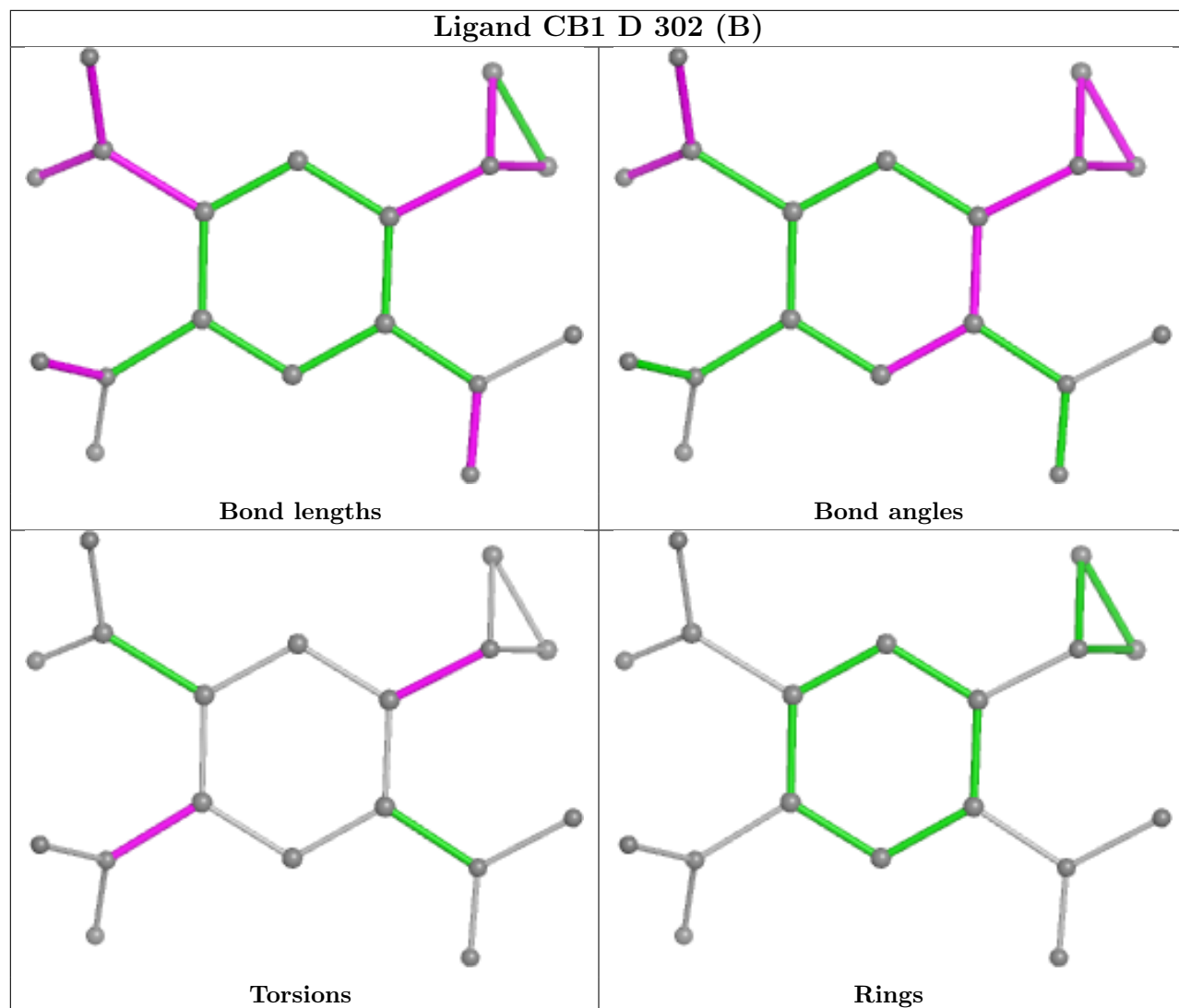


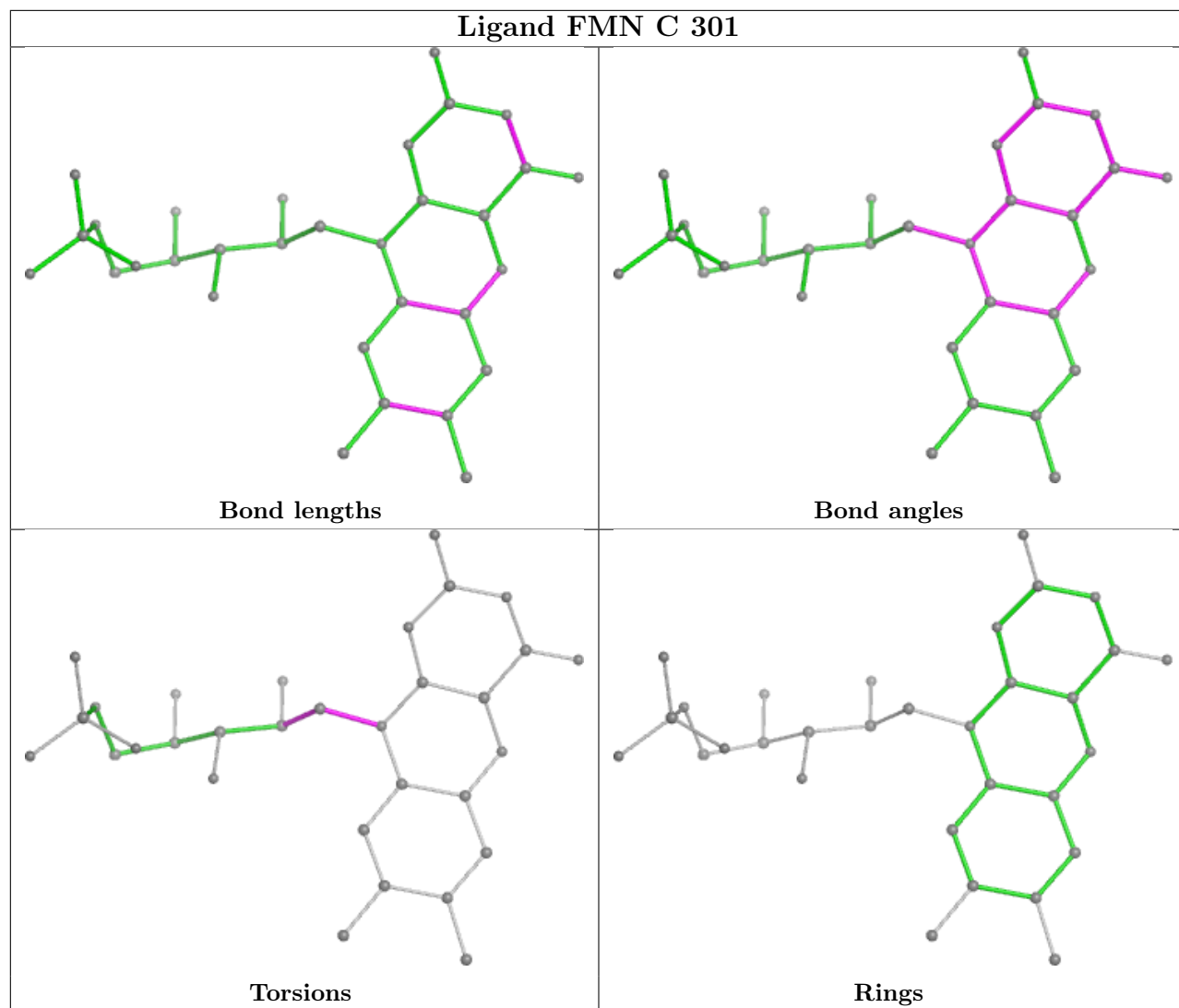


Ligand CB1 A 306 (B)

