



Full wwPDB X-ray Structure Validation Report

May 14, 2020 – 02:21 am BST

PDB ID : 5HEI
Title : Structure of B. megaterium NfrA2
Authors : Vigouroux, A.; Morera, S.
Deposited on : 2016-01-06
Resolution : 2.84 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 following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

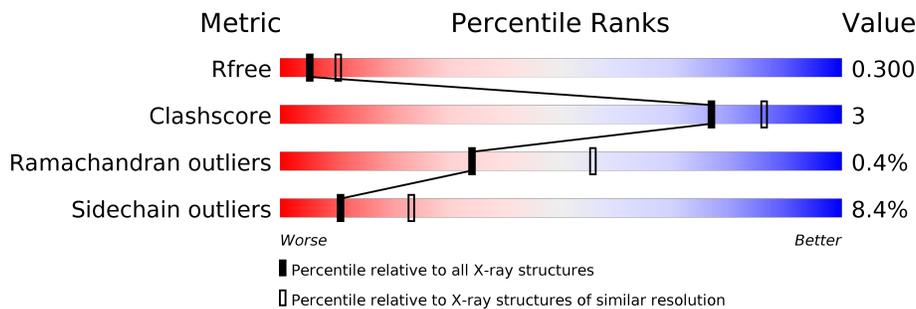
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)

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 on 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	253	
1	B	253	
1	C	253	
1	D	253	
1	E	253	
1	F	253	
1	G	253	

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Mol	Chain	Length	Quality of chain
1	H	253	 80% 15% ••

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15833 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 NfrA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	246	Total 1913	C 1202	N 332	O 374	S 5	0	0	0
1	B	246	Total 1913	C 1202	N 332	O 374	S 5	0	0	0
1	C	245	Total 1905	C 1197	N 331	O 373	S 4	0	0	0
1	D	246	Total 1913	C 1202	N 332	O 374	S 5	0	0	0
1	E	246	Total 1913	C 1202	N 332	O 374	S 5	0	0	0
1	F	246	Total 1913	C 1202	N 332	O 374	S 5	0	0	0
1	G	246	Total 1913	C 1202	N 332	O 374	S 5	0	0	0
1	H	246	Total 1913	C 1202	N 332	O 374	S 5	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	LYS	-	expression tag	UNP A0A0K0VJM8
A	247	GLY	-	expression tag	UNP A0A0K0VJM8
A	248	HIS	-	expression tag	UNP A0A0K0VJM8
A	249	HIS	-	expression tag	UNP A0A0K0VJM8
A	250	HIS	-	expression tag	UNP A0A0K0VJM8
A	251	HIS	-	expression tag	UNP A0A0K0VJM8
A	252	HIS	-	expression tag	UNP A0A0K0VJM8
A	253	HIS	-	expression tag	UNP A0A0K0VJM8
B	246	LYS	-	expression tag	UNP A0A0K0VJM8
B	247	GLY	-	expression tag	UNP A0A0K0VJM8
B	248	HIS	-	expression tag	UNP A0A0K0VJM8
B	249	HIS	-	expression tag	UNP A0A0K0VJM8
B	250	HIS	-	expression tag	UNP A0A0K0VJM8

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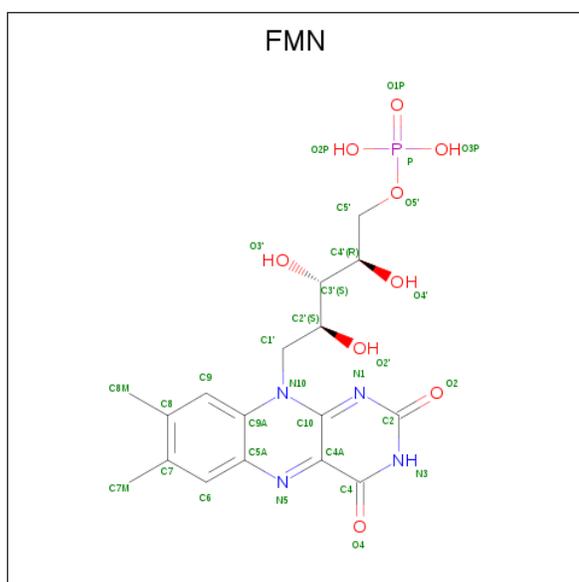
Chain	Residue	Modelled	Actual	Comment	Reference
B	251	HIS	-	expression tag	UNP A0A0K0VJM8
B	252	HIS	-	expression tag	UNP A0A0K0VJM8
B	253	HIS	-	expression tag	UNP A0A0K0VJM8
C	246	LYS	-	expression tag	UNP A0A0K0VJM8
C	247	GLY	-	expression tag	UNP A0A0K0VJM8
C	248	HIS	-	expression tag	UNP A0A0K0VJM8
C	249	HIS	-	expression tag	UNP A0A0K0VJM8
C	250	HIS	-	expression tag	UNP A0A0K0VJM8
C	251	HIS	-	expression tag	UNP A0A0K0VJM8
C	252	HIS	-	expression tag	UNP A0A0K0VJM8
C	253	HIS	-	expression tag	UNP A0A0K0VJM8
D	246	LYS	-	expression tag	UNP A0A0K0VJM8
D	247	GLY	-	expression tag	UNP A0A0K0VJM8
D	248	HIS	-	expression tag	UNP A0A0K0VJM8
D	249	HIS	-	expression tag	UNP A0A0K0VJM8
D	250	HIS	-	expression tag	UNP A0A0K0VJM8
D	251	HIS	-	expression tag	UNP A0A0K0VJM8
D	252	HIS	-	expression tag	UNP A0A0K0VJM8
D	253	HIS	-	expression tag	UNP A0A0K0VJM8
E	246	LYS	-	expression tag	UNP A0A0K0VJM8
E	247	GLY	-	expression tag	UNP A0A0K0VJM8
E	248	HIS	-	expression tag	UNP A0A0K0VJM8
E	249	HIS	-	expression tag	UNP A0A0K0VJM8
E	250	HIS	-	expression tag	UNP A0A0K0VJM8
E	251	HIS	-	expression tag	UNP A0A0K0VJM8
E	252	HIS	-	expression tag	UNP A0A0K0VJM8
E	253	HIS	-	expression tag	UNP A0A0K0VJM8
F	246	LYS	-	expression tag	UNP A0A0K0VJM8
F	247	GLY	-	expression tag	UNP A0A0K0VJM8
F	248	HIS	-	expression tag	UNP A0A0K0VJM8
F	249	HIS	-	expression tag	UNP A0A0K0VJM8
F	250	HIS	-	expression tag	UNP A0A0K0VJM8
F	251	HIS	-	expression tag	UNP A0A0K0VJM8
F	252	HIS	-	expression tag	UNP A0A0K0VJM8
F	253	HIS	-	expression tag	UNP A0A0K0VJM8
G	246	LYS	-	expression tag	UNP A0A0K0VJM8
G	247	GLY	-	expression tag	UNP A0A0K0VJM8
G	248	HIS	-	expression tag	UNP A0A0K0VJM8
G	249	HIS	-	expression tag	UNP A0A0K0VJM8
G	250	HIS	-	expression tag	UNP A0A0K0VJM8
G	251	HIS	-	expression tag	UNP A0A0K0VJM8
G	252	HIS	-	expression tag	UNP A0A0K0VJM8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	253	HIS	-	expression tag	UNP A0A0K0VJM8
H	246	LYS	-	expression tag	UNP A0A0K0VJM8
H	247	GLY	-	expression tag	UNP A0A0K0VJM8
H	248	HIS	-	expression tag	UNP A0A0K0VJM8
H	249	HIS	-	expression tag	UNP A0A0K0VJM8
H	250	HIS	-	expression tag	UNP A0A0K0VJM8
H	251	HIS	-	expression tag	UNP A0A0K0VJM8
H	252	HIS	-	expression tag	UNP A0A0K0VJM8
H	253	HIS	-	expression tag	UNP A0A0K0VJM8

