



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2024 – 10:23 PM EDT

PDB ID : 1QXO
Title : Crystal structure of Chorismate synthase complexed with oxidized FMN and EPSP
Authors : Maclean, J.; Ali, S.
Deposited on : 2003-09-08
Resolution : 2.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

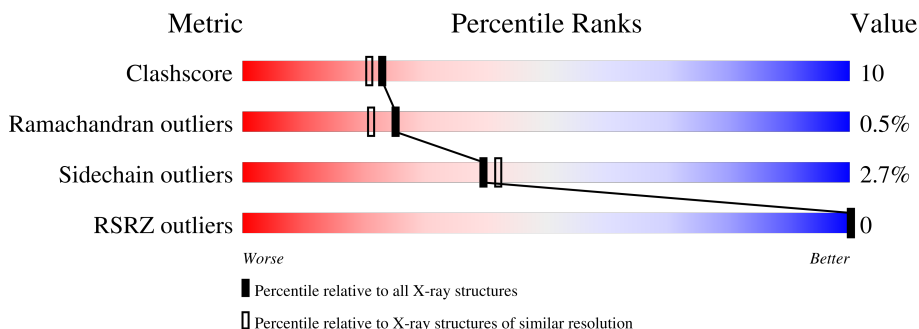
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	388	<div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	B	388	<div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	C	388	<div> <div>78%</div> <div>18%</div> <div>..</div> </div>
1	D	388	<div> <div>73%</div> <div>21%</div> <div>..</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14427 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	Se	0	8	0
			3037	1892	546	587	12			
1	B	388	Total	C	N	O	Se	0	8	0
			3043	1892	549	590	12			
1	C	388	Total	C	N	O	Se	0	8	0
			3035	1893	543	587	12			
1	D	388	Total	C	N	O	Se	0	4	0
			3022	1884	543	583	12			

There are 48 discrepancies between the modelled and reference sequences:

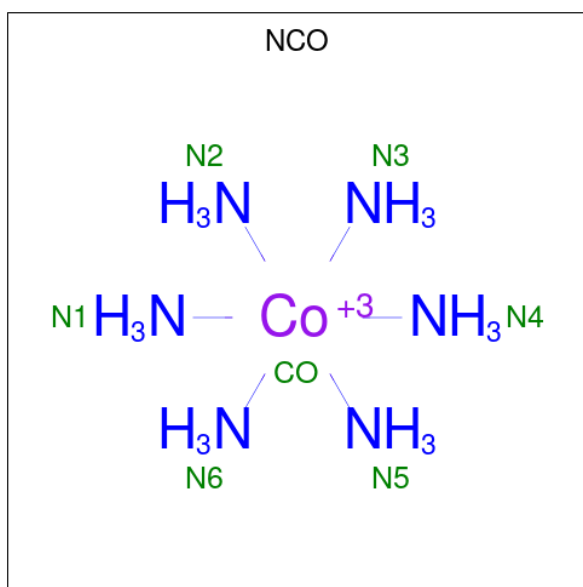
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P0A2Y6
A	49	MSE	MET	modified residue	UNP P0A2Y6
A	74	MSE	MET	modified residue	UNP P0A2Y6
A	88	MSE	MET	modified residue	UNP P0A2Y6
A	138	MSE	MET	modified residue	UNP P0A2Y6
A	155	MSE	MET	modified residue	UNP P0A2Y6
A	273	MSE	MET	modified residue	UNP P0A2Y6
A	298	MSE	MET	modified residue	UNP P0A2Y6
A	310	MSE	MET	modified residue	UNP P0A2Y6
A	321	MSE	MET	modified residue	UNP P0A2Y6
A	348	MSE	MET	modified residue	UNP P0A2Y6
A	350	MSE	MET	modified residue	UNP P0A2Y6
B	1	MSE	MET	modified residue	UNP P0A2Y6
B	49	MSE	MET	modified residue	UNP P0A2Y6
B	74	MSE	MET	modified residue	UNP P0A2Y6
B	88	MSE	MET	modified residue	UNP P0A2Y6
B	138	MSE	MET	modified residue	UNP P0A2Y6
B	155	MSE	MET	modified residue	UNP P0A2Y6
B	273	MSE	MET	modified residue	UNP P0A2Y6
B	298	MSE	MET	modified residue	UNP P0A2Y6
B	310	MSE	MET	modified residue	UNP P0A2Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	321	MSE	MET	modified residue	UNP P0A2Y6
B	348	MSE	MET	modified residue	UNP P0A2Y6
B	350	MSE	MET	modified residue	UNP P0A2Y6
C	1	MSE	MET	modified residue	UNP P0A2Y6
C	49	MSE	MET	modified residue	UNP P0A2Y6
C	74	MSE	MET	modified residue	UNP P0A2Y6
C	88	MSE	MET	modified residue	UNP P0A2Y6
C	138	MSE	MET	modified residue	UNP P0A2Y6
C	155	MSE	MET	modified residue	UNP P0A2Y6
C	273	MSE	MET	modified residue	UNP P0A2Y6
C	298	MSE	MET	modified residue	UNP P0A2Y6
C	310	MSE	MET	modified residue	UNP P0A2Y6
C	321	MSE	MET	modified residue	UNP P0A2Y6
C	348	MSE	MET	modified residue	UNP P0A2Y6
C	350	MSE	MET	modified residue	UNP P0A2Y6
D	1	MSE	MET	modified residue	UNP P0A2Y6
D	49	MSE	MET	modified residue	UNP P0A2Y6
D	74	MSE	MET	modified residue	UNP P0A2Y6
D	88	MSE	MET	modified residue	UNP P0A2Y6
D	138	MSE	MET	modified residue	UNP P0A2Y6
D	155	MSE	MET	modified residue	UNP P0A2Y6
D	273	MSE	MET	modified residue	UNP P0A2Y6
D	298	MSE	MET	modified residue	UNP P0A2Y6
D	310	MSE	MET	modified residue	UNP P0A2Y6
D	321	MSE	MET	modified residue	UNP P0A2Y6
D	348	MSE	MET	modified residue	UNP P0A2Y6
D	350	MSE	MET	modified residue	UNP P0A2Y6

- Molecule 2 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $\text{CoH}_{18}\text{N}_6$).



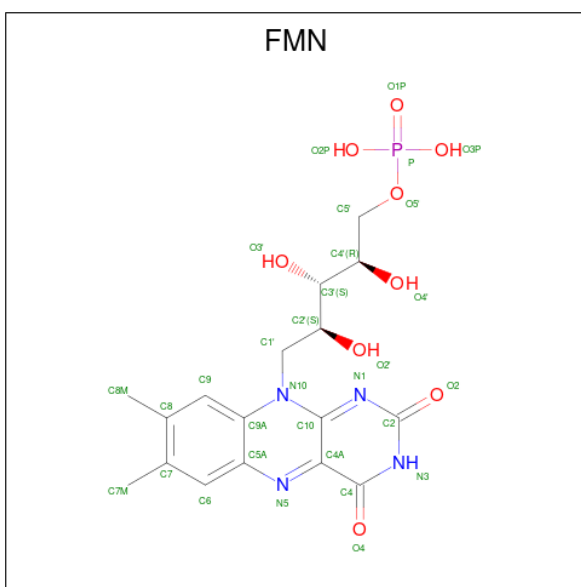
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Co	N	0	0
			7	1	6		
2	A	1	Total	Co	N	0	0
			7	1	6		
2	A	1	Total	Co	N	0	0
			7	1	6		
2	B	1	Total	Co	N	0	0
			7	1	6		
2	B	1	Total	Co	N	0	0
			7	1	6		
2	C	1	Total	Co	N	0	0
			7	1	6		
2	C	1	Total	Co	N	0	0
			7	1	6		
2	D	1	Total	Co	N	0	0
			7	1	6		
2	D	1	Total	Co	N	0	0
			7	1	6		

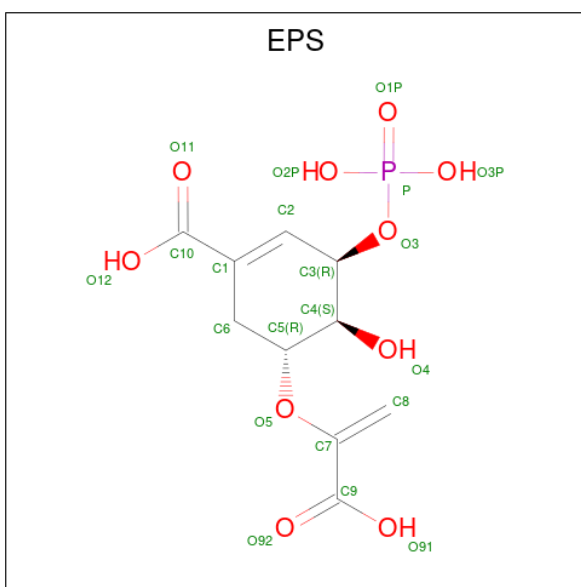
- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	P	
			21	10	10	1	
5	B	1	Total	C	O	P	
			21	10	10	1	
5	C	1	Total	C	O	P	
			21	10	10	1	
5	D	1	Total	C	O	P	
			21	10	10	1	

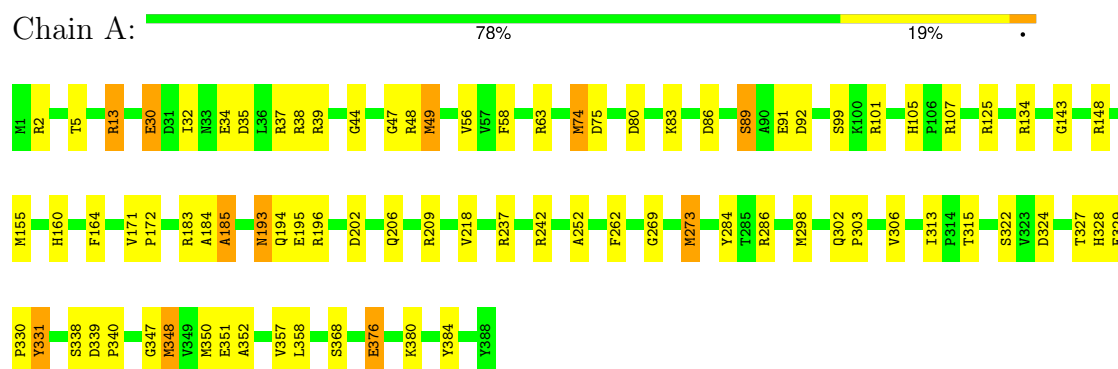
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	453	Total	O		
			453	453	0	0
6	B	528	Total	O		
			528	528	0	0
6	C	469	Total	O		
			469	469	0	0
6	D	479	Total	O		
			479	479	0	0