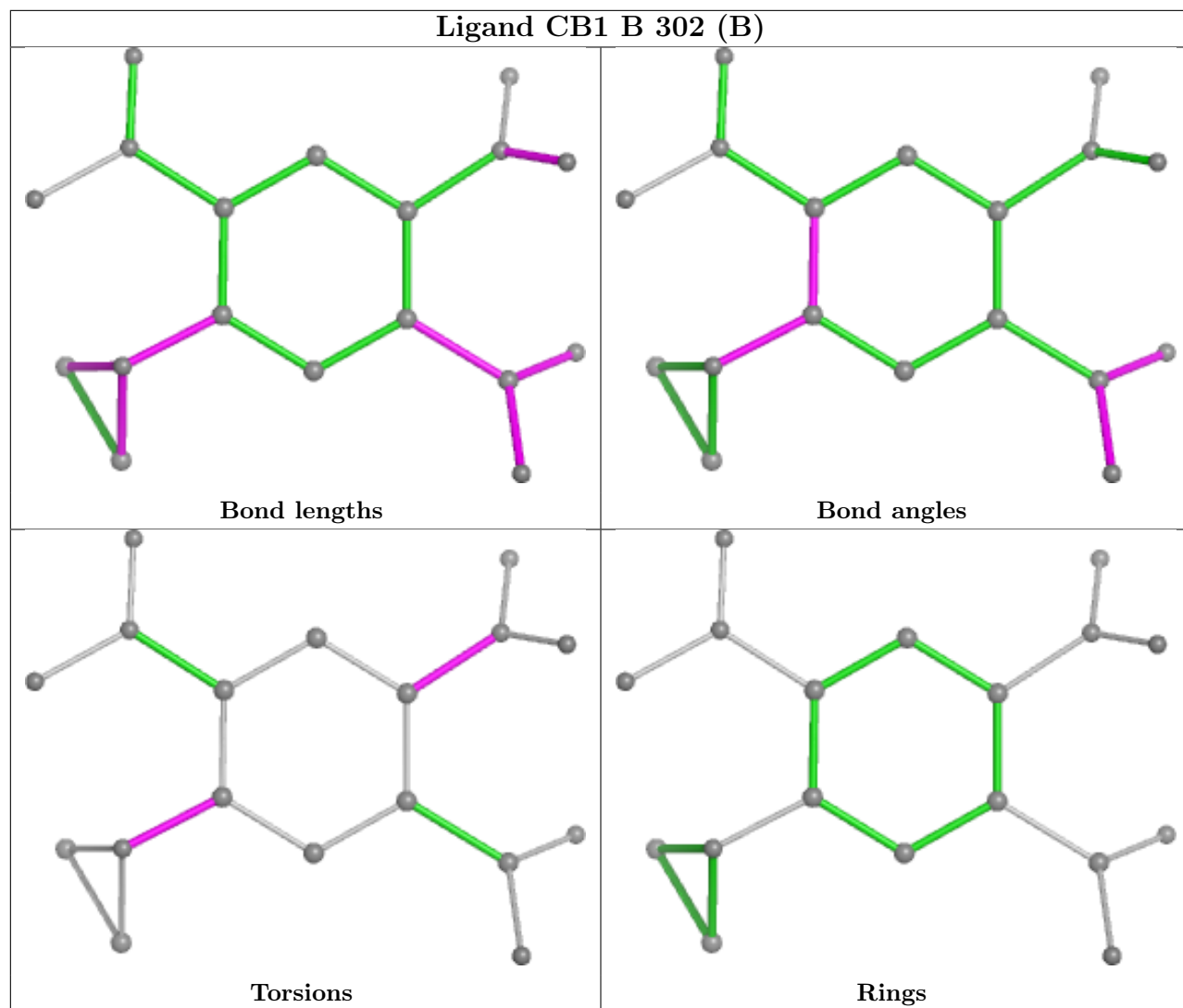


Ligand CB1 D 302 (B)