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



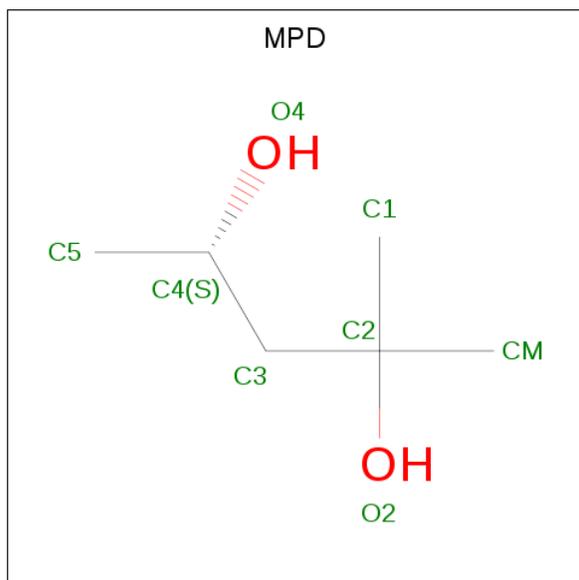
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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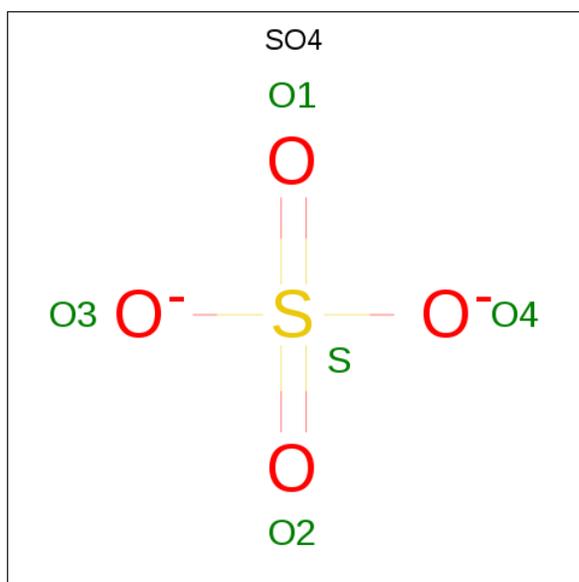
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	H	1	31	17	4	9	1	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	C	1	8	6	2	0	0
3	H	1	8	6	2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	26	Total	O	0	0
			26	26		
5	C	41	Total	O	0	0
			41	41		
5	D	40	Total	O	0	0
			40	40		
5	E	19	Total	O	0	0
			19	19		
5	F	16	Total	O	0	0
			16	16		
5	G	36	Total	O	0	0
			36	36		

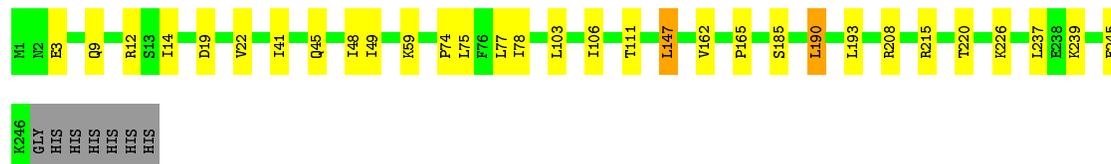
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	47	Total	O	0	0
			47	47		

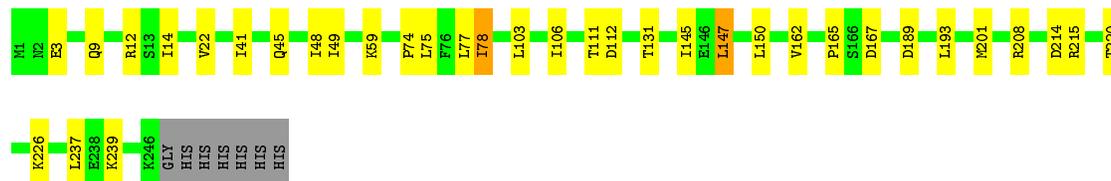
- Molecule 1: NfrA2

Chain E: 85% 11% ..



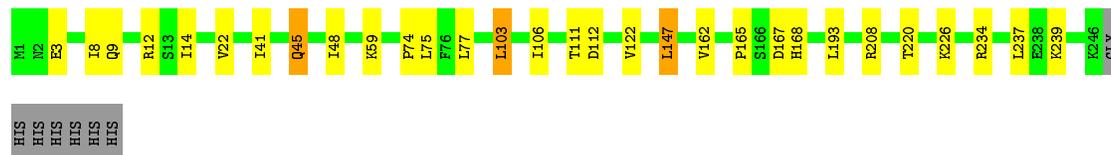
- Molecule 1: NfrA2

Chain F: 83% 13% ..



- Molecule 1: NfrA2

Chain G: 85% 11% ..



- Molecule 1: NfrA2

Chain H: 80% 15% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.44Å 158.19Å 103.86Å 90.00° 102.21° 90.00°	Depositor
Resolution (Å)	28.63 – 2.84 48.33 – 2.84	Depositor EDS
% Data completeness (in resolution range)	97.2 (28.63-2.84) 97.3 (48.33-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.86Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.203 , 0.247 0.251 , 0.300	Depositor DCC
R_{free} test set	2222 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtrriage
Anisotropy	0.909	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15833	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4182e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, MPD, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/1947	0.63	0/2636
1	B	0.41	0/1947	0.63	0/2636
1	C	0.42	0/1939	0.64	0/2626
1	D	0.41	0/1947	0.64	0/2636
1	E	0.41	0/1947	0.65	1/2636 (0.0%)
1	F	0.40	0/1947	0.62	0/2636
1	G	0.42	0/1947	0.63	0/2636
1	H	0.41	0/1947	0.63	0/2636
All	All	0.41	0/15568	0.63	1/21078 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	LEU	CA-CB-CG	6.03	129.17	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1913	0	1906	16	0
1	B	1913	0	1906	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1905	0	1894	11	0
1	D	1913	0	1906	12	0
1	E	1913	0	1906	9	0
1	F	1913	0	1906	11	0
1	G	1913	0	1906	13	0
1	H	1913	0	1906	20	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
2	G	31	0	19	0	0
2	H	31	0	19	0	0
3	C	8	0	14	0	0
3	H	8	0	14	1	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	A	23	0	0	0	0
5	B	26	0	0	0	0
5	C	41	0	0	0	0
5	D	40	0	0	0	0
5	E	19	0	0	0	0
5	F	16	0	0	0	0
5	G	36	0	0	0	0
5	H	47	0	0	0	0
All	All	15833	0	15416	92	0