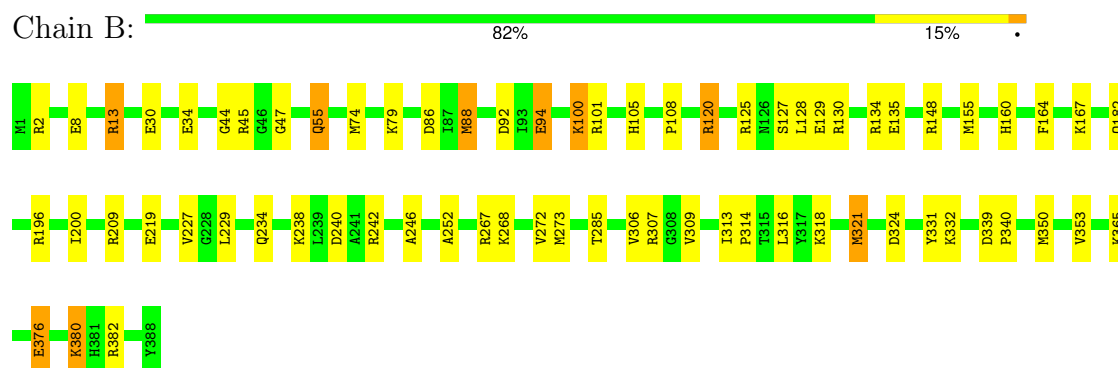
3 Residue-property plots

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: Chorismate synthase



• Molecule 1: Chorismate synthase

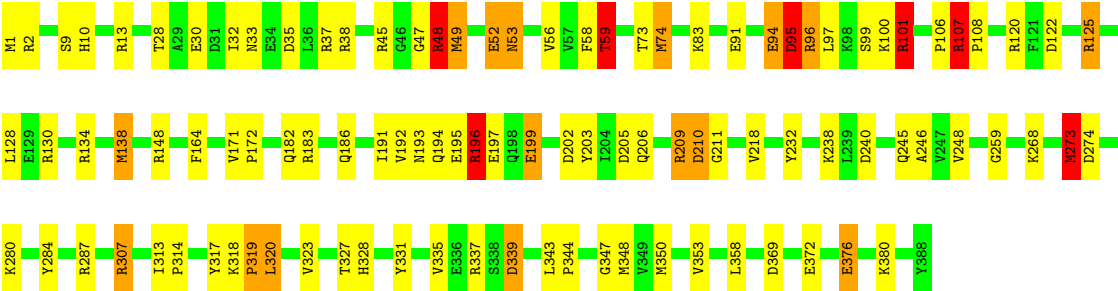


• Molecule 1: Chorismate synthase





● Molecule 1: Chorismate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.06Å 124.58Å 85.16Å 90.00° 115.15° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.00) 97.4 (25.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.30 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.157 , 0.222 0.145 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	7.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14427	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, NCO, EDO, EPS

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	0.75	5/3115 (0.2%)	1.43	38/4185 (0.9%)
1	B	0.79	4/3119 (0.1%)	1.37	26/4188 (0.6%)
1	C	0.78	8/3111 (0.3%)	1.49	38/4180 (0.9%)
1	D	0.78	4/3078 (0.1%)	1.62	53/4134 (1.3%)
All	All	0.78	21/12423 (0.2%)	1.48	155/16687 (0.9%)

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	D	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	MSE	CG-SE	13.31	2.40	1.95
1	D	273	MSE	CG-SE	13.14	2.40	1.95
1	C	273	MSE	CG-SE	12.20	2.37	1.95
1	D	49	MSE	CG-SE	9.80	2.28	1.95
1	B	88	MSE	CG-SE	9.58	2.28	1.95

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	48	ARG	NE-CZ-NH2	-20.75	109.92	120.30
1	D	196	ARG	NE-CZ-NH2	-17.53	111.53	120.30
1	D	196	ARG	NE-CZ-NH1	14.18	127.39	120.30
1	D	2	ARG	NE-CZ-NH1	-13.76	113.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	130	ARG	NE-CZ-NH2	-13.60	113.50	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	10	HIS	Mainchain
1	D	248	VAL	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3037	0	3050	49	0
1	B	3043	0	3053	48	0
1	C	3035	0	3054	71	0
1	D	3022	0	3038	86	0
2	A	21	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	1	0
3	A	12	0	18	4	0
3	B	4	0	6	1	0
3	C	4	0	6	2	0
3	D	8	0	12	2	0
4	A	31	0	19	5	0
4	B	31	0	19	4	0
4	C	62	0	38	7	0
4	D	62	0	38	6	0
5	A	21	0	8	0	0
5	B	21	0	8	1	0
5	C	21	0	8	0	0
5	D	21	0	8	0	0
6	A	453	0	0	7	0
6	B	528	0	0	12	0
6	C	469	0	0	16	0
6	D	479	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14427	0	12383	255	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 255 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:348:MSE:SE	1:D:348:MSE:CE	2.14	1.45
1:C:138:MSE:CG	1:C:138:MSE:SE	2.15	1.45
1:D:273:MSE:SE	1:D:273:MSE:CE	2.14	1.45
1:D:138:MSE:SE	1:D:138:MSE:CG	2.16	1.42
1:B:88:MSE:SE	1:B:88:MSE:CE	2.16	1.42

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/388 (102%)	386 (98%)	7 (2%)	1 (0%)	37	35
1	B	394/388 (102%)	387 (98%)	6 (2%)	1 (0%)	37	35
1	C	394/388 (102%)	383 (97%)	10 (2%)	1 (0%)	37	35
1	D	390/388 (100%)	375 (96%)	10 (3%)	5 (1%)	10	5
All	All	1572/1552 (101%)	1531 (97%)	33 (2%)	8 (0%)	25	21

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	GLY
1	D	319	PRO

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Mol	Chain	Res	Type
1	D	47	GLY
1	D	320	LEU
1	C	210	ASP

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	327/308 (106%)	321 (98%)	6 (2%)	54	59
1	B	327/308 (106%)	321 (98%)	6 (2%)	54	59
1	C	327/308 (106%)	321 (98%)	6 (2%)	54	59
1	D	323/308 (105%)	307 (95%)	16 (5%)	20	18
All	All	1304/1232 (106%)	1270 (97%)	34 (3%)	40	44

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	164	PHE
1	D	196	ARG
1	D	280	LYS
1	C	59	THR
1	B	164	PHE

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	C	33	ASN
1	D	194	GLN
1	C	182	GLN
1	D	302	GLN
1	D	55	GLN

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 ⓘ

26 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$
3	EDO	C	3003	-	3,3,3	0.44	0	2,2,2	0.60	0
4	FMN	C	4005	-	33,33,33	1.20	5 (15%)	48,50,50	1.55	10 (20%)
2	NCO	A	2004	-	6,6,6	0.51	0	-		
5	EPS	C	5003	-	20,21,21	4.34	14 (70%)	26,31,31	4.37	17 (65%)
3	EDO	A	3005	-	3,3,3	0.65	0	2,2,2	0.52	0
2	NCO	D	2006	-	6,6,6	0.54	0	-		
3	EDO	D	3007	-	3,3,3	0.51	0	2,2,2	0.61	0
4	FMN	B	4002	-	33,33,33	1.36	4 (12%)	48,50,50	1.76	13 (27%)
5	EPS	B	5002	-	20,21,21	4.31	15 (75%)	26,31,31	5.00	18 (69%)
2	NCO	A	2007	-	6,6,6	0.57	0	-		
2	NCO	B	2003	-	6,6,6	0.69	0	-		
5	EPS	A	5001	-	20,21,21	4.34	14 (70%)	26,31,31	4.12	15 (57%)
2	NCO	C	2005	-	6,6,6	0.63	0	-		
4	FMN	C	4003	-	33,33,33	1.43	4 (12%)	48,50,50	1.72	11 (22%)
5	EPS	D	5004	-	20,21,21	4.22	14 (70%)	26,31,31	4.45	17 (65%)
4	FMN	D	4006	-	33,33,33	1.30	4 (12%)	48,50,50	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMN	D	4004	-	33,33,33	1.24	2 (6%)	48,50,50	1.70	15 (31%)
4	FMN	A	4001	-	33,33,33	1.45	5 (15%)	48,50,50	1.48	8 (16%)
2	NCO	D	2009	-	6,6,6	0.65	0	-		
3	EDO	B	3002	-	3,3,3	0.52	0	2,2,2	0.70	0
2	NCO	B	2008	-	6,6,6	0.52	0	-		
3	EDO	A	3006	-	3,3,3	0.76	0	2,2,2	1.16	0
2	NCO	A	2002	-	6,6,6	0.55	0	-		
3	EDO	D	3004	-	3,3,3	0.51	0	2,2,2	0.11	0
3	EDO	A	3001	-	3,3,3	0.49	0	2,2,2	0.47	0
2	NCO	C	2001	-	6,6,6	0.75	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	FMN	C	4003	-	-	0/18/18/18	0/3/3/3
5	EPS	D	5004	-	-	0/15/33/33	0/1/1/1
4	FMN	D	4006	-	-	1/18/18/18	0/3/3/3
3	EDO	D	3004	-	-	0/1/1/1	-
3	EDO	D	3007	-	-	1/1/1/1	-
4	FMN	D	4004	-	-	1/18/18/18	0/3/3/3
4	FMN	A	4001	-	-	1/18/18/18	0/3/3/3
4	FMN	B	4002	-	-	1/18/18/18	0/3/3/3
3	EDO	B	3002	-	-	1/1/1/1	-
5	EPS	B	5002	-	-	0/15/33/33	0/1/1/1
5	EPS	C	5003	-	-	0/15/33/33	0/1/1/1
3	EDO	A	3001	-	-	0/1/1/1	-
3	EDO	C	3003	-	-	1/1/1/1	-
4	FMN	C	4005	-	-	11/18/18/18	0/3/3/3
5	EPS	A	5001	-	-	0/15/33/33	0/1/1/1
3	EDO	A	3005	-	-	1/1/1/1	-
3	EDO	A	3006	-	-	1/1/1/1	-

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5003	EPS	C7-C9	-10.49	1.39	1.49
5	A	5001	EPS	C7-C9	-10.40	1.39	1.49
5	B	5002	EPS	C7-C9	-10.07	1.39	1.49
5	D	5004	EPS	C7-C9	-9.81	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5002	EPS	O11-C10	6.18	1.37	1.22

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5002	EPS	C2-C1-C10	13.19	138.02	119.99
5	B	5002	EPS	O12-C10-O11	-10.83	98.13	123.90
5	D	5004	EPS	O12-C10-O11	-10.62	98.61	123.90
5	D	5004	EPS	C2-C1-C10	10.20	133.93	119.99
5	B	5002	EPS	O12-C10-C1	10.00	136.55	115.43

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	4005	FMN	C1'-C2'-C3'-O3'
4	C	4005	FMN	C1'-C2'-C3'-C4'
4	C	4005	FMN	O2'-C2'-C3'-O3'
4	C	4005	FMN	O2'-C2'-C3'-C4'
4	C	4005	FMN	C2'-C3'-C4'-O4'