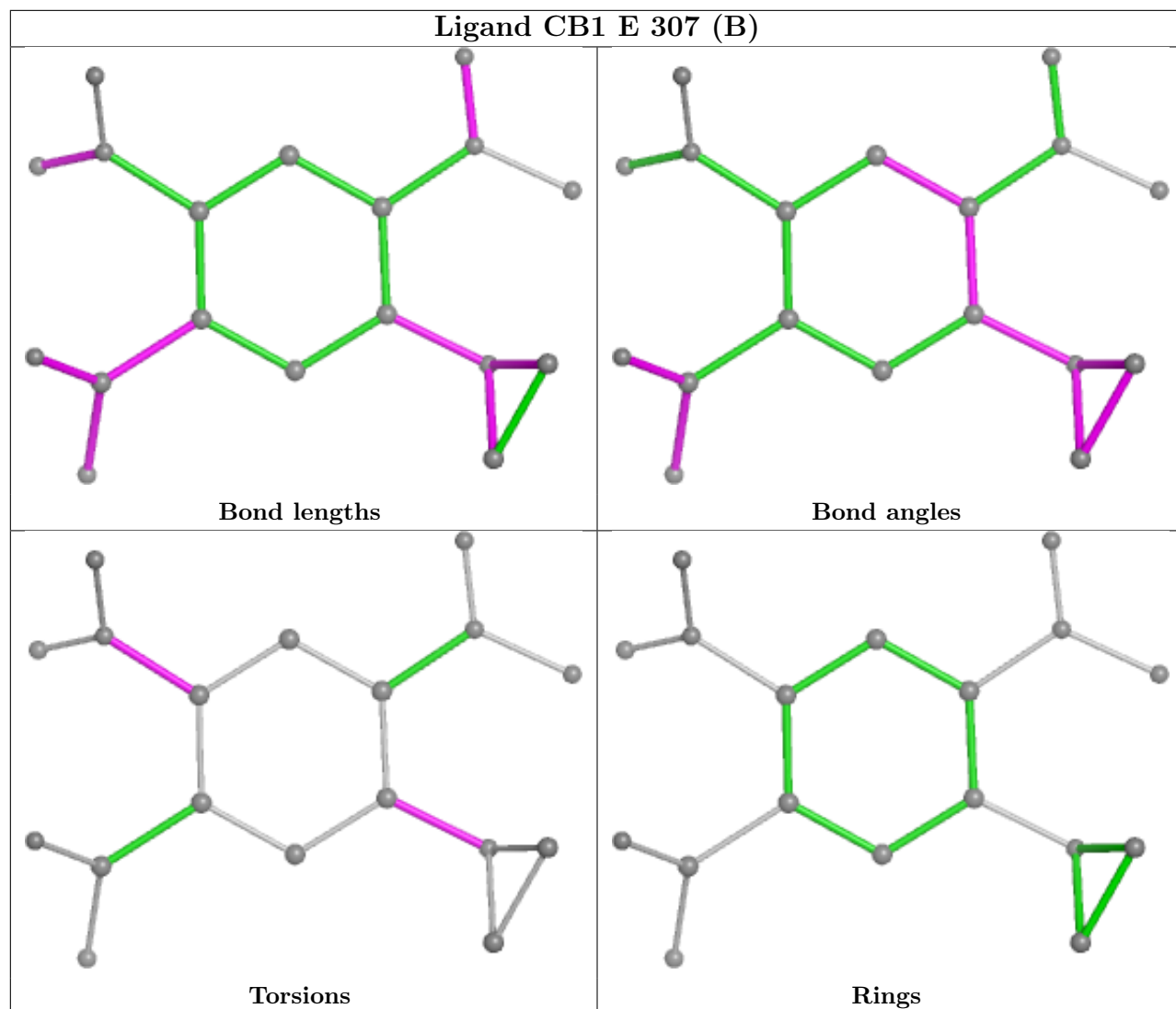


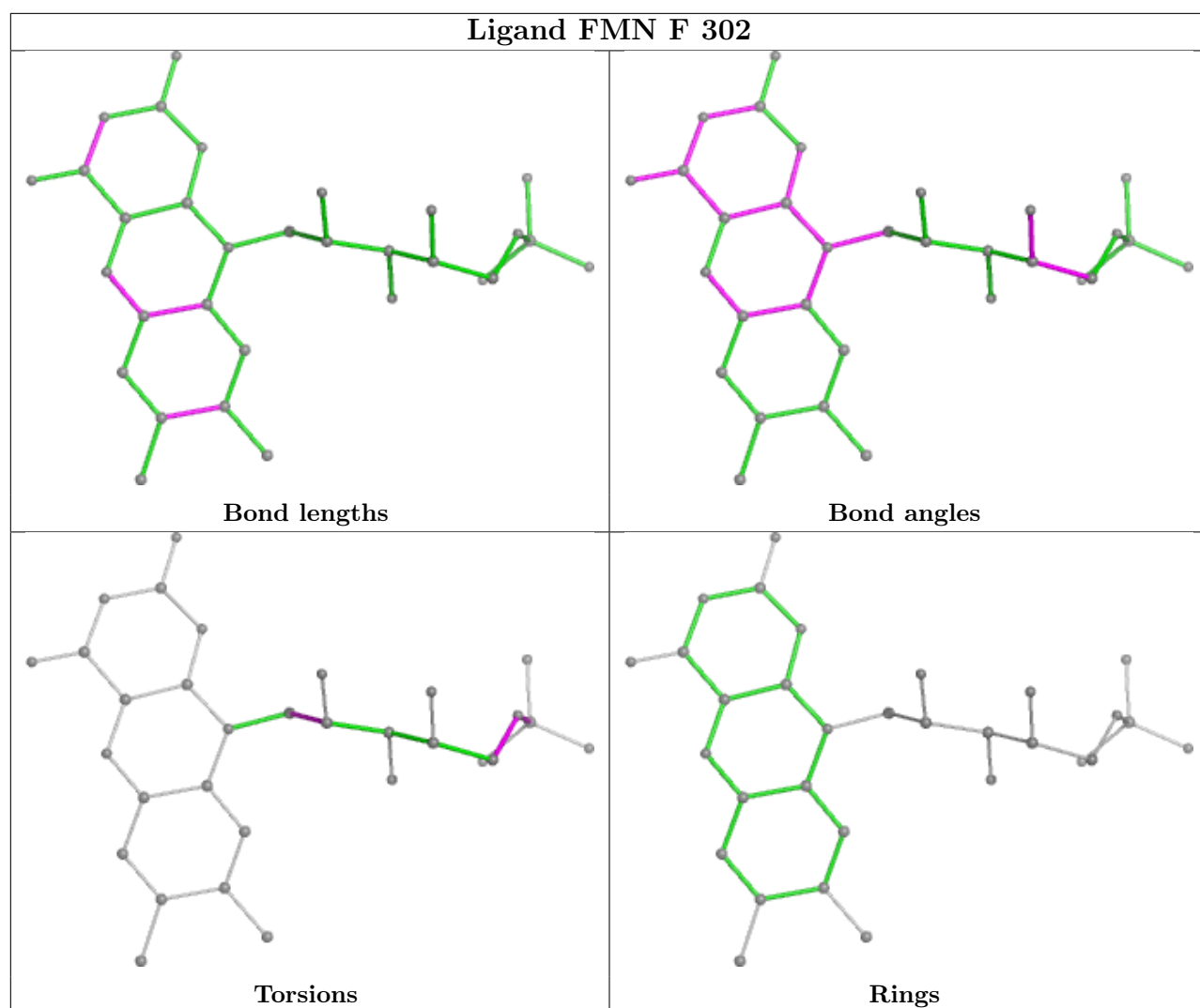


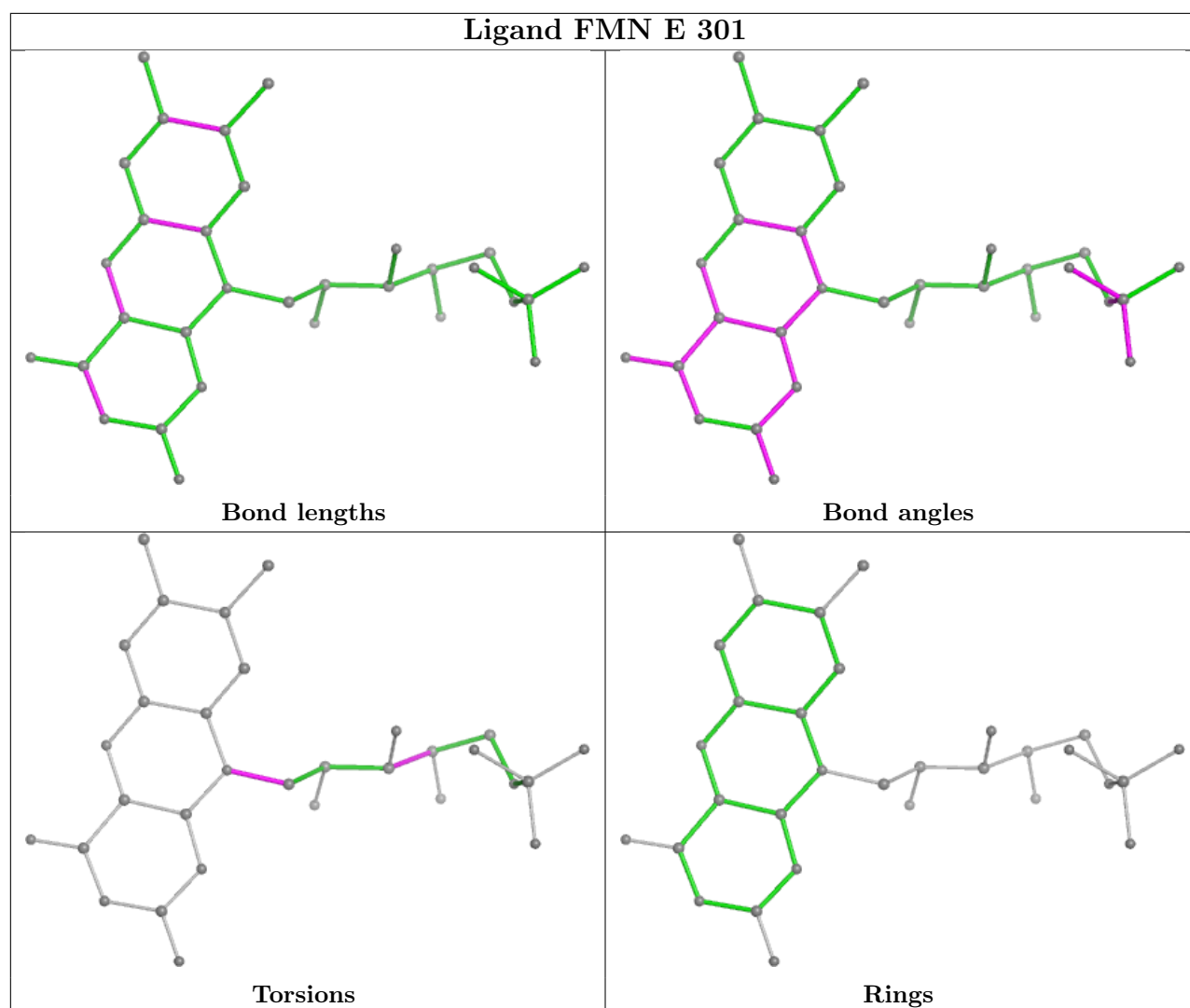
Ligand CB1 B 302 (B)