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

All (92) 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:E:3:GLU:HB3	1:F:3:GLU:HB3	1.63	0.80
1:G:103:LEU:HD11	1:H:244:PHE:CZ	2.19	0.77
1:D:48:ILE:HD11	1:D:77:LEU:HB3	1.66	0.76
1:H:48:ILE:HD11	1:H:77:LEU:HB3	1.67	0.76
1:C:14:ILE:HG21	1:C:165:PRO:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ILE:HD11	1:E:77:LEU:HB3	1.67	0.76
1:G:48:ILE:HD11	1:G:77:LEU:HB3	1.67	0.75
1:F:48:ILE:HD11	1:F:77:LEU:HB3	1.68	0.73
1:A:48:ILE:HD11	1:A:77:LEU:HB3	1.68	0.73
1:G:103:LEU:HD11	1:H:244:PHE:HZ	1.52	0.72
1:A:3:GLU:HB3	1:B:3:GLU:HB3	1.72	0.71
1:A:205:MET:O	1:A:209:THR:HG22	1.89	0.71
1:G:3:GLU:HB3	1:H:3:GLU:HB3	1.74	0.68
1:B:48:ILE:HD11	1:B:77:LEU:HB3	1.76	0.67
1:A:209:THR:HG21	1:A:213:ASP:H	1.60	0.66
1:D:106:ILE:HD12	1:D:237:LEU:HD22	1.77	0.65
1:H:106:ILE:HD12	1:H:237:LEU:HD22	1.78	0.64
1:D:49:ILE:HB	1:D:78:ILE:HG23	1.79	0.64
1:F:49:ILE:HB	1:F:78:ILE:HG23	1.80	0.63
1:C:106:ILE:HD12	1:C:237:LEU:HD22	1.80	0.63
1:H:41:ILE:HG22	3:H:302:MPD:H32	1.81	0.63
1:H:49:ILE:HB	1:H:78:ILE:HG23	1.80	0.62
1:F:106:ILE:HD12	1:F:237:LEU:HD22	1.82	0.62
1:G:106:ILE:HD12	1:G:237:LEU:HD22	1.82	0.62
1:A:106:ILE:HD12	1:A:237:LEU:HD22	1.82	0.61
1:B:106:ILE:HD12	1:B:237:LEU:HD22	1.82	0.61
1:E:106:ILE:HD12	1:E:237:LEU:HD22	1.82	0.61
1:A:209:THR:OG1	1:A:212:ALA:HB3	2.01	0.60
1:G:122:VAL:HG23	1:H:8:ILE:HD11	1.84	0.59
1:C:8:ILE:HD11	1:D:122:VAL:HG23	1.84	0.58
1:A:209:THR:CG2	1:A:213:ASP:H	2.17	0.58
1:G:8:ILE:HD11	1:H:122:VAL:HG23	1.86	0.58
1:E:49:ILE:HB	1:E:78:ILE:HG23	1.87	0.57
1:G:75:LEU:HD23	1:G:162:VAL:HB	1.89	0.55
1:B:12:ARG:HD2	1:B:168:HIS:O	2.07	0.54
1:B:49:ILE:HB	1:B:78:ILE:HG23	1.89	0.54
1:C:75:LEU:HD23	1:C:162:VAL:HB	1.90	0.54
1:F:75:LEU:HD23	1:F:162:VAL:HB	1.91	0.53
1:E:75:LEU:HD23	1:E:162:VAL:HB	1.91	0.53
1:D:75:LEU:HD23	1:D:162:VAL:HB	1.91	0.53
1:C:3:GLU:HB3	1:D:3:GLU:HB3	1.91	0.52
1:H:75:LEU:HD23	1:H:162:VAL:HB	1.91	0.52
1:H:78:ILE:HD13	1:H:137:ILE:HG12	1.91	0.52
1:B:75:LEU:HD23	1:B:162:VAL:HB	1.91	0.52
1:H:14:ILE:HG21	1:H:165:PRO:HB3	1.92	0.52
1:E:14:ILE:HG21	1:E:165:PRO:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ILE:HG21	1:B:165:PRO:HB3	1.93	0.51
1:D:14:ILE:HG21	1:D:165:PRO:HB3	1.92	0.51
1:G:14:ILE:HG21	1:G:165:PRO:HB3	1.93	0.51
1:F:14:ILE:HG21	1:F:165:PRO:HB3	1.93	0.50
1:C:59:LYS:HB3	1:C:147:LEU:HD11	1.92	0.50
1:A:59:LYS:HB3	1:A:147:LEU:HD11	1.93	0.49
1:F:145:ILE:HG23	1:F:150:LEU:HB2	1.95	0.49
1:A:209:THR:HG21	1:A:213:ASP:N	2.27	0.49
1:D:59:LYS:HB3	1:D:147:LEU:HD11	1.95	0.48
1:B:10:ASP:HA	1:B:171:LYS:HD2	1.96	0.48
1:B:59:LYS:HB3	1:B:147:LEU:HD11	1.95	0.48
1:G:59:LYS:HB3	1:G:147:LEU:HD11	1.94	0.48
1:H:77:LEU:HB2	1:H:160:LEU:HB3	1.96	0.48
1:F:59:LYS:HB3	1:F:147:LEU:HD11	1.96	0.47
1:C:99:VAL:HG22	1:C:105:SER:HB3	1.98	0.46
1:A:131:THR:HG22	1:A:162:VAL:HG22	1.97	0.46
1:H:59:LYS:HB3	1:H:147:LEU:HD11	1.97	0.46
1:C:215:ARG:HD2	1:C:220:THR:HG22	1.97	0.46
1:E:59:LYS:HB3	1:E:147:LEU:HD11	1.97	0.45
1:E:215:ARG:HD2	1:E:220:THR:HG22	1.97	0.45
1:A:209:THR:HG23	1:A:212:ALA:H	1.82	0.45
1:A:209:THR:HG1	1:A:212:ALA:HB3	1.81	0.44
1:A:67:GLN:HB2	1:A:70:ILE:HD12	1.98	0.44
1:H:215:ARG:HD2	1:H:220:THR:HG22	1.99	0.44
1:C:131:THR:HA	1:C:161:VAL:O	2.18	0.44
1:D:208:ARG:HH12	1:H:10:ASP:CG	2.21	0.43
1:H:22:VAL:HG23	1:H:74:PRO:HG2	2.00	0.43
1:D:22:VAL:HG23	1:D:74:PRO:HG2	2.01	0.43
1:F:215:ARG:HD2	1:F:220:THR:HG22	2.00	0.42
1:G:234:ARG:HH11	1:H:244:PHE:HB3	1.84	0.42
1:E:22:VAL:HG23	1:E:74:PRO:HG2	2.01	0.42
1:C:22:VAL:HG23	1:C:74:PRO:HG2	2.01	0.42
1:F:22:VAL:HG23	1:F:74:PRO:HG2	2.01	0.42
1:G:22:VAL:HG23	1:G:74:PRO:HG2	2.02	0.42
1:B:131:THR:HG22	1:B:162:VAL:HG22	2.02	0.41
1:A:22:VAL:HG23	1:A:74:PRO:HG2	2.02	0.41
1:G:45:GLN:HB2	1:G:45:GLN:HE21	1.72	0.41
1:D:131:THR:HG22	1:D:162:VAL:HG22	2.02	0.41
1:F:131:THR:HG22	1:F:162:VAL:HG22	2.02	0.41
1:H:179:ALA:HA	1:H:190:LEU:HD22	2.02	0.41
1:A:131:THR:HA	1:A:161:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:HIS:O	1:B:49:ILE:HA	2.21	0.40
1:C:182:HIS:O	1:D:49:ILE:HA	2.20	0.40
1:H:145:ILE:HG23	1:H:150:LEU:HB2	2.03	0.40
1:B:131:THR:HA	1:B:161:VAL:O	2.22	0.40
1:B:22:VAL:HG23	1:B:74:PRO:HG2	2.02	0.40

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	244/253 (96%)	234 (96%)	9 (4%)	1 (0%)	34	56
1	B	244/253 (96%)	234 (96%)	9 (4%)	1 (0%)	34	56
1	C	243/253 (96%)	234 (96%)	8 (3%)	1 (0%)	34	56
1	D	244/253 (96%)	236 (97%)	7 (3%)	1 (0%)	34	56
1	E	244/253 (96%)	236 (97%)	7 (3%)	1 (0%)	34	56
1	F	244/253 (96%)	236 (97%)	7 (3%)	1 (0%)	34	56
1	G	244/253 (96%)	235 (96%)	8 (3%)	1 (0%)	34	56
1	H	244/253 (96%)	235 (96%)	8 (3%)	1 (0%)	34	56
All	All	1951/2024 (96%)	1880 (96%)	63 (3%)	8 (0%)	34	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	B	41	ILE
1	E	41	ILE
1	F	41	ILE
1	H	41	ILE