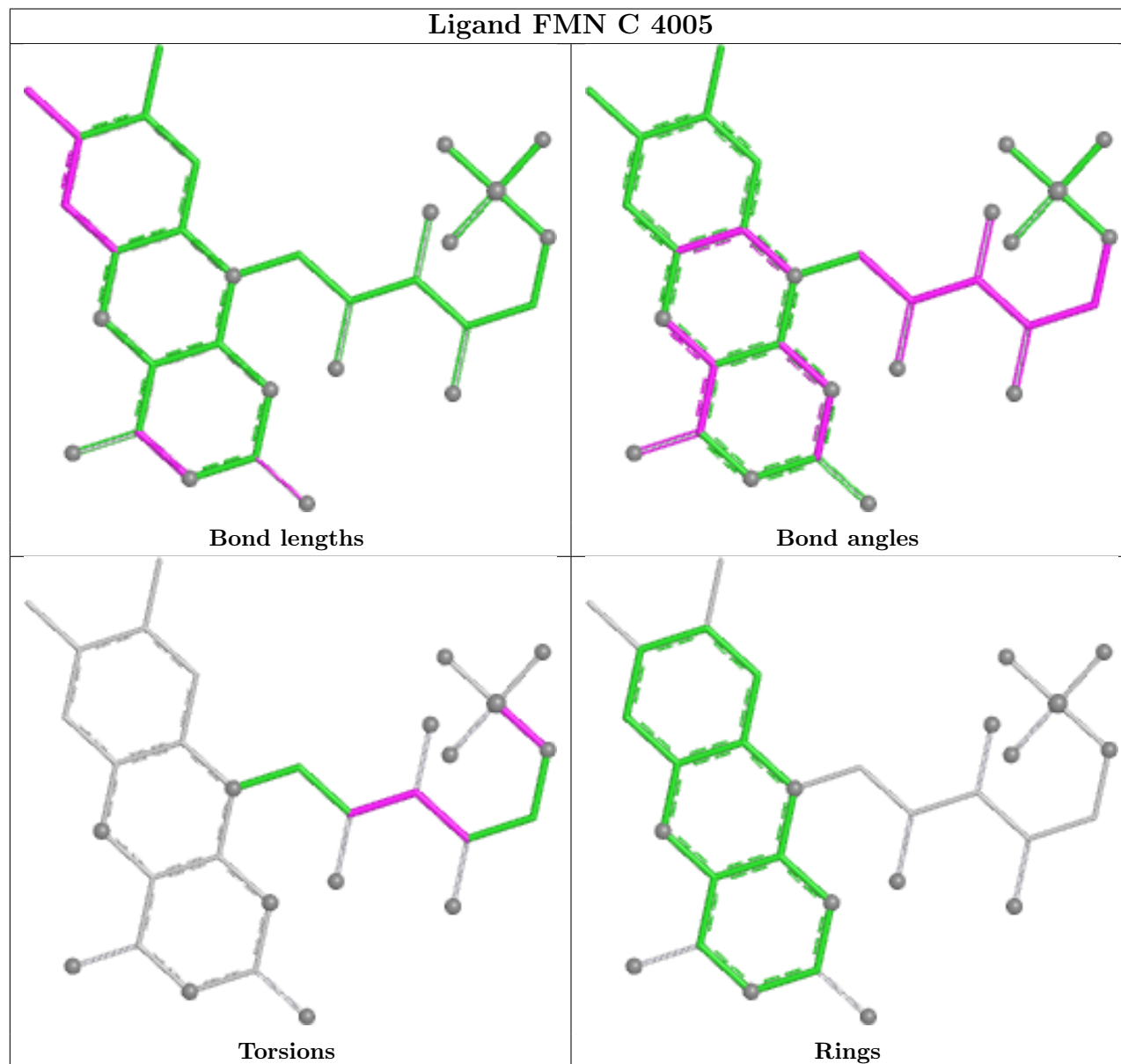
There are no ring outliers.

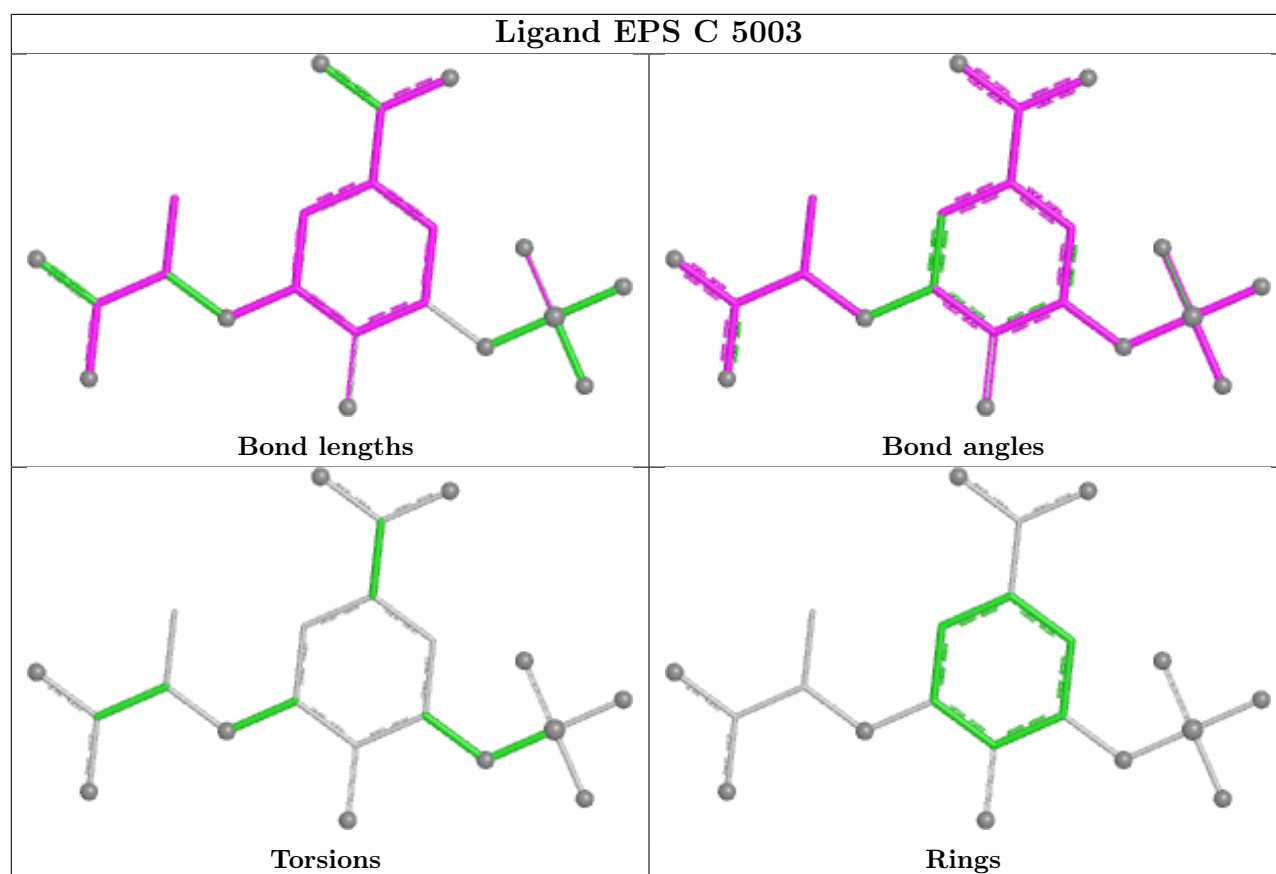
13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3003	EDO	2	0
4	C	4005	FMN	4	0
2	D	2006	NCO	1	0
4	B	4002	FMN	4	0
5	B	5002	EPS	1	0
4	C	4003	FMN	3	0
4	D	4006	FMN	4	0
4	D	4004	FMN	2	0
4	A	4001	FMN	5	0
3	B	3002	EDO	1	0
3	A	3006	EDO	2	0
3	D	3004	EDO	2	0
3	A	3001	EDO	2	0

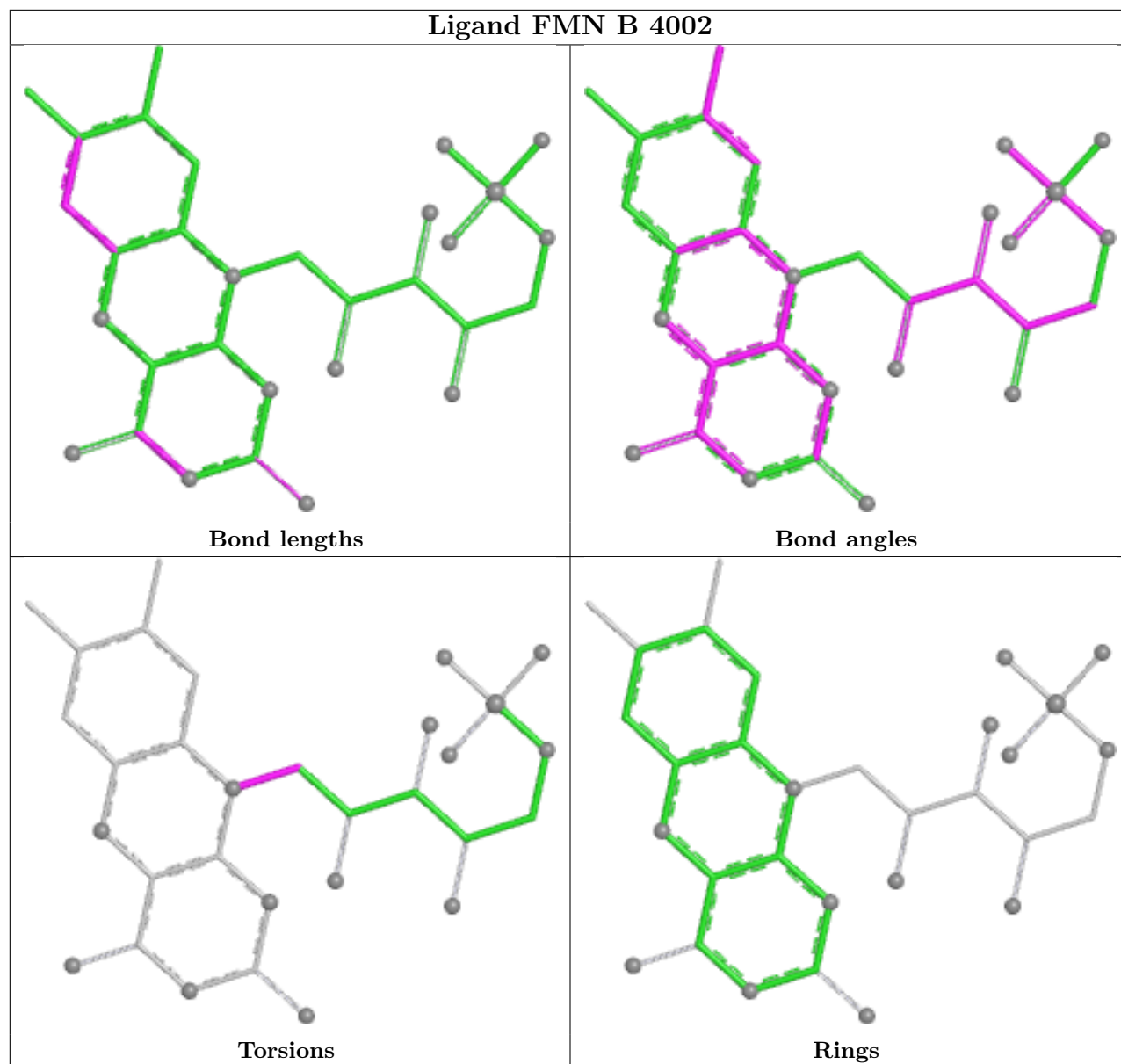
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