Ligand CB1 E 307 (B)







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	226/248 (91%)	-0.76	0	100 100	29, 51, 85, 101	1 (0%)
1	B	228/248 (91%)	-0.77	1 (0%)	89 87	29, 53, 76, 86	4 (1%)
1	C	228/248 (91%)	-0.65	1 (0%)	89 87	33, 59, 86, 97	2 (0%)
1	D	229/248 (92%)	-0.66	2 (0%)	81 78	33, 58, 86, 102	3 (1%)
1	E	228/248 (91%)	-0.53	2 (0%)	81 78	43, 61, 101, 112	1 (0%)
1	F	227/248 (91%)	-0.58	2 (0%)	81 78	31, 61, 94, 111	2 (0%)
All	All	1366/1488 (91%)	-0.66	8 (0%)	85 83	29, 57, 89, 112	13 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	MET	4.0
1	D	0	MET	3.3
1	B	0	MET	3.1
1	D	-1	HIS	2.8
1	C	0	MET	2.7
1	F	72	TRP	2.6
1	E	0	MET	2.5
1	E	72	TRP	2.2

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 ⓘ

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
3	GOL	E	306[A]	6/6	0.53	0.79	89,139,167,182	14
3	GOL	C	303[A]	6/6	0.73	0.31	75,95,114,114	14
6	CB1	C	304[B]	18/18	0.73	0.29	76,128,189,216	26
4	EDO	F	305	4/4	0.74	0.14	61,73,84,84	0
6	CB1	E	307[B]	18/18	0.76	0.21	77,130,189,215	0
4	EDO	B	306	4/4	0.78	0.13	63,76,85,90	0
5	PEG	A	304	7/7	0.80	0.16	49,70,85,85	0
6	CB1	A	306[B]	18/18	0.80	0.23	66,127,189,215	0
3	GOL	B	301[A]	6/6	-	-	70,92,135,135	14
6	CB1	B	302[B]	18/18	0.80	0.24	50,127,189,215	0
4	EDO	F	301	4/4	0.80	0.21	73,87,105,105	0
3	GOL	D	301[A]	6/6	-	-	74,100,132,132	14
3	GOL	A	302	6/6	0.80	0.12	62,77,106,106	0
6	CB1	D	302[B]	18/18	0.81	0.21	69,127,189,215	0
7	SO4	C	306	5/5	0.81	0.11	85,88,125,133	0
5	PEG	E	305	7/7	0.82	0.18	66,96,144,144	0
5	PEG	B	309	7/7	0.83	0.17	67,80,94,96	0
4	EDO	F	304	4/4	0.83	0.13	64,78,93,93	0
3	GOL	E	302	6/6	0.84	0.17	61,85,114,116	0
4	EDO	E	308	4/4	0.84	0.13	59,75,90,93	0
3	GOL	E	303	6/6	0.85	0.13	56,78,94,106	0
4	EDO	C	305	4/4	0.86	0.17	77,93,102,102	0
4	EDO	D	307	4/4	0.86	0.13	60,78,93,97	0
4	EDO	E	304	4/4	0.86	0.13	61,74,87,91	0
4	EDO	B	307	4/4	0.86	0.12	62,81,85,97	0
4	EDO	D	306	4/4	0.87	0.16	63,79,95,100	0
4	EDO	A	307	4/4	0.88	0.16	49,66,81,81	0
7	SO4	A	309	5/5	0.88	0.10	65,77,102,109	0
4	EDO	A	303	4/4	0.88	0.10	66,80,83,95	0
4	EDO	B	310	4/4	0.89	0.10	50,60,65,71	0
4	EDO	C	302	4/4	0.89	0.10	63,76,83,91	0
4	EDO	B	308	4/4	0.89	0.15	61,87,105,105	0
5	PEG	D	305	7/7	0.89	0.11	57,83,99,101	0
4	EDO	B	304	4/4	0.90	0.10	51,62,74,74	0
4	EDO	D	308	4/4	0.90	0.10	50,68,80,82	0
3	GOL	B	305	6/6	0.91	0.10	56,70,83,87	0
7	SO4	D	309	5/5	0.93	0.07	63,72,106,115	0