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Mol	Chain	Res	Type
1	C	41	ILE
1	D	41	ILE
1	G	41	ILE

5.3.2 Protein sidechains [i](#)

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	205/211 (97%)	184 (90%)	21 (10%)	7	15
1	B	205/211 (97%)	187 (91%)	18 (9%)	10	21
1	C	204/211 (97%)	187 (92%)	17 (8%)	11	24
1	D	205/211 (97%)	185 (90%)	20 (10%)	8	16
1	E	205/211 (97%)	191 (93%)	14 (7%)	16	31
1	F	205/211 (97%)	189 (92%)	16 (8%)	12	26
1	G	205/211 (97%)	191 (93%)	14 (7%)	16	31
1	H	205/211 (97%)	187 (91%)	18 (9%)	10	21
All	All	1639/1688 (97%)	1501 (92%)	138 (8%)	11	23

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	10	ASP
1	A	12	ARG
1	A	19	ASP
1	A	24	ASP
1	A	25	GLU
1	A	45	GLN
1	A	60	LEU
1	A	103	LEU
1	A	111	THR
1	A	112	ASP
1	A	147	LEU

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Mol	Chain	Res	Type
1	A	168	HIS
1	A	193	LEU
1	A	205	MET
1	A	208	ARG
1	A	219	GLN
1	A	220	THR
1	A	226	LYS
1	A	239	LYS
1	A	245	GLU
1	B	6	ARG
1	B	9	GLN
1	B	16	GLN
1	B	25	GLU
1	B	45	GLN
1	B	103	LEU
1	B	116	SER
1	B	147	LEU
1	B	167	ASP
1	B	175	LEU
1	B	193	LEU
1	B	200	GLU
1	B	205	MET
1	B	214	ASP
1	B	220	THR
1	B	226	LYS
1	B	239	LYS
1	B	245	GLU
1	C	6	ARG
1	C	12	ARG
1	C	45	GLN
1	C	46	VAL
1	C	53	ASP
1	C	60	LEU
1	C	80	CYS
1	C	103	LEU
1	C	112	ASP
1	C	116	SER
1	C	147	LEU
1	C	193	LEU
1	C	205	MET
1	C	208	ARG
1	C	214	ASP

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Mol	Chain	Res	Type
1	C	226	LYS
1	C	239	LYS
1	D	6	ARG
1	D	9	GLN
1	D	12	ARG
1	D	53	ASP
1	D	78	ILE
1	D	94	ASP
1	D	103	LEU
1	D	112	ASP
1	D	142	LEU
1	D	147	LEU
1	D	167	ASP
1	D	185	SER
1	D	189	ASP
1	D	193	LEU
1	D	203	GLU
1	D	208	ARG
1	D	220	THR
1	D	226	LYS
1	D	239	LYS
1	D	245	GLU
1	E	9	GLN
1	E	12	ARG
1	E	19	ASP
1	E	45	GLN
1	E	103	LEU
1	E	111	THR
1	E	147	LEU
1	E	185	SER
1	E	190	LEU
1	E	193	LEU
1	E	208	ARG
1	E	226	LYS
1	E	239	LYS
1	E	245	GLU
1	F	9	GLN
1	F	12	ARG
1	F	45	GLN
1	F	78	ILE
1	F	103	LEU
1	F	111	THR

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Mol	Chain	Res	Type
1	F	112	ASP
1	F	147	LEU
1	F	167	ASP
1	F	189	ASP
1	F	193	LEU
1	F	201	MET
1	F	208	ARG
1	F	214	ASP
1	F	226	LYS
1	F	239	LYS
1	G	9	GLN
1	G	12	ARG
1	G	45	GLN
1	G	103	LEU
1	G	111	THR
1	G	112	ASP
1	G	147	LEU
1	G	167	ASP
1	G	168	HIS
1	G	193	LEU
1	G	208	ARG
1	G	220	THR
1	G	226	LYS
1	G	239	LYS
1	H	6	ARG
1	H	9	GLN
1	H	12	ARG
1	H	45	GLN
1	H	53	ASP
1	H	60	LEU
1	H	78	ILE
1	H	103	LEU
1	H	112	ASP
1	H	137	ILE
1	H	147	LEU
1	H	167	ASP
1	H	189	ASP
1	H	193	LEU
1	H	208	ARG
1	H	214	ASP
1	H	226	LYS
1	H	239	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	52	GLN
1	A	188	HIS
1	B	9	GLN
1	B	210	ASN
1	D	9	GLN
1	D	188	HIS
1	D	210	ASN
1	E	9	GLN
1	F	9	GLN
1	F	187	ASN
1	F	210	ASN
1	G	9	GLN
1	H	9	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	SO4	D	302	-	4,4,4	0.44	0	6,6,6	0.55	0
4	SO4	G	302	-	4,4,4	0.12	0	6,6,6	0.10	0
2	FMN	B	301	-	31,33,33	1.82	5 (16%)	40,50,50	2.62	7 (17%)
2	FMN	D	301	-	31,33,33	1.83	5 (16%)	40,50,50	2.61	7 (17%)
2	FMN	F	301	-	31,33,33	1.90	5 (16%)	40,50,50	2.62	7 (17%)
4	SO4	H	303	-	4,4,4	0.16	0	6,6,6	0.15	0
2	FMN	H	301	-	31,33,33	1.91	5 (16%)	40,50,50	2.64	7 (17%)
4	SO4	D	303	-	4,4,4	0.20	0	6,6,6	0.17	0
3	MPD	C	302	-	7,7,7	1.04	1 (14%)	9,10,10	0.43	0
3	MPD	H	302	-	7,7,7	0.69	0	9,10,10	0.52	0
4	SO4	C	303	-	4,4,4	0.16	0	6,6,6	0.09	0
2	FMN	A	301	-	31,33,33	1.90	5 (16%)	40,50,50	2.64	7 (17%)
2	FMN	C	301	-	31,33,33	1.88	5 (16%)	40,50,50	2.63	7 (17%)
2	FMN	E	301	-	31,33,33	1.83	5 (16%)	40,50,50	2.62	7 (17%)
2	FMN	G	301	-	31,33,33	1.81	5 (16%)	40,50,50	2.64	7 (17%)