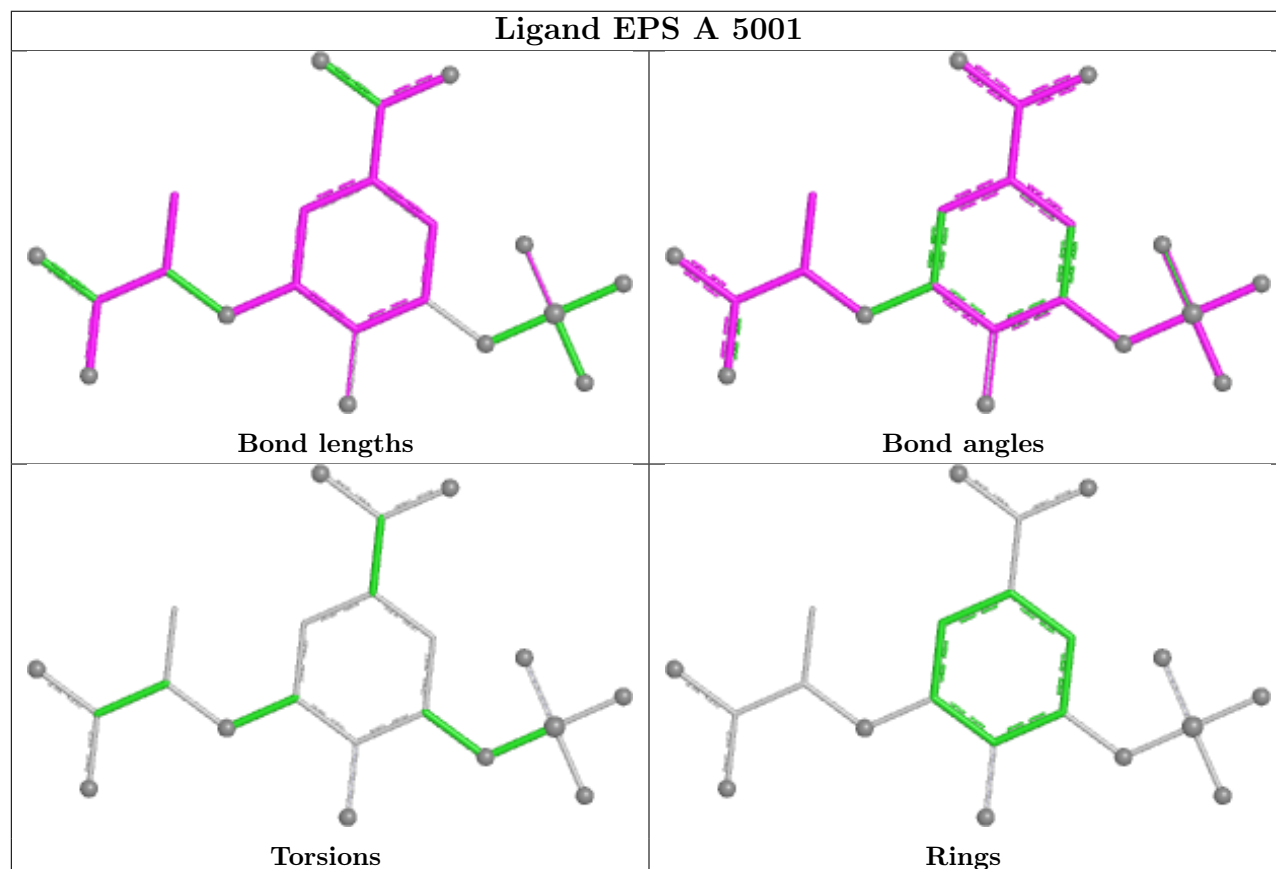
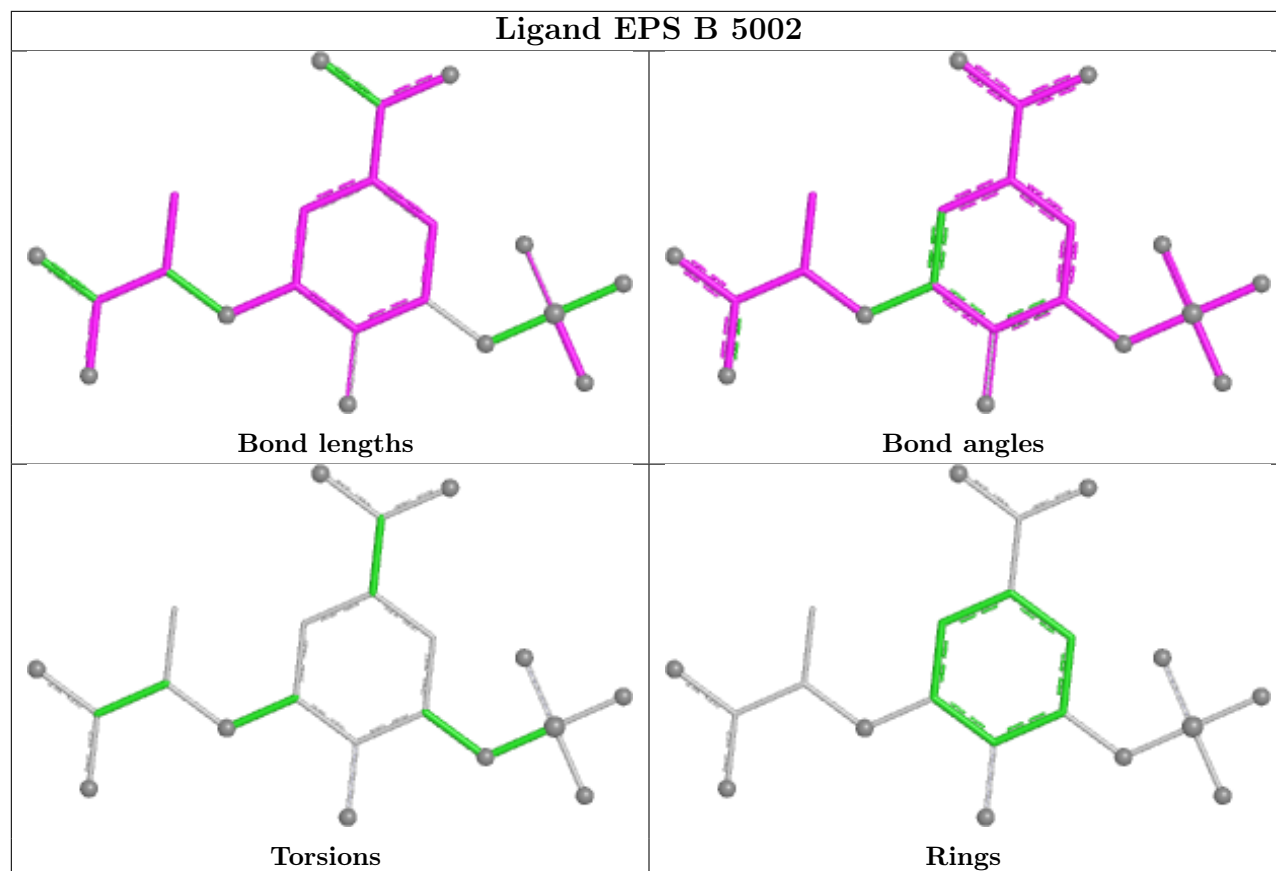
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