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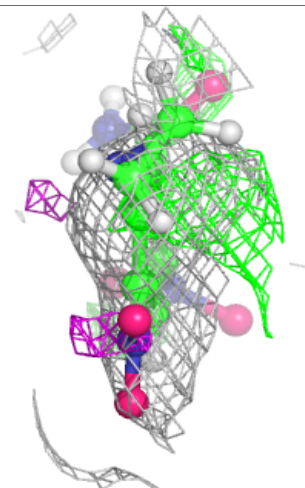
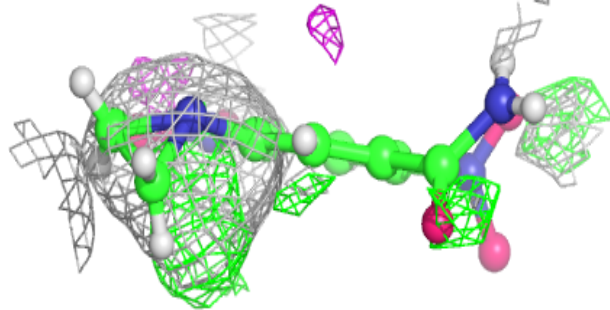
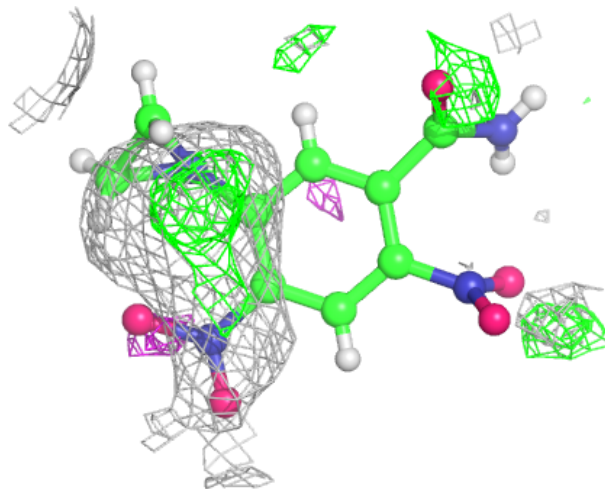
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	308	4/4	0.94	0.11	50,61,82,99	0
4	EDO	F	303	4/4	0.94	0.09	57,79,80,97	0
3	GOL	A	305[A]	6/6	0.96	0.32	80,102,138,138	14
2	FMN	E	301	31/31	0.96	0.06	34,50,64,69	0
4	EDO	D	304	4/4	0.96	0.08	46,69,74,83	0
7	SO4	B	311	5/5	0.97	0.06	51,53,68,71	0
2	FMN	F	302	31/31	0.97	0.07	40,53,67,75	0
2	FMN	D	303	31/31	0.97	0.06	34,50,71,75	0
2	FMN	B	303	31/31	0.98	0.05	32,46,58,67	0
2	FMN	C	301	31/31	0.98	0.06	36,47,58,62	0
2	FMN	A	301	31/31	0.98	0.05	29,45,59,64	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.

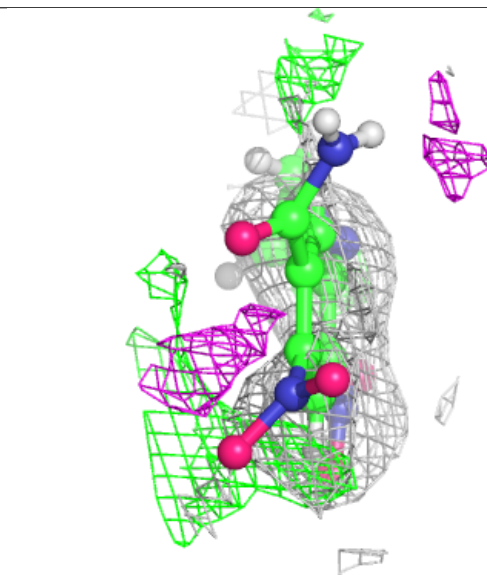
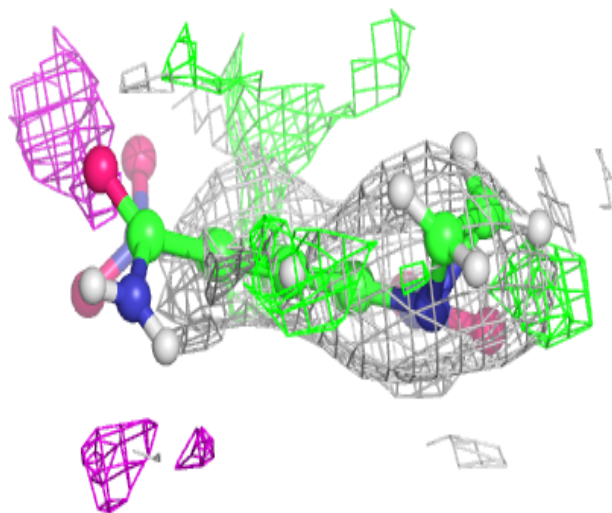
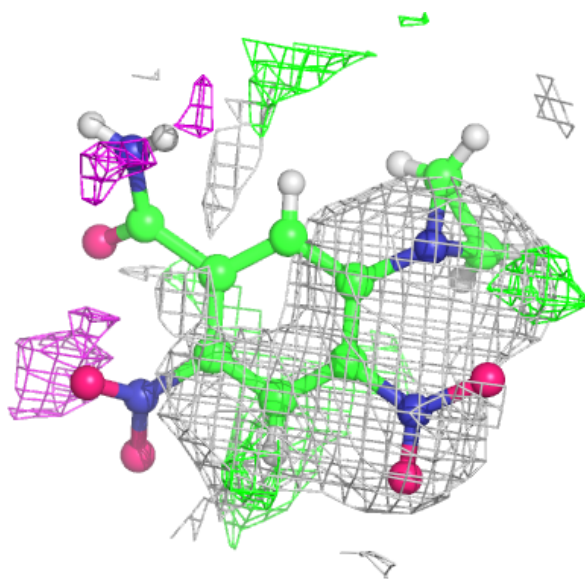
Electron density around CB1 C 304 (B):

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



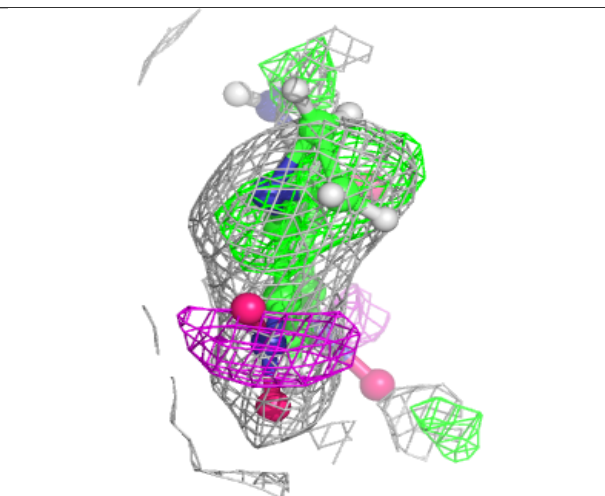
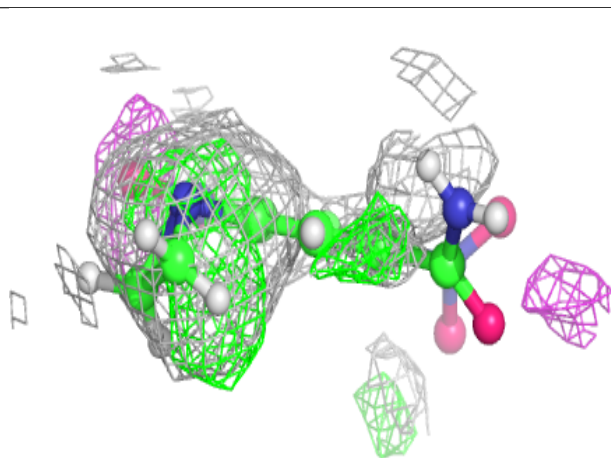
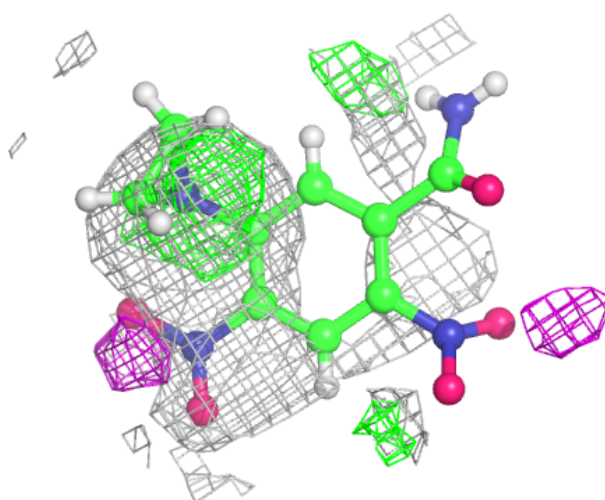
Electron density around CB1 E 307 (B):