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
2	FMN	B	301	-	-	3/18/18/18	0/3/3/3
2	FMN	D	301	-	-	3/18/18/18	0/3/3/3
2	FMN	F	301	-	-	3/18/18/18	0/3/3/3
2	FMN	H	301	-	-	3/18/18/18	0/3/3/3
3	MPD	C	302	-	-	2/5/5/5	-
3	MPD	H	302	-	-	3/5/5/5	-
2	FMN	A	301	-	-	3/18/18/18	0/3/3/3
2	FMN	C	301	-	-	2/18/18/18	0/3/3/3
2	FMN	E	301	-	-	3/18/18/18	0/3/3/3
2	FMN	G	301	-	-	3/18/18/18	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	FMN	C4A-C10	8.28	1.47	1.38
2	F	301	FMN	C4A-C10	8.13	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	FMN	C4A-C10	7.99	1.46	1.38
2	C	301	FMN	C4A-C10	7.89	1.46	1.38
2	D	301	FMN	C4A-C10	7.77	1.46	1.38
2	B	301	FMN	C4A-C10	7.70	1.46	1.38
2	G	301	FMN	C4A-C10	7.56	1.46	1.38
2	E	301	FMN	C4A-C10	7.56	1.46	1.38
2	E	301	FMN	C4-C4A	3.82	1.47	1.41
2	A	301	FMN	C4-C4A	3.60	1.47	1.41
2	C	301	FMN	C4-C4A	3.59	1.47	1.41
2	A	301	FMN	C4-N3	3.51	1.39	1.33
2	F	301	FMN	C4-C4A	3.49	1.47	1.41
2	D	301	FMN	C4-C4A	3.42	1.47	1.41
2	G	301	FMN	C4-C4A	3.41	1.47	1.41
2	B	301	FMN	C4-N3	3.41	1.39	1.33
2	H	301	FMN	C4-C4A	3.40	1.47	1.41
2	G	301	FMN	C4-N3	3.39	1.38	1.33
2	F	301	FMN	C4-N3	3.38	1.38	1.33
2	C	301	FMN	C4-N3	3.36	1.38	1.33
2	H	301	FMN	C4-N3	3.30	1.38	1.33
2	E	301	FMN	C4-N3	3.26	1.38	1.33
2	B	301	FMN	C4-C4A	3.25	1.47	1.41
2	D	301	FMN	C4-N3	3.25	1.38	1.33
2	C	301	FMN	C9A-N10	3.17	1.42	1.38
2	G	301	FMN	C9A-N10	3.06	1.42	1.38
2	A	301	FMN	C9A-N10	3.06	1.42	1.38
2	H	301	FMN	C9A-N10	3.04	1.42	1.38
2	E	301	FMN	C9A-N10	3.03	1.42	1.38
2	F	301	FMN	C9A-N10	3.00	1.42	1.38
2	D	301	FMN	C9A-N10	2.91	1.42	1.38
2	B	301	FMN	C5A-N5	2.78	1.39	1.35
2	B	301	FMN	C9A-N10	2.77	1.42	1.38
2	H	301	FMN	C5A-N5	2.70	1.39	1.35
2	C	301	FMN	C5A-N5	2.69	1.39	1.35
2	A	301	FMN	C5A-N5	2.67	1.39	1.35
2	E	301	FMN	C5A-N5	2.64	1.39	1.35
2	D	301	FMN	C5A-N5	2.63	1.39	1.35
2	F	301	FMN	C5A-N5	2.61	1.39	1.35
3	C	302	MPD	C3-C2	2.49	1.60	1.53
2	G	301	FMN	C5A-N5	2.44	1.39	1.35

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	FMN	C4-N3-C2	12.88	126.01	115.14
2	E	301	FMN	C4-N3-C2	12.76	125.92	115.14
2	G	301	FMN	C4-N3-C2	12.75	125.91	115.14
2	B	301	FMN	C4-N3-C2	12.74	125.90	115.14
2	F	301	FMN	C4-N3-C2	12.72	125.88	115.14
2	D	301	FMN	C4-N3-C2	12.72	125.88	115.14
2	C	301	FMN	C4-N3-C2	12.71	125.87	115.14
2	A	301	FMN	C4-N3-C2	12.69	125.86	115.14
2	F	301	FMN	C4A-C4-N3	-6.97	113.89	123.43
2	A	301	FMN	C4A-C4-N3	-6.95	113.92	123.43
2	C	301	FMN	C4A-C4-N3	-6.95	113.92	123.43
2	G	301	FMN	C4A-C4-N3	-6.95	113.92	123.43
2	B	301	FMN	C4A-C4-N3	-6.95	113.93	123.43
2	E	301	FMN	C4A-C4-N3	-6.95	113.93	123.43
2	H	301	FMN	C4A-C4-N3	-6.91	113.98	123.43
2	D	301	FMN	C4A-C4-N3	-6.86	114.05	123.43
2	G	301	FMN	C10-C4A-N5	4.26	124.20	121.26
2	A	301	FMN	C10-C4A-N5	4.22	124.17	121.26
2	E	301	FMN	C10-C4A-N5	4.15	124.13	121.26
2	C	301	FMN	C10-C4A-N5	4.14	124.12	121.26
2	D	301	FMN	C10-C4A-N5	4.09	124.08	121.26
2	F	301	FMN	C10-C4A-N5	4.06	124.06	121.26
2	H	301	FMN	C10-C4A-N5	4.03	124.05	121.26
2	B	301	FMN	C10-C4A-N5	4.01	124.03	121.26
2	B	301	FMN	C4-C4A-C10	-3.79	117.44	119.95
2	A	301	FMN	C4-C4A-C10	-3.79	117.44	119.95
2	H	301	FMN	C4-C4A-C10	-3.75	117.47	119.95
2	C	301	FMN	C4-C4A-C10	-3.74	117.47	119.95
2	D	301	FMN	C4-C4A-C10	-3.67	117.52	119.95
2	E	301	FMN	C4-C4A-C10	-3.63	117.55	119.95
2	G	301	FMN	C4-C4A-C10	-3.63	117.55	119.95
2	F	301	FMN	C4-C4A-C10	-3.59	117.58	119.95
2	G	301	FMN	C4A-C10-N10	-3.38	116.83	120.30
2	A	301	FMN	C4A-C10-N10	-3.35	116.86	120.30
2	H	301	FMN	C4A-C10-N10	-3.34	116.87	120.30
2	F	301	FMN	C4A-C10-N10	-3.32	116.89	120.30
2	E	301	FMN	C4A-C10-N10	-3.28	116.93	120.30
2	D	301	FMN	C4A-C10-N10	-3.27	116.94	120.30
2	B	301	FMN	C4A-C10-N10	-3.26	116.95	120.30
2	C	301	FMN	C4A-C10-N10	-3.25	116.96	120.30
2	H	301	FMN	P-O5'-C5'	2.88	126.24	118.30
2	A	301	FMN	P-O5'-C5'	2.76	125.90	118.30
2	F	301	FMN	P-O5'-C5'	2.73	125.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	FMN	C1'-N10-C9A	2.69	120.41	118.29
2	C	301	FMN	P-O5'-C5'	2.66	125.62	118.30
2	B	301	FMN	P-O5'-C5'	2.65	125.60	118.30
2	E	301	FMN	P-O5'-C5'	2.61	125.48	118.30
2	G	301	FMN	P-O5'-C5'	2.60	125.45	118.30
2	D	301	FMN	P-O5'-C5'	2.57	125.36	118.30
2	C	301	FMN	C1'-N10-C9A	2.53	120.29	118.29
2	A	301	FMN	C1'-N10-C9A	2.53	120.28	118.29
2	D	301	FMN	C1'-N10-C9A	2.43	120.20	118.29
2	F	301	FMN	C1'-N10-C9A	2.29	120.09	118.29
2	H	301	FMN	C1'-N10-C9A	2.11	119.95	118.29
2	B	301	FMN	C1'-N10-C9A	2.10	119.94	118.29
2	E	301	FMN	C1'-N10-C9A	2.03	119.89	118.29

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	FMN	C5'-O5'-P-O1P
2	B	301	FMN	C5'-O5'-P-O2P
2	D	301	FMN	C5'-O5'-P-O2P
2	F	301	FMN	C5'-O5'-P-O1P
2	F	301	FMN	C5'-O5'-P-O2P
2	H	301	FMN	C5'-O5'-P-O1P
2	H	301	FMN	C5'-O5'-P-O2P
3	C	302	MPD	C2-C3-C4-O4
3	H	302	MPD	C1-C2-C3-C4
3	H	302	MPD	O2-C2-C3-C4
2	A	301	FMN	C5'-O5'-P-O1P
2	A	301	FMN	C5'-O5'-P-O2P
2	C	301	FMN	C5'-O5'-P-O1P
2	C	301	FMN	C5'-O5'-P-O2P
2	E	301	FMN	C5'-O5'-P-O1P
2	E	301	FMN	C5'-O5'-P-O2P
2	G	301	FMN	C5'-O5'-P-O1P
2	G	301	FMN	C5'-O5'-P-O2P
2	D	301	FMN	C5'-O5'-P-O1P
3	H	302	MPD	CM-C2-C3-C4
2	B	301	FMN	C5'-O5'-P-O3P
2	D	301	FMN	C5'-O5'-P-O3P
2	F	301	FMN	C5'-O5'-P-O3P
2	H	301	FMN	C5'-O5'-P-O3P