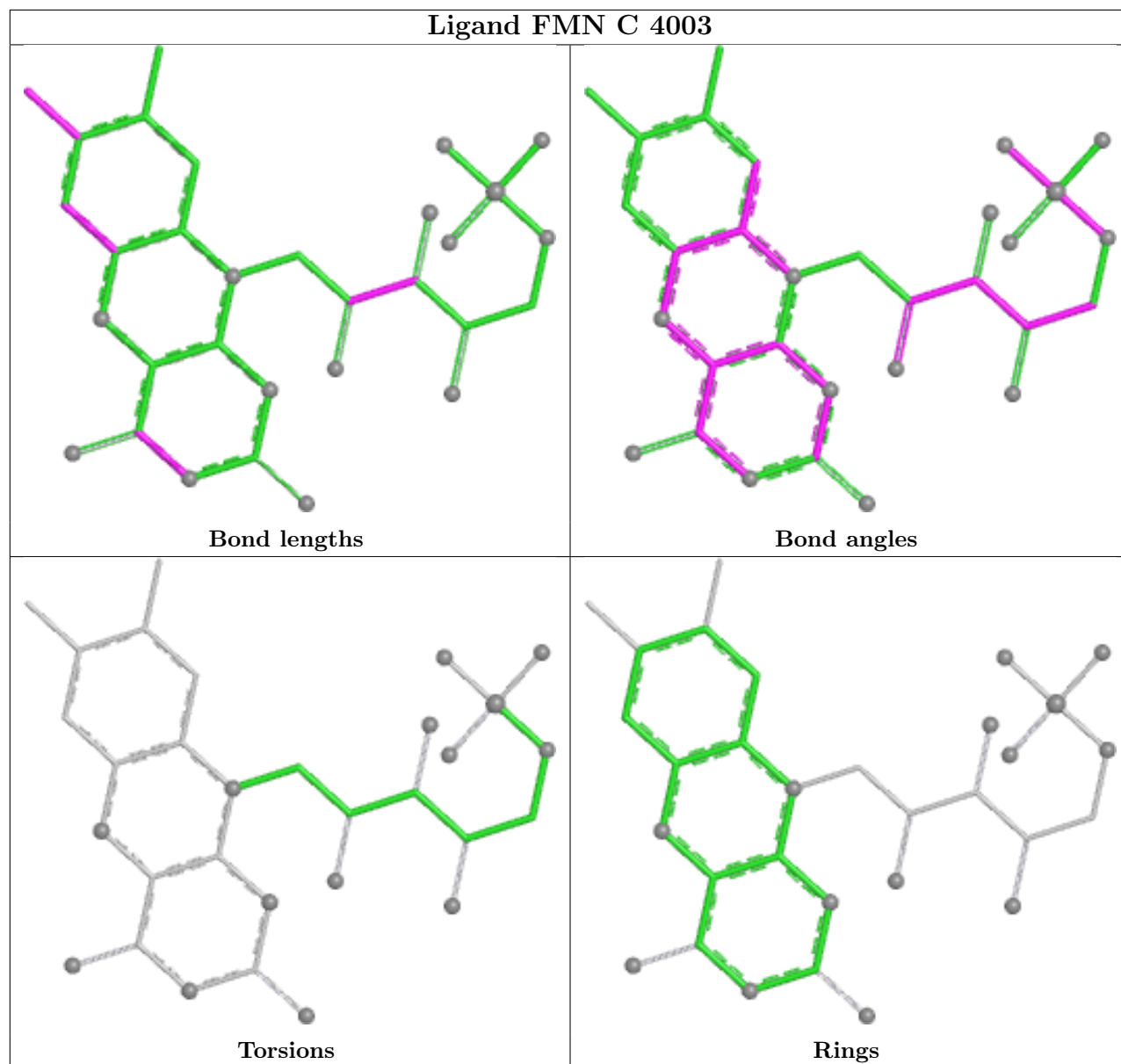


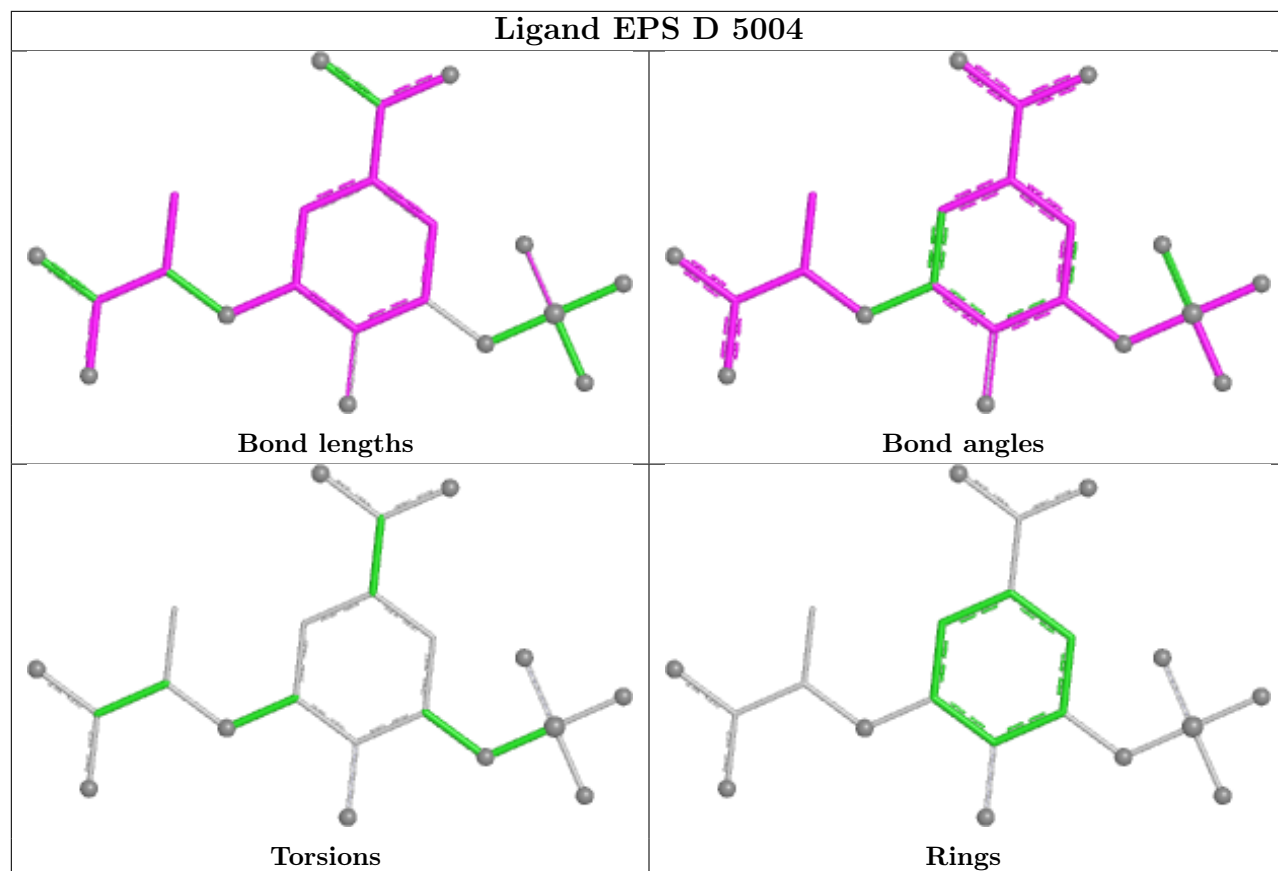


Ligand FMN B 4002

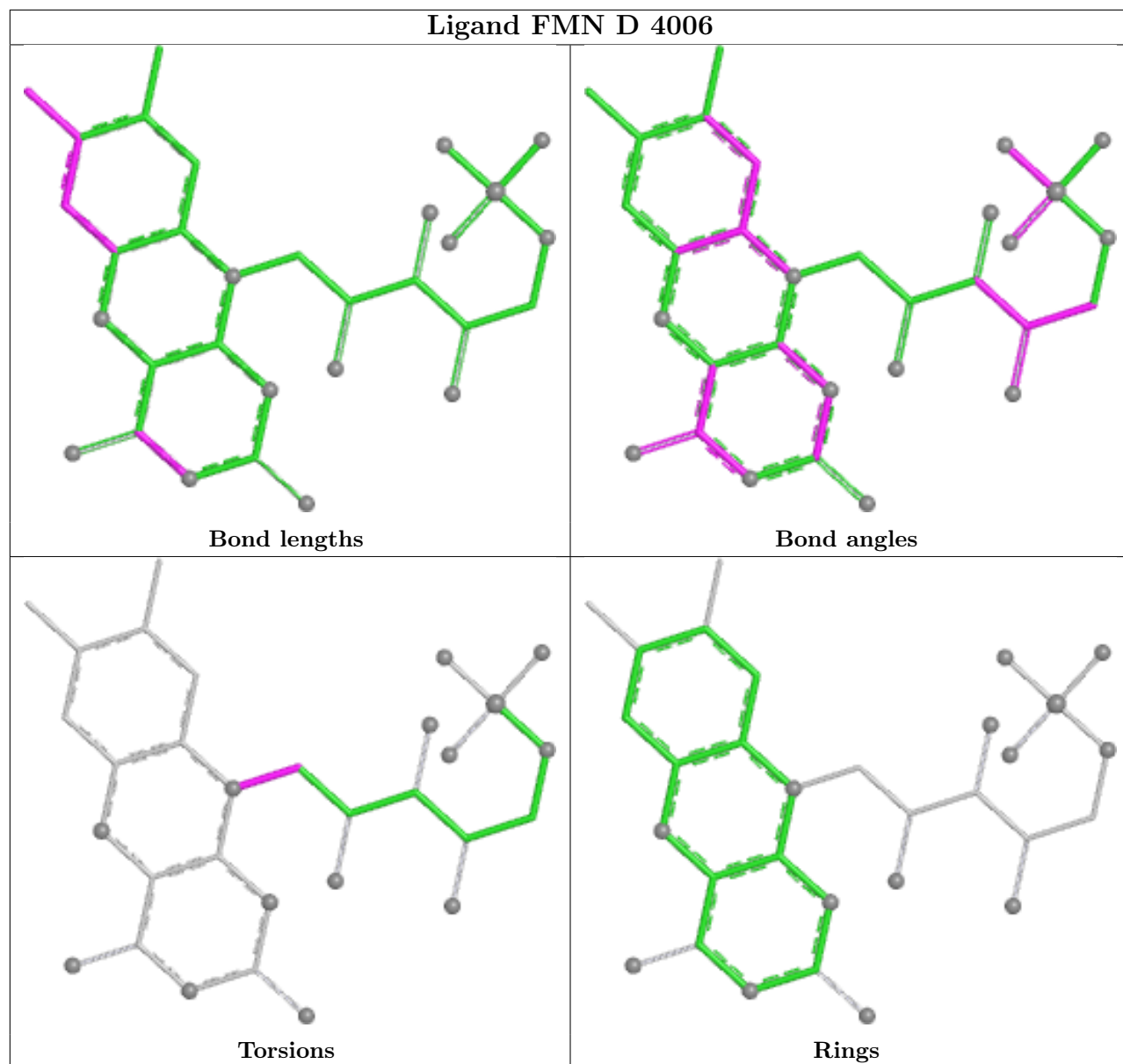


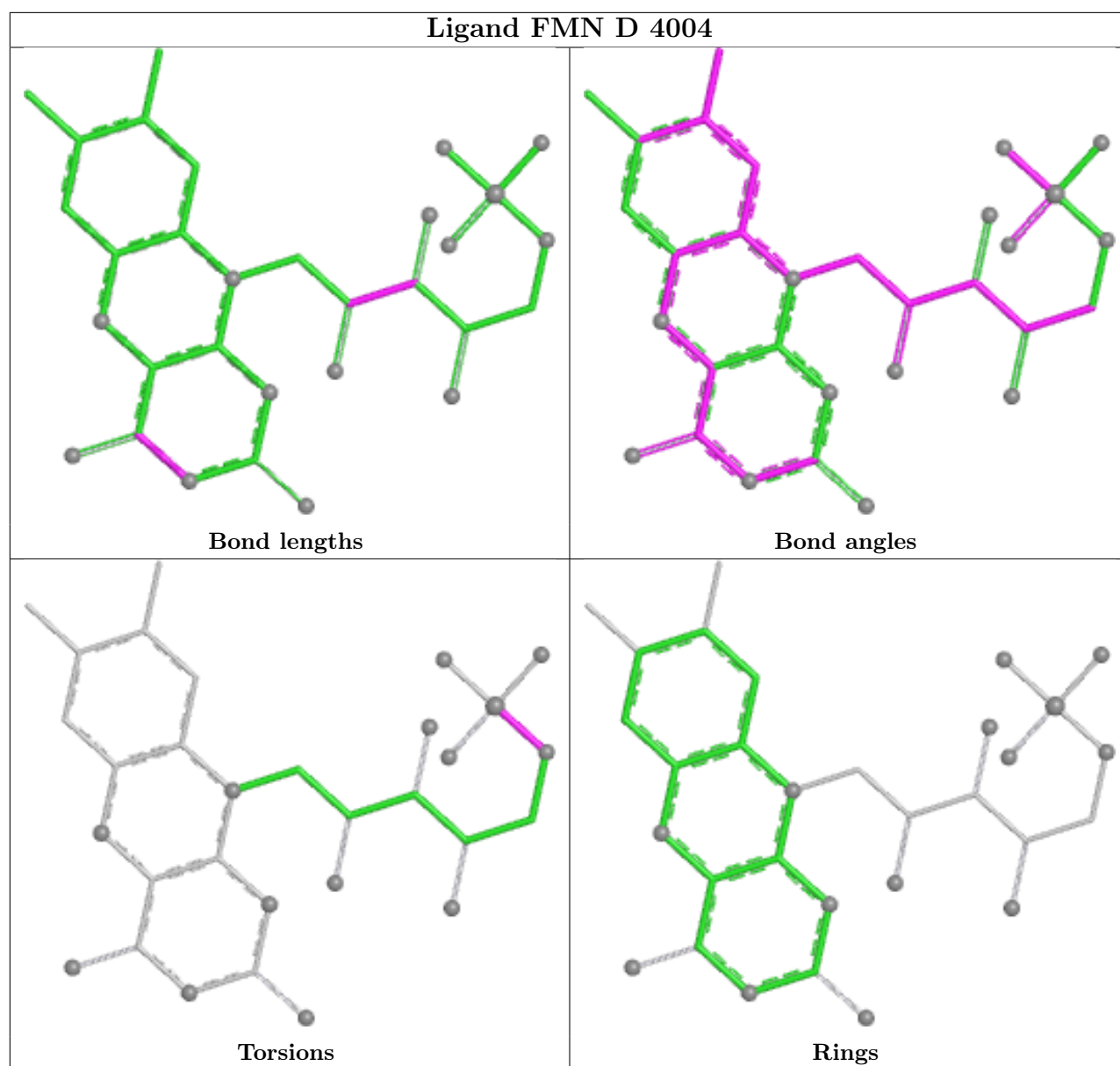


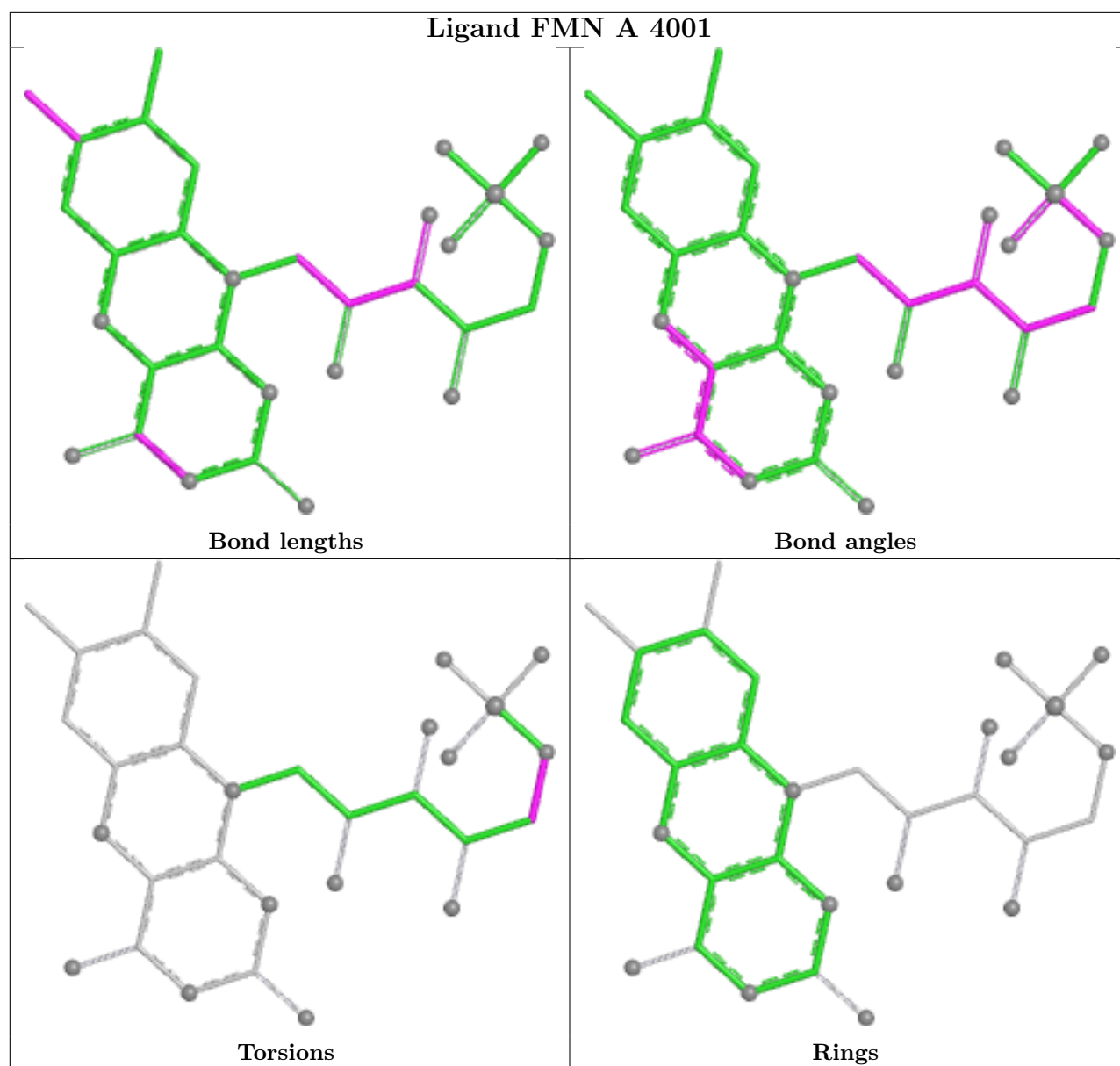




Ligand FMN D 4006







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	376/388 (96%)	-1.49	0 100 100	12, 22, 46, 65	8 (2%)
1	B	376/388 (96%)	-1.53	0 100 100	12, 22, 36, 59	8 (2%)
1	C	376/388 (96%)	-1.46	0 100 100	15, 23, 50, 79	8 (2%)
1	D	376/388 (96%)	-1.45	0 100 100	14, 23, 53, 83	4 (1%)
All	All	1504/1552 (96%)	-1.48	0 100 100	12, 22, 46, 83	28 (1%)

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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NCO	A	2002	7/7	0.97	0.06	86,86,86,86	0
2	NCO	B	2008	7/7	0.97	0.06	73,73,74,74	0
2	NCO	A	2007	7/7	0.98	0.06	80,80,80,80	0
3	EDO	A	3001	4/4	0.98	0.05	25,29,30,34	0

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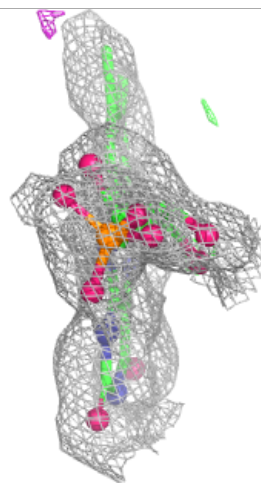
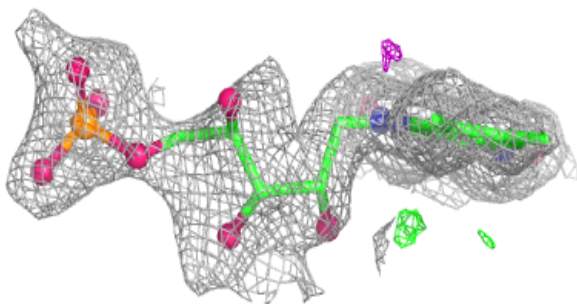
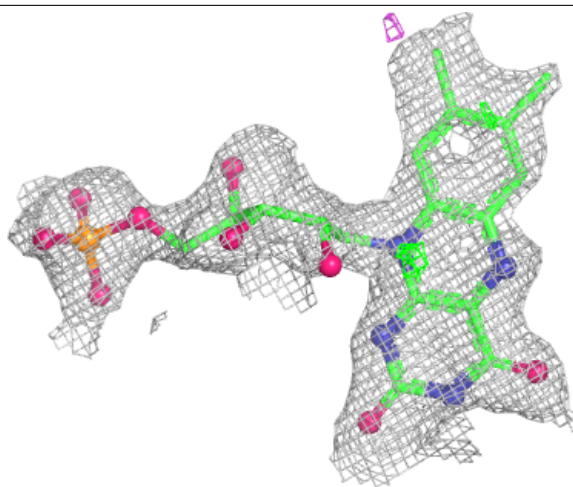