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



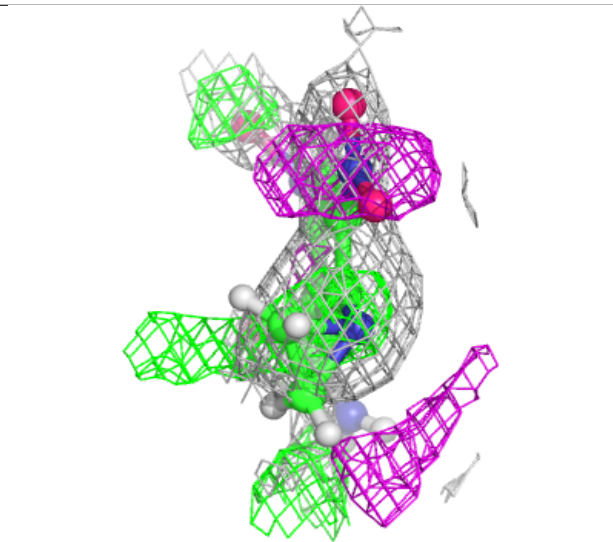
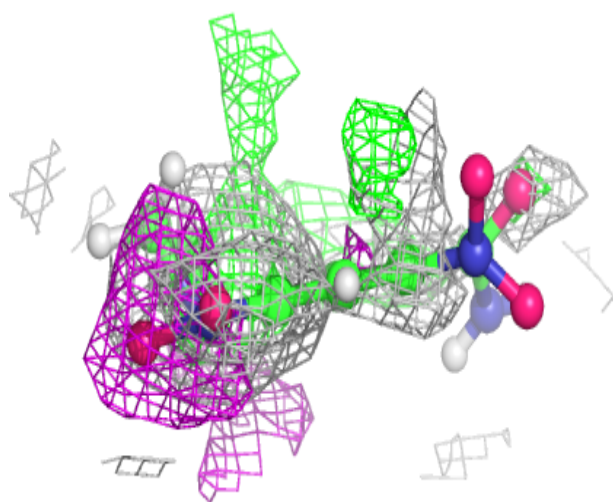
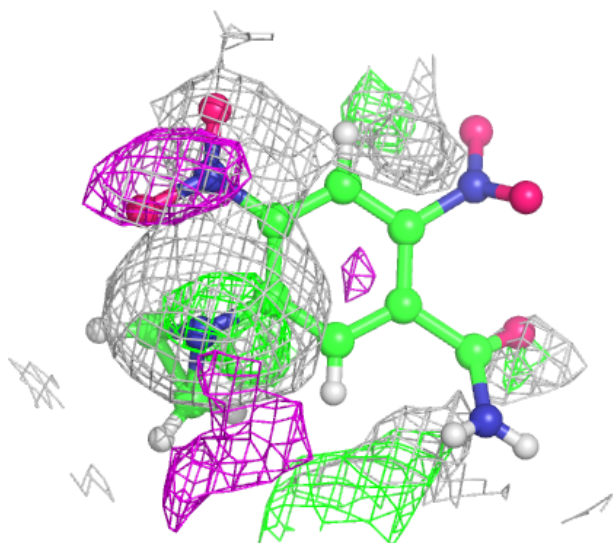
Electron density around CB1 A 306 (B):

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



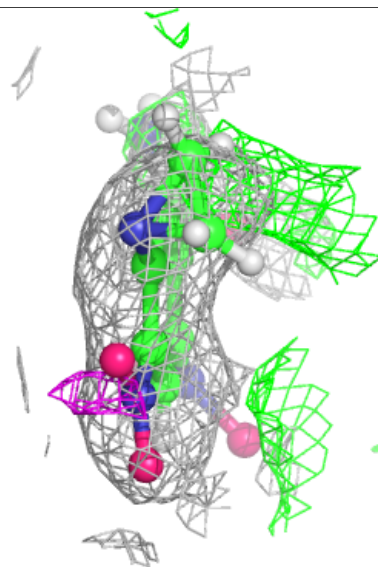
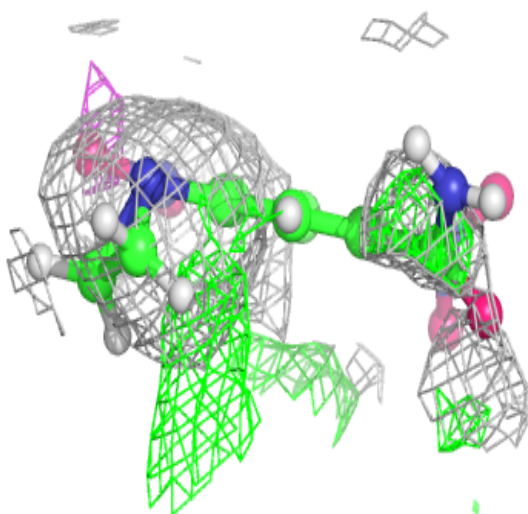
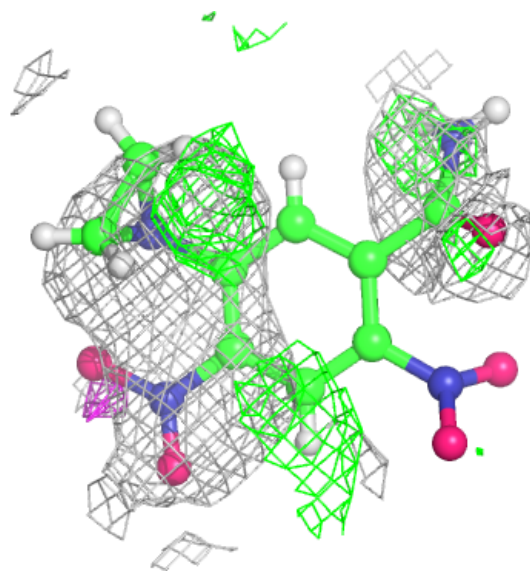
Electron density around CB1 B 302 (B):