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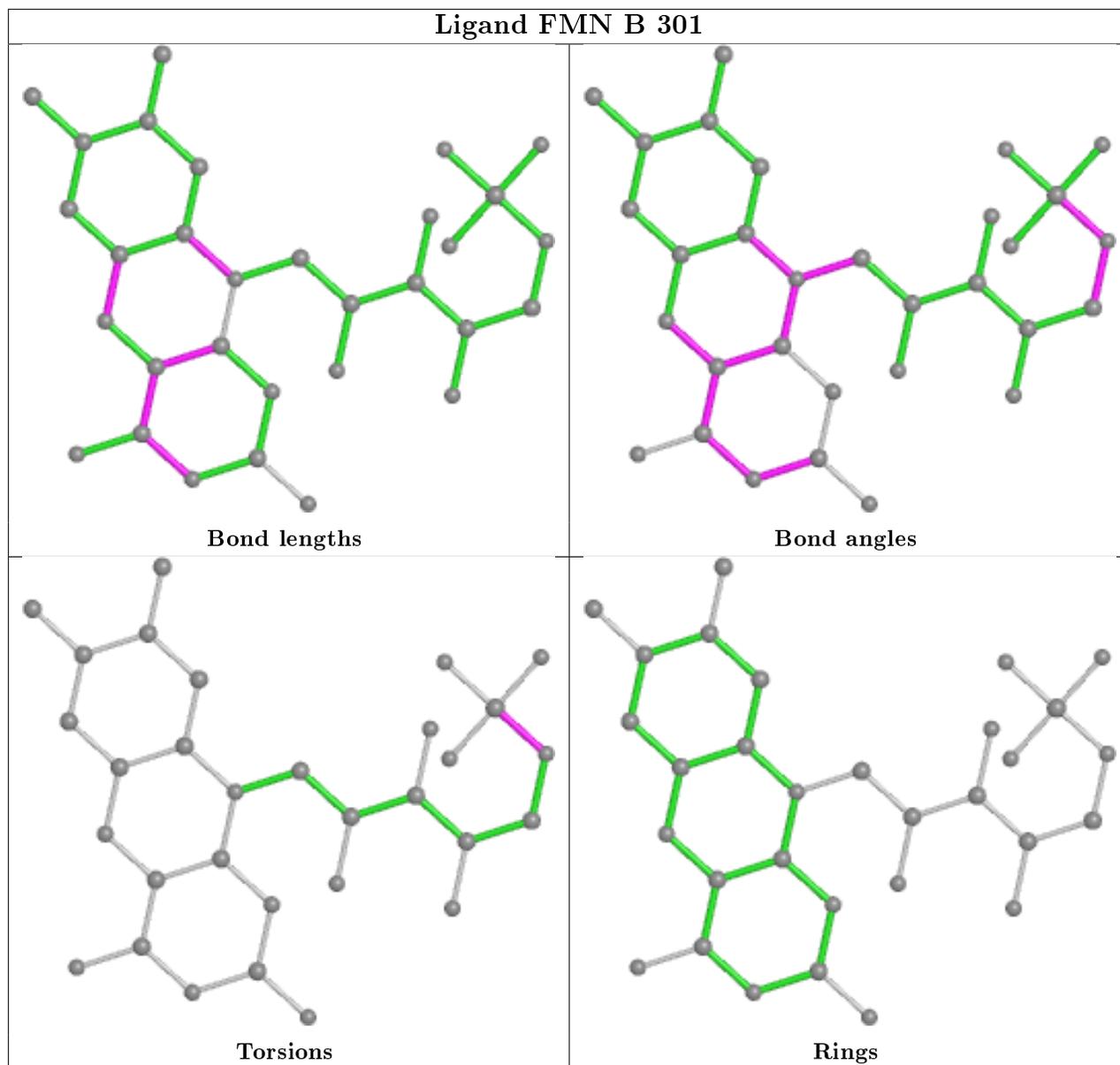
Mol	Chain	Res	Type	Atoms
2	A	301	FMN	C5'-O5'-P-O3P
2	E	301	FMN	C5'-O5'-P-O3P
2	G	301	FMN	C5'-O5'-P-O3P
3	C	302	MPD	C2-C3-C4-C5

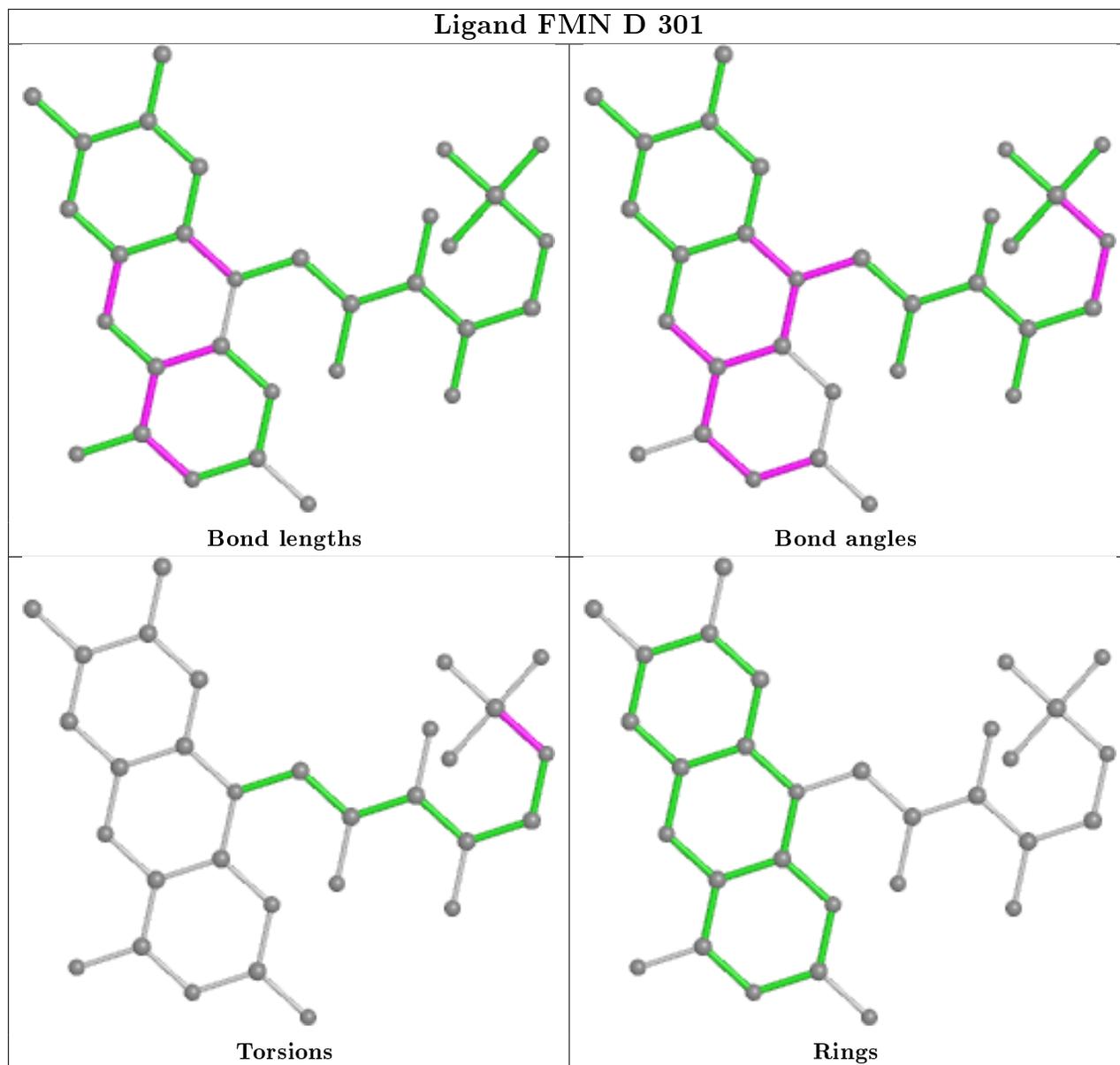
There are no ring outliers.