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	3005	4/4	0.98	0.04	31,31,33,35	0
3	EDO	D	3007	4/4	0.98	0.04	28,29,30,33	0
4	FMN	C	4005	31/31	0.98	0.05	46,53,62,63	0
4	FMN	D	4006	31/31	0.98	0.04	46,50,51,51	0
2	NCO	C	2005	7/7	0.99	0.04	52,53,53,53	0
3	EDO	A	3006	4/4	0.99	0.07	38,38,39,39	0
3	EDO	B	3002	4/4	0.99	0.05	23,27,29,29	0
3	EDO	C	3003	4/4	0.99	0.04	26,32,32,33	0
3	EDO	D	3004	4/4	0.99	0.03	20,26,28,28	0
2	NCO	D	2006	7/7	0.99	0.05	47,47,47,48	0
4	FMN	A	4001	31/31	0.99	0.03	17,20,23,24	0
4	FMN	B	4002	31/31	0.99	0.03	17,20,22,23	0
4	FMN	C	4003	31/31	0.99	0.03	18,22,25,28	0
2	NCO	D	2009	7/7	0.99	0.04	25,26,28,29	0
4	FMN	D	4004	31/31	0.99	0.03	16,20,24,26	0
2	NCO	B	2003	7/7	0.99	0.04	40,41,41,42	0
5	EPS	A	5001	21/21	0.99	0.03	19,26,41,42	0
5	EPS	B	5002	21/21	0.99	0.03	21,27,37,39	0
5	EPS	C	5003	21/21	0.99	0.03	23,29,42,43	0
5	EPS	D	5004	21/21	0.99	0.03	22,33,43,44	0
2	NCO	A	2004	7/7	1.00	0.04	39,40,41,42	0
2	NCO	C	2001	7/7	1.00	0.04	34,34,35,36	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.