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



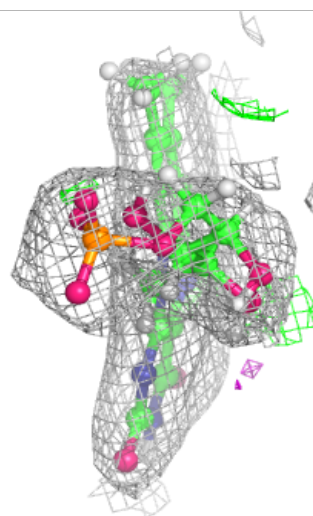
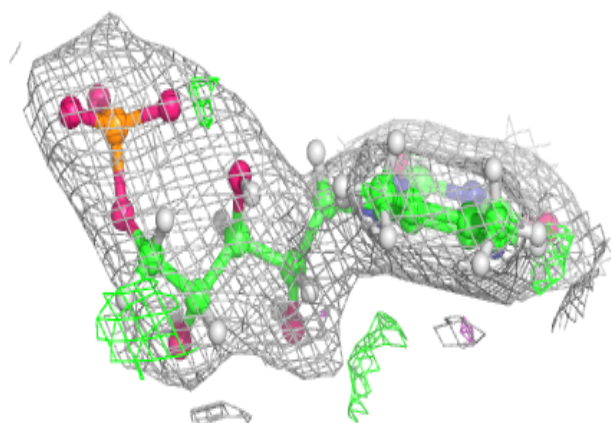
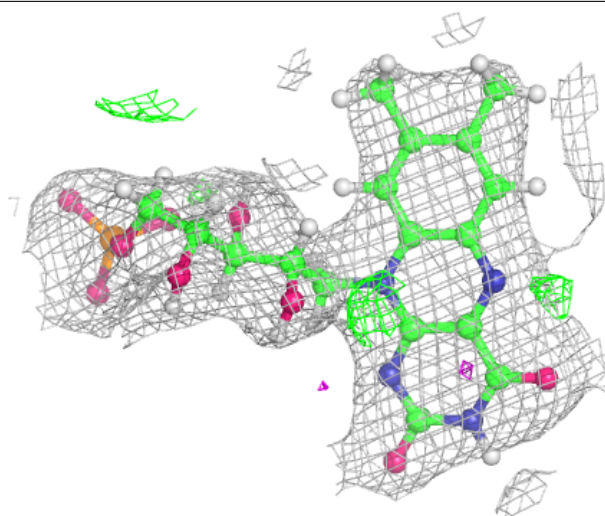
Electron density around CB1 D 302 (B):

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



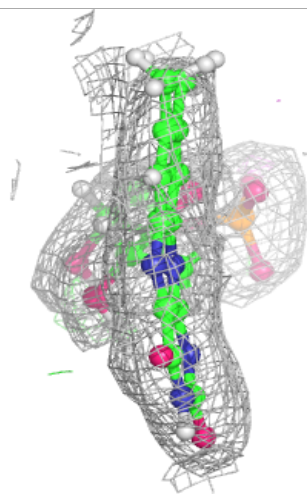
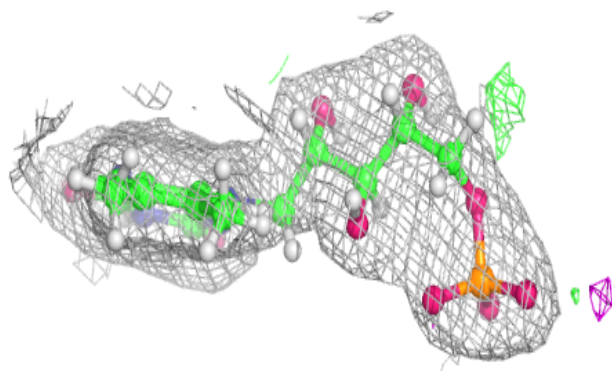
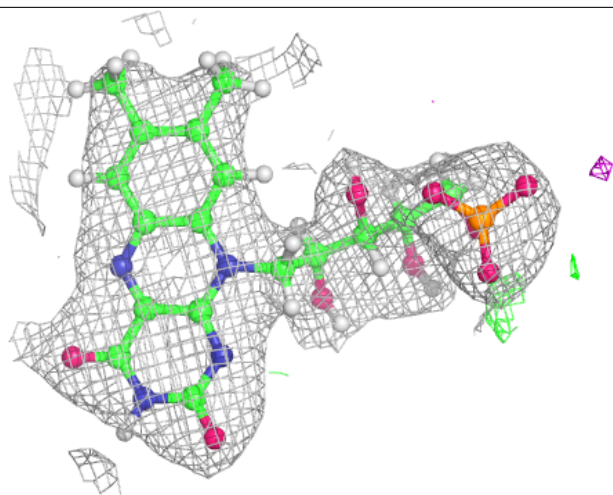
Electron density around FMN E 301:

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



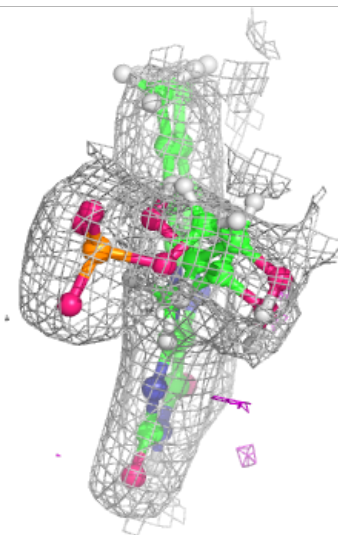
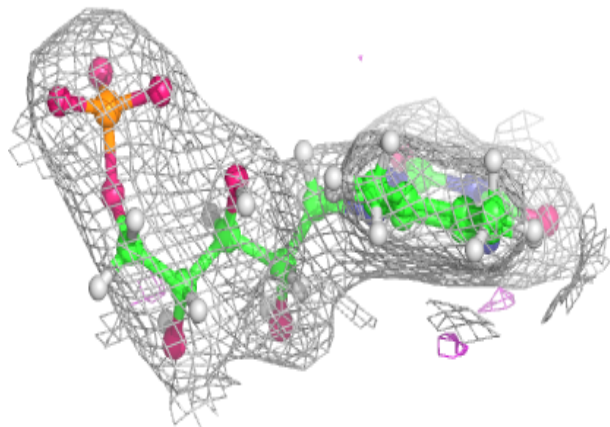
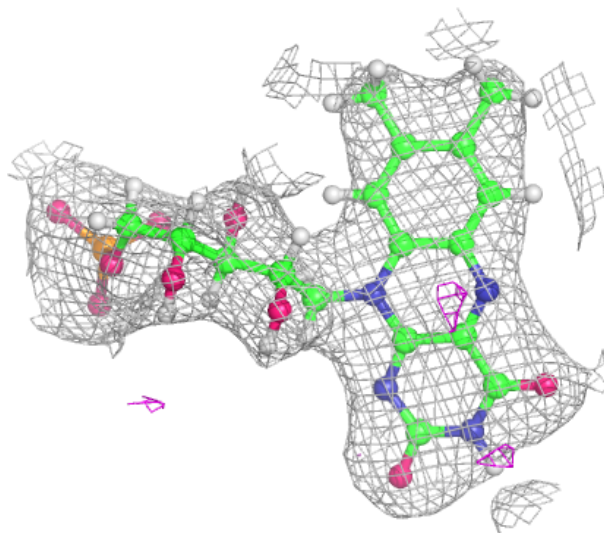
Electron density around FMN F 302:

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



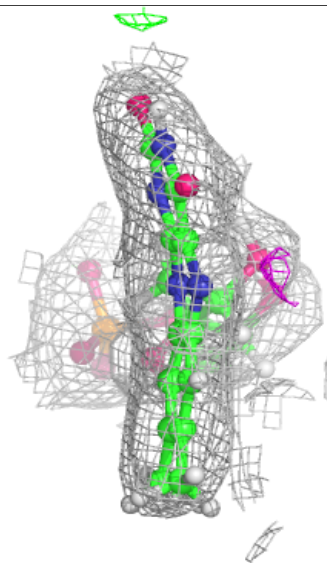
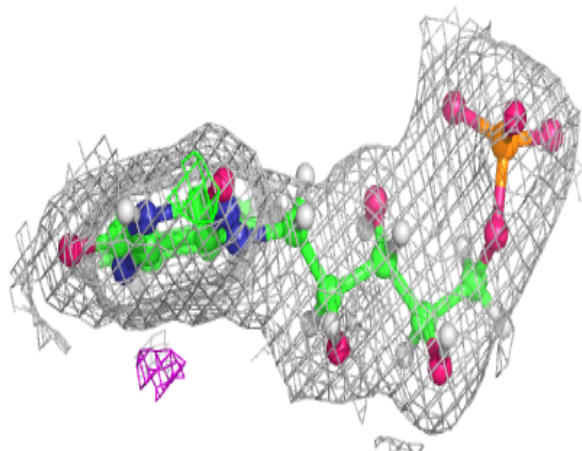
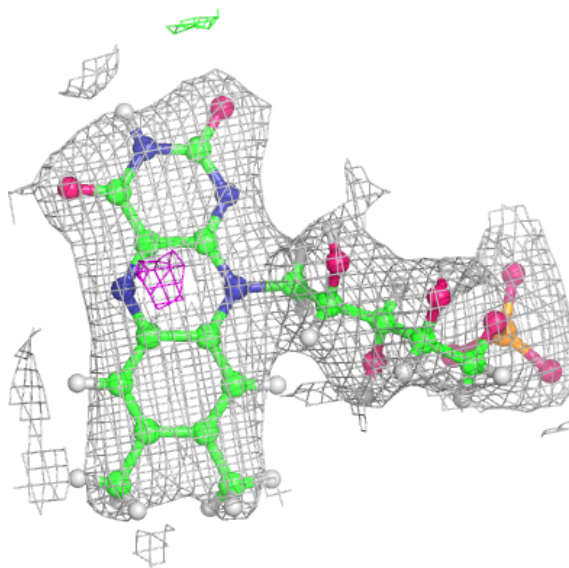
Electron density around FMN D 303:

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



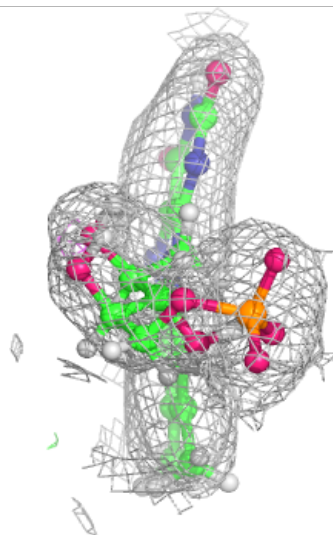
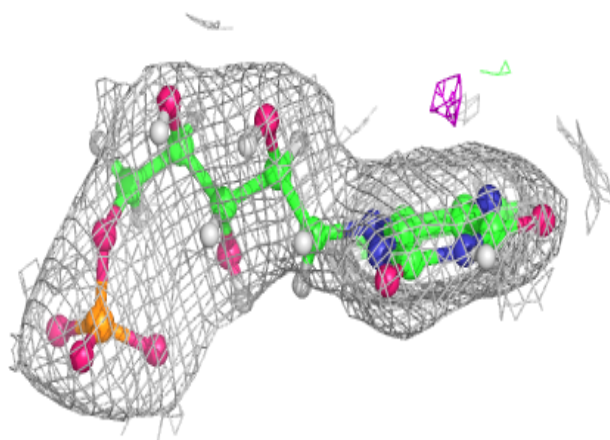
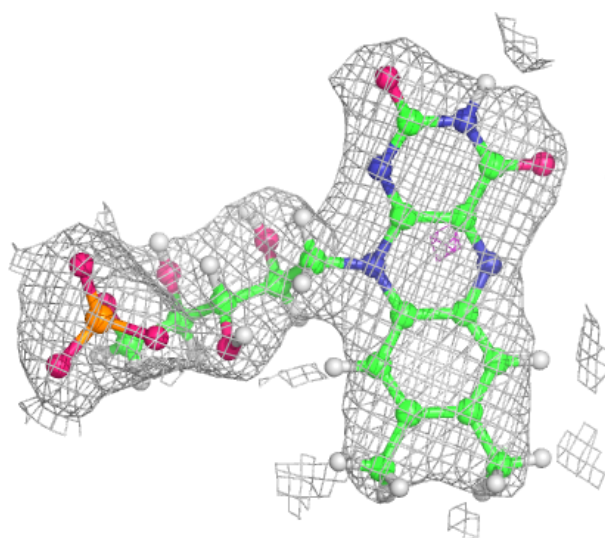
Electron density around FMN B 303:

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



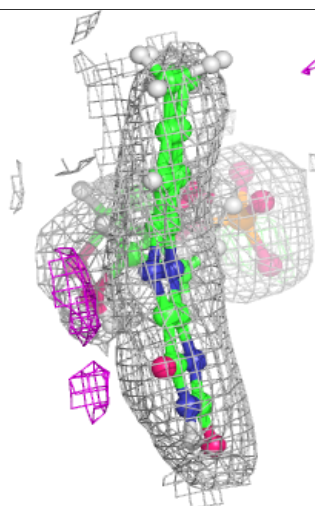
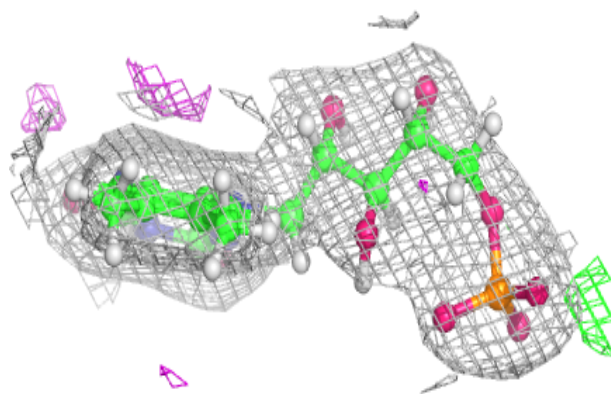
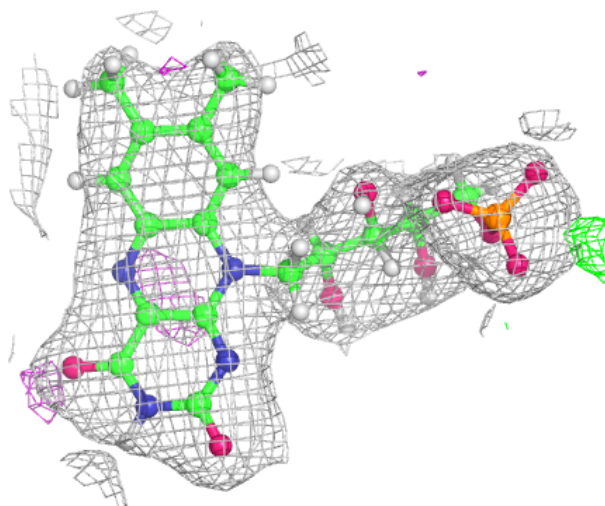
Electron density around FMN C 301:

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



Electron density around FMN A 301:

$2mF_o-DF_c$ (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.