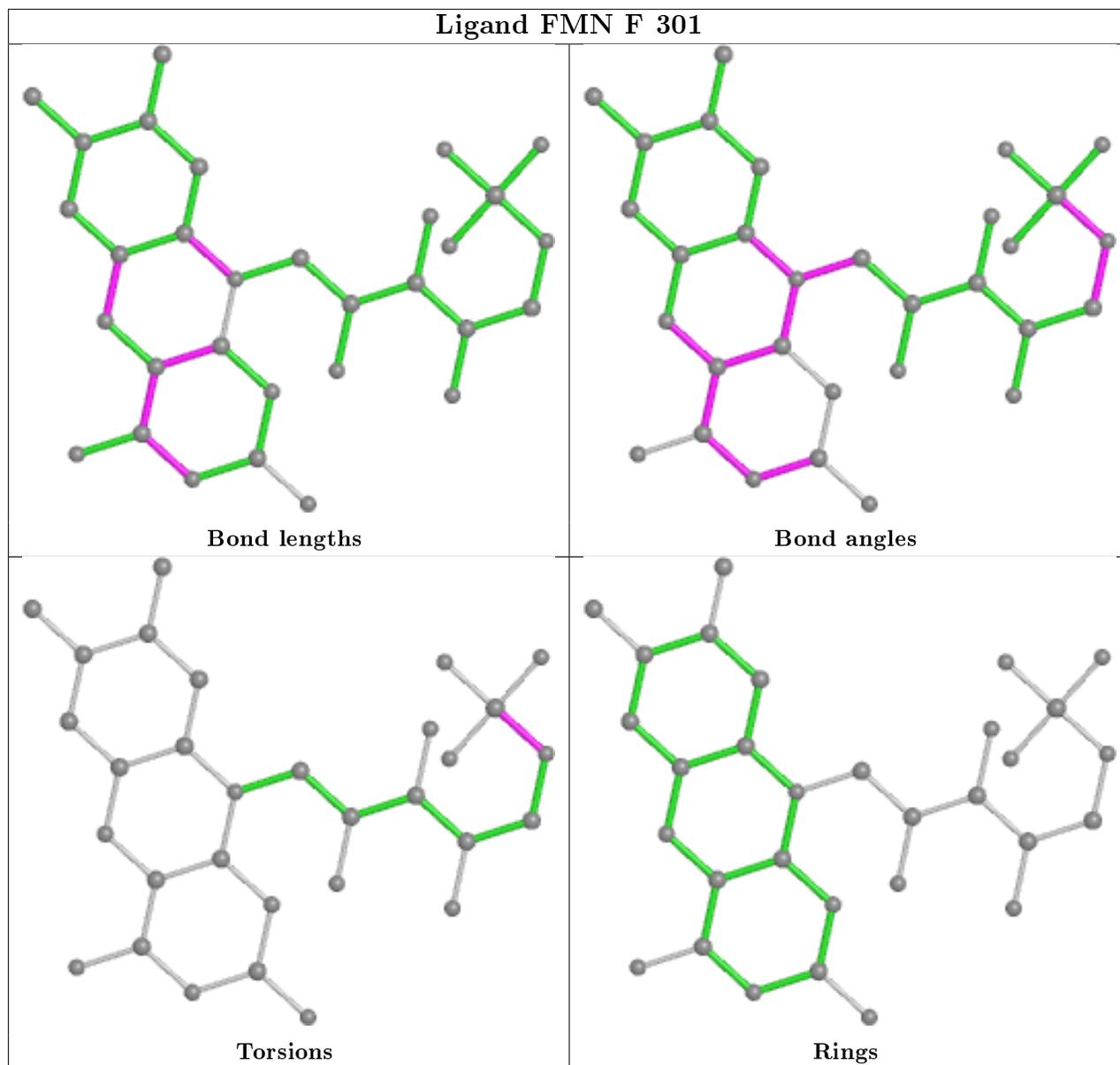
1 monomer is involved in 1 short contact:

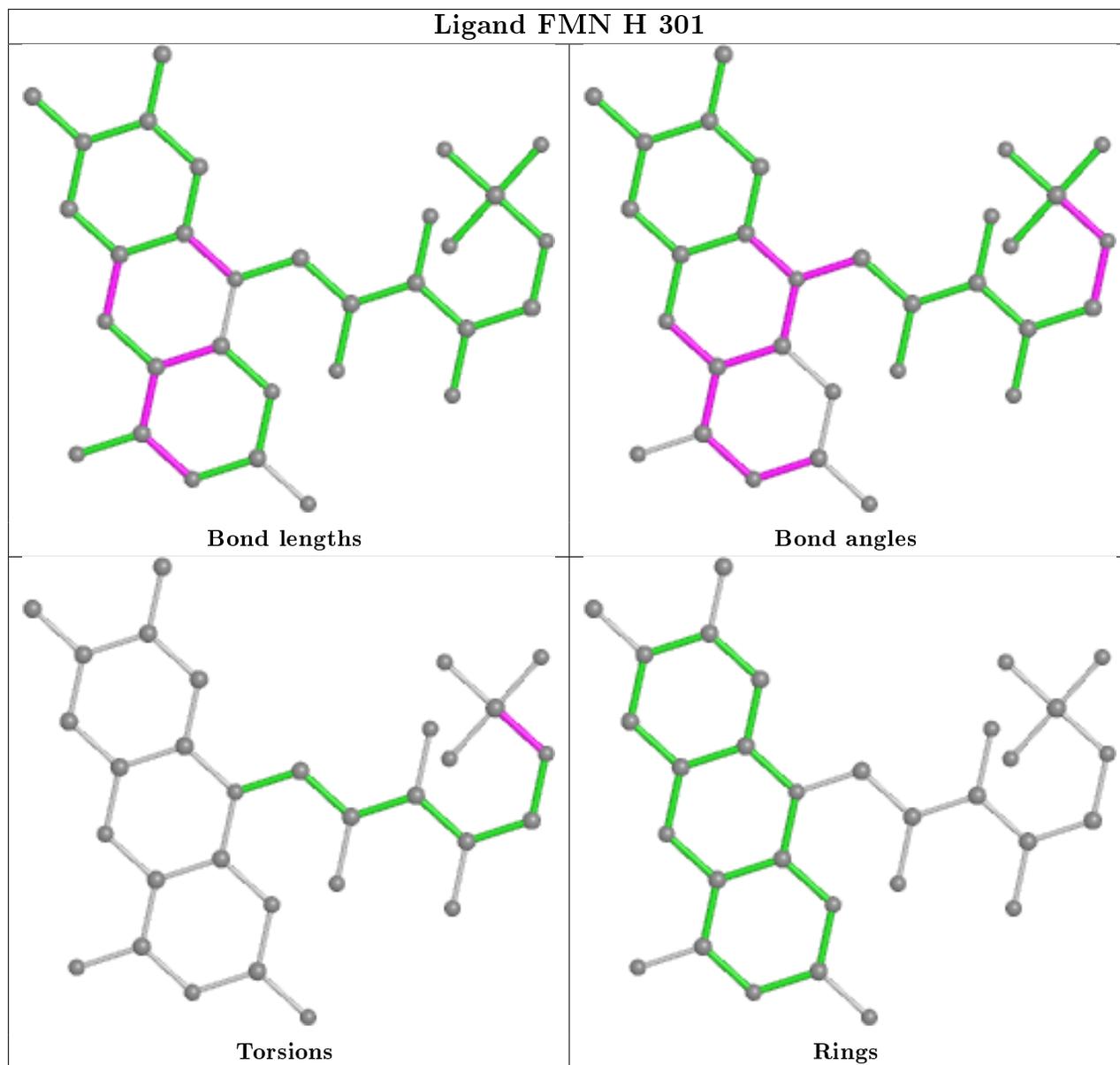
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	302	MPD	1	0

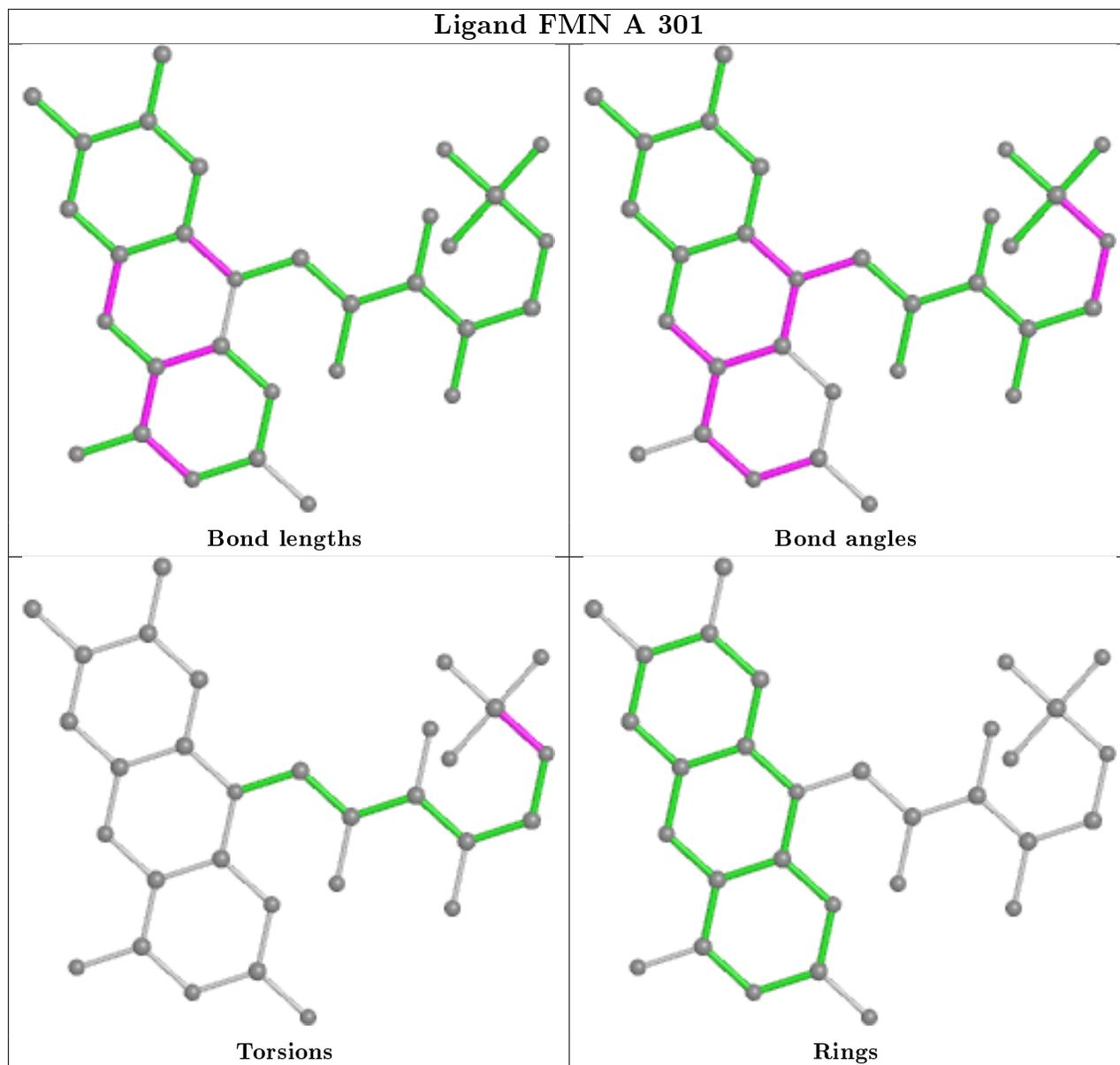
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

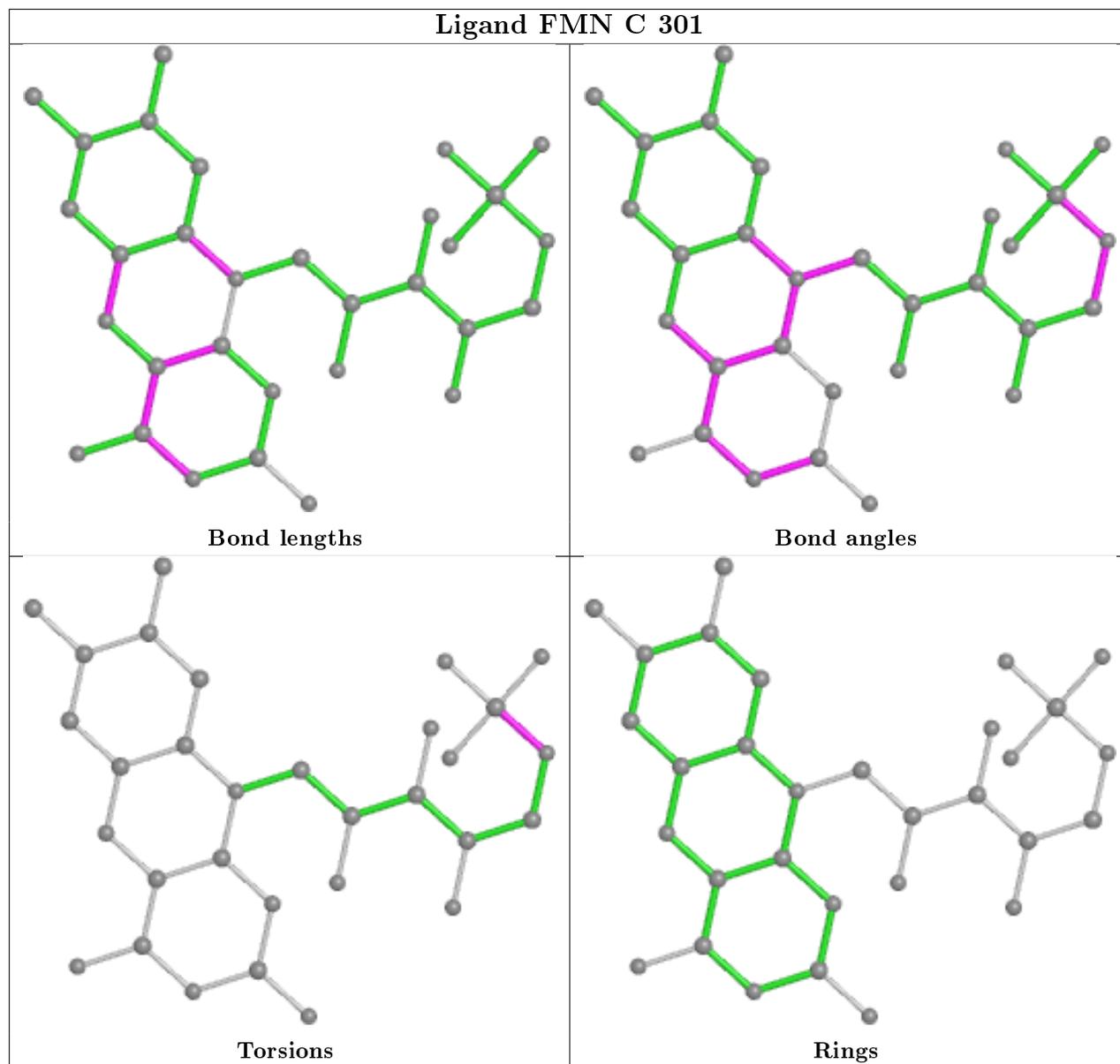