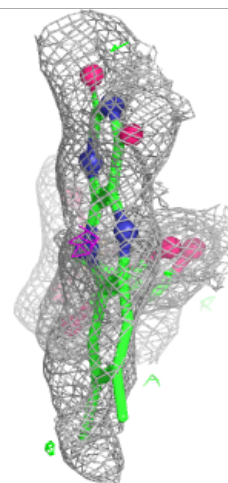
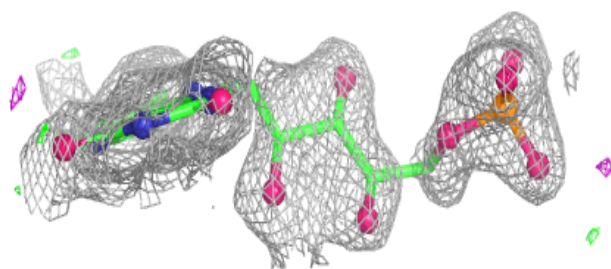
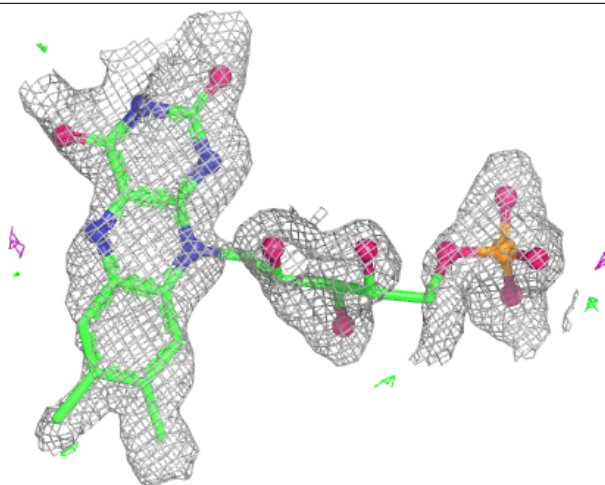
Electron density around FMN C 4005:

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



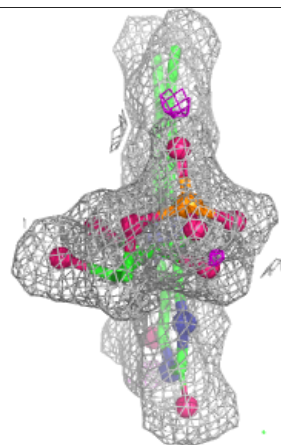
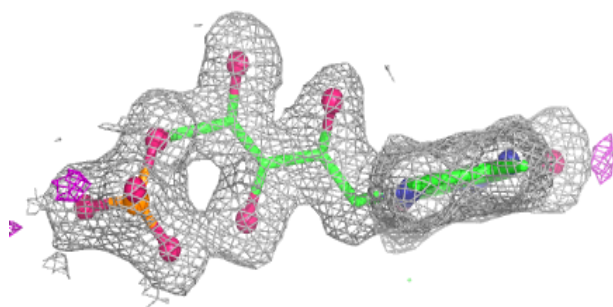
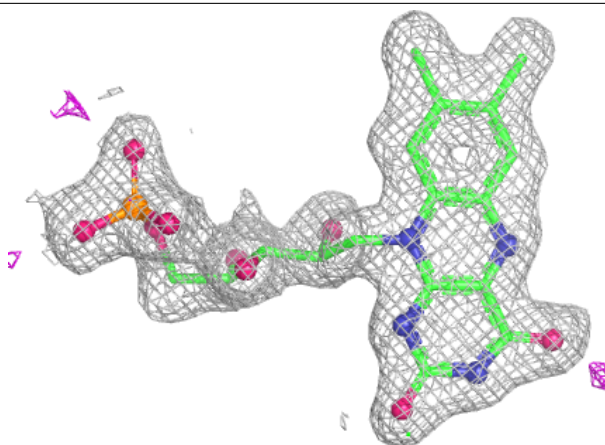
Electron density around FMN D 4006:

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



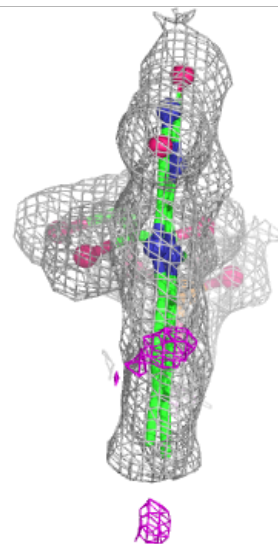
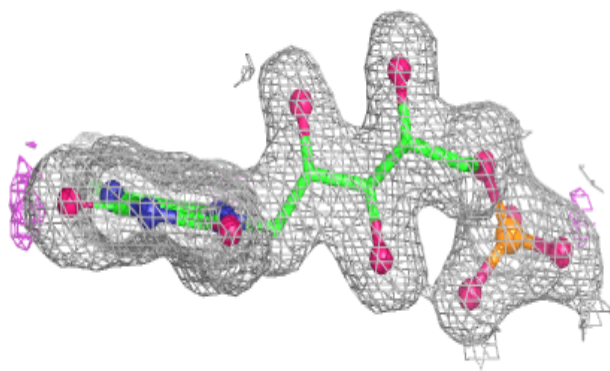
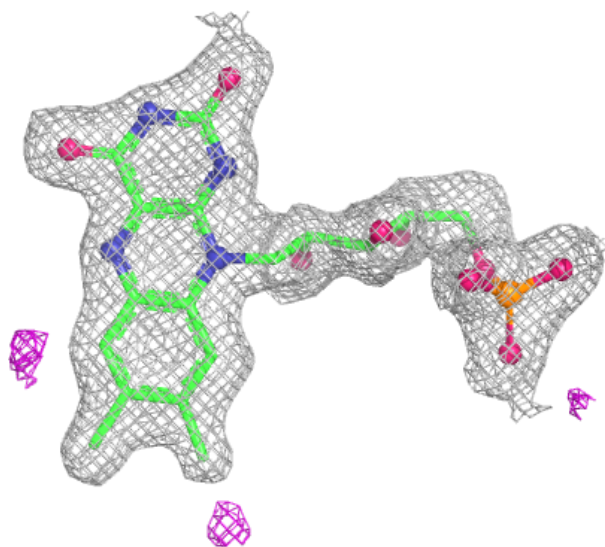
Electron density around FMN A 4001:

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



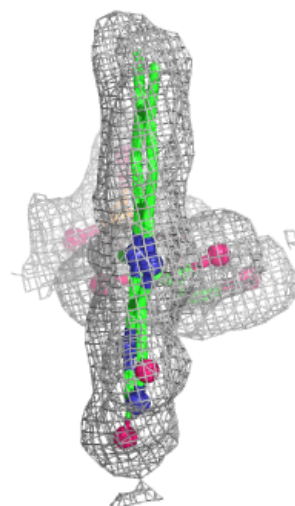
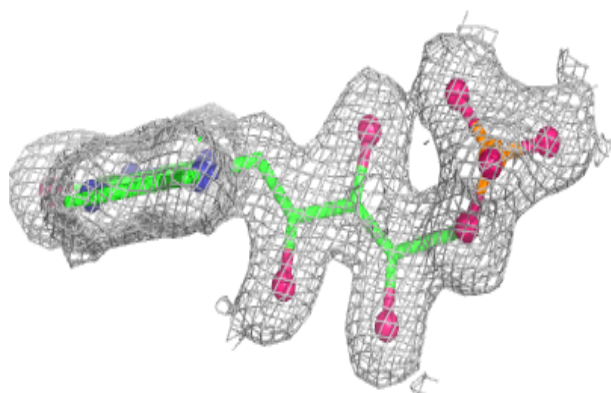
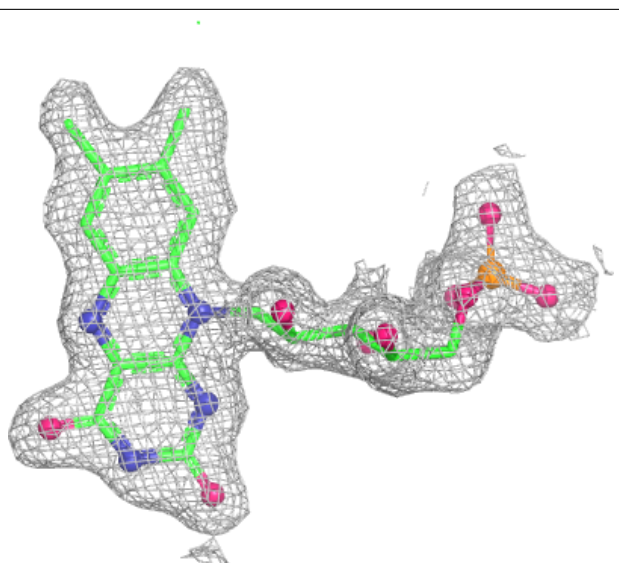
Electron density around FMN B 4002:

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



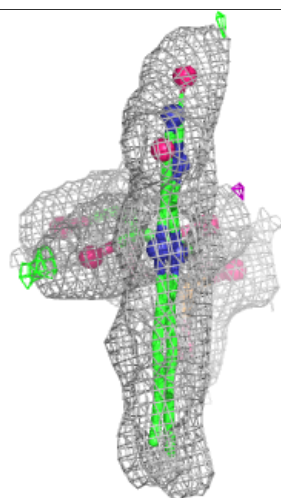
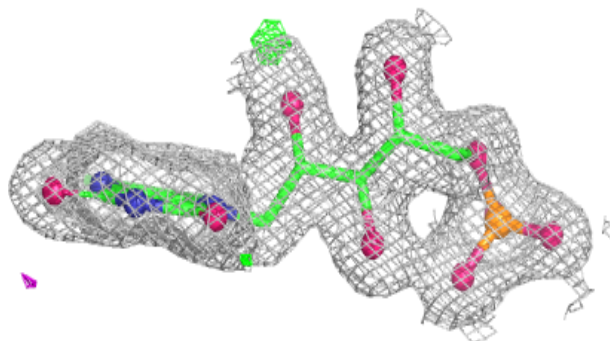
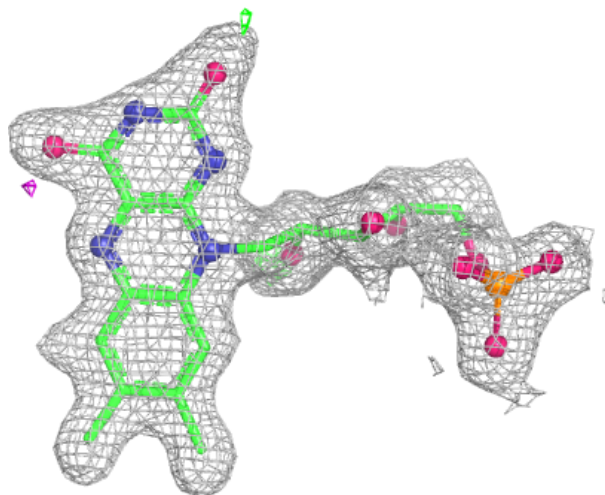
Electron density around FMN C 4003:

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



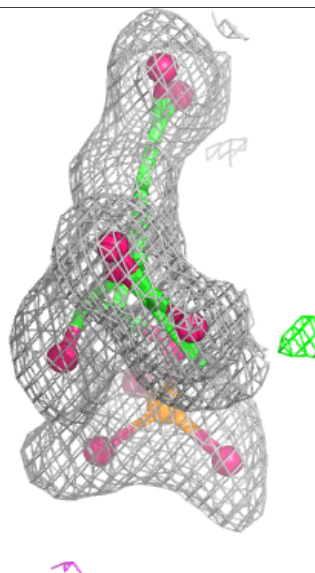
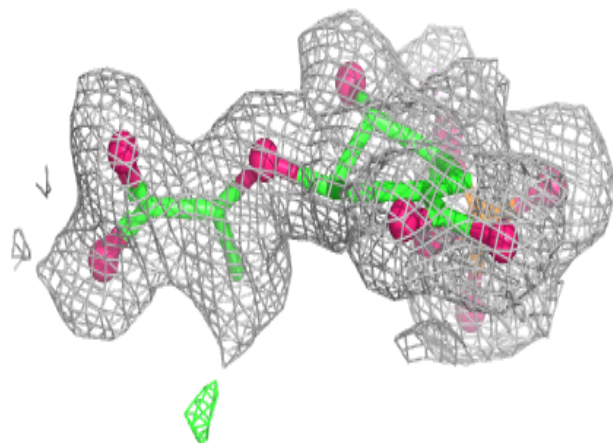
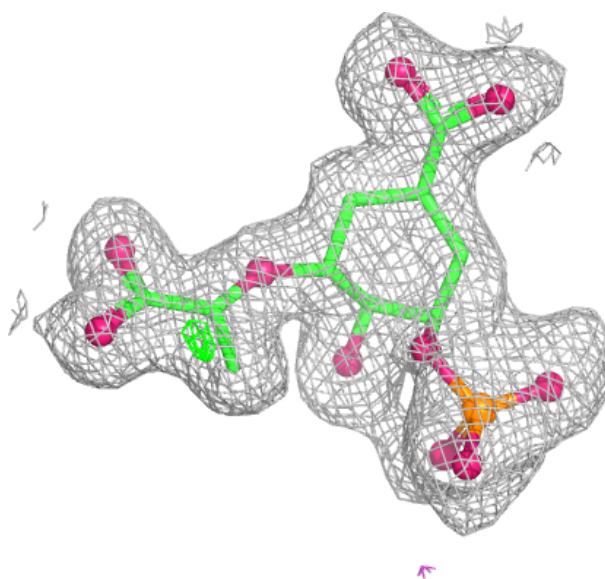
Electron density around FMN D 4004:

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



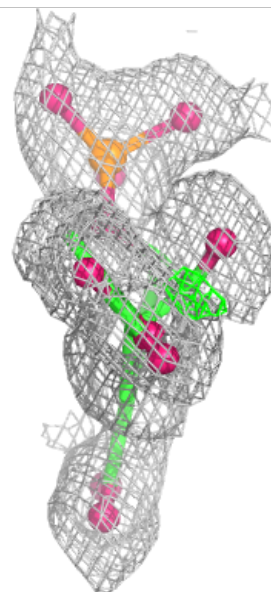
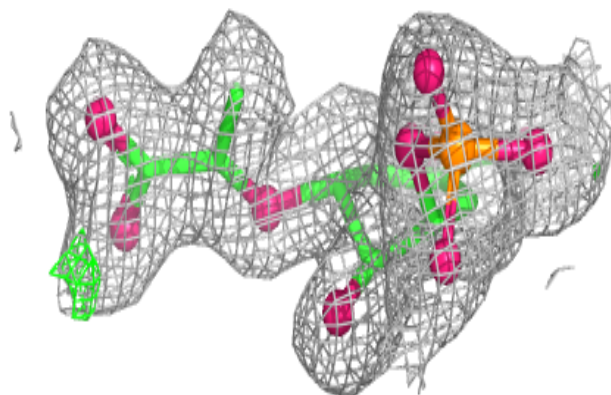
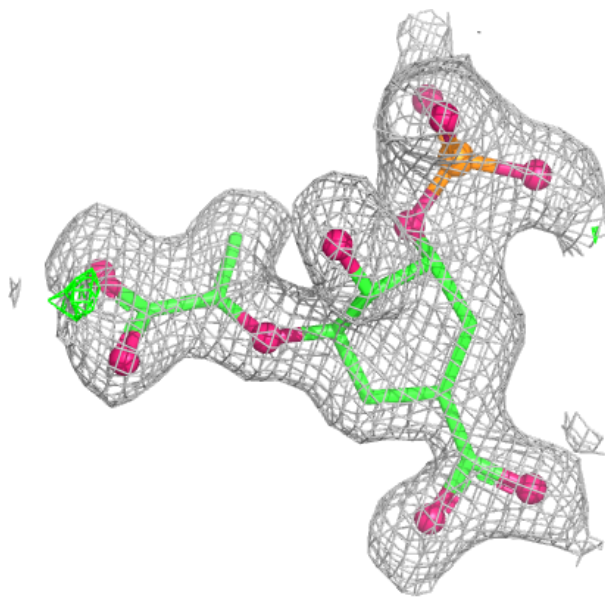
Electron density around EPS A 5001:

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



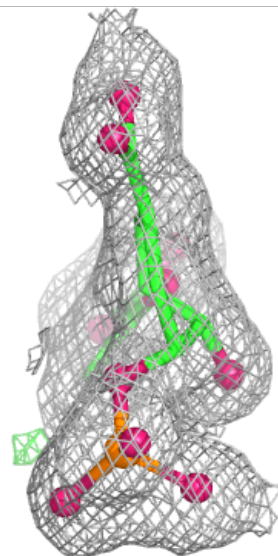
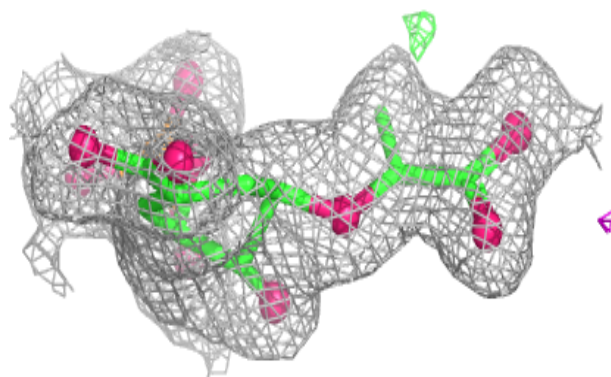
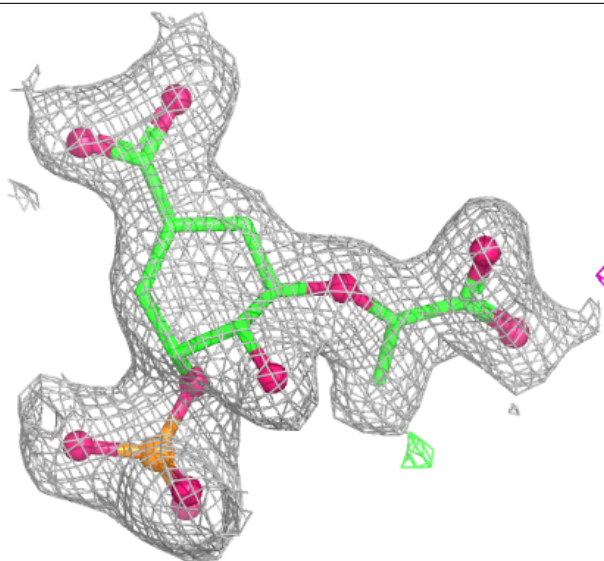
Electron density around EPS B 5002:

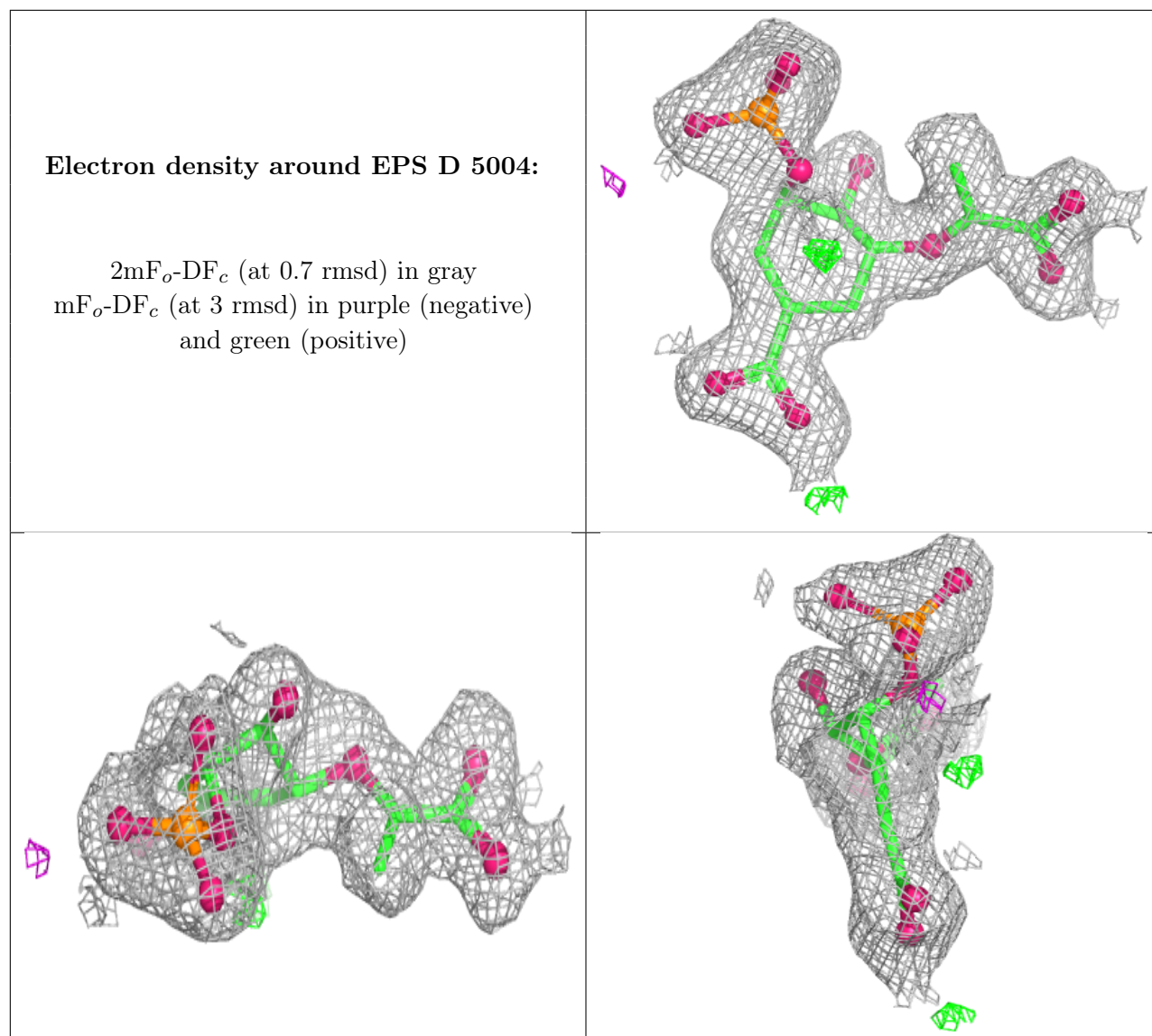
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around EPS C 5003:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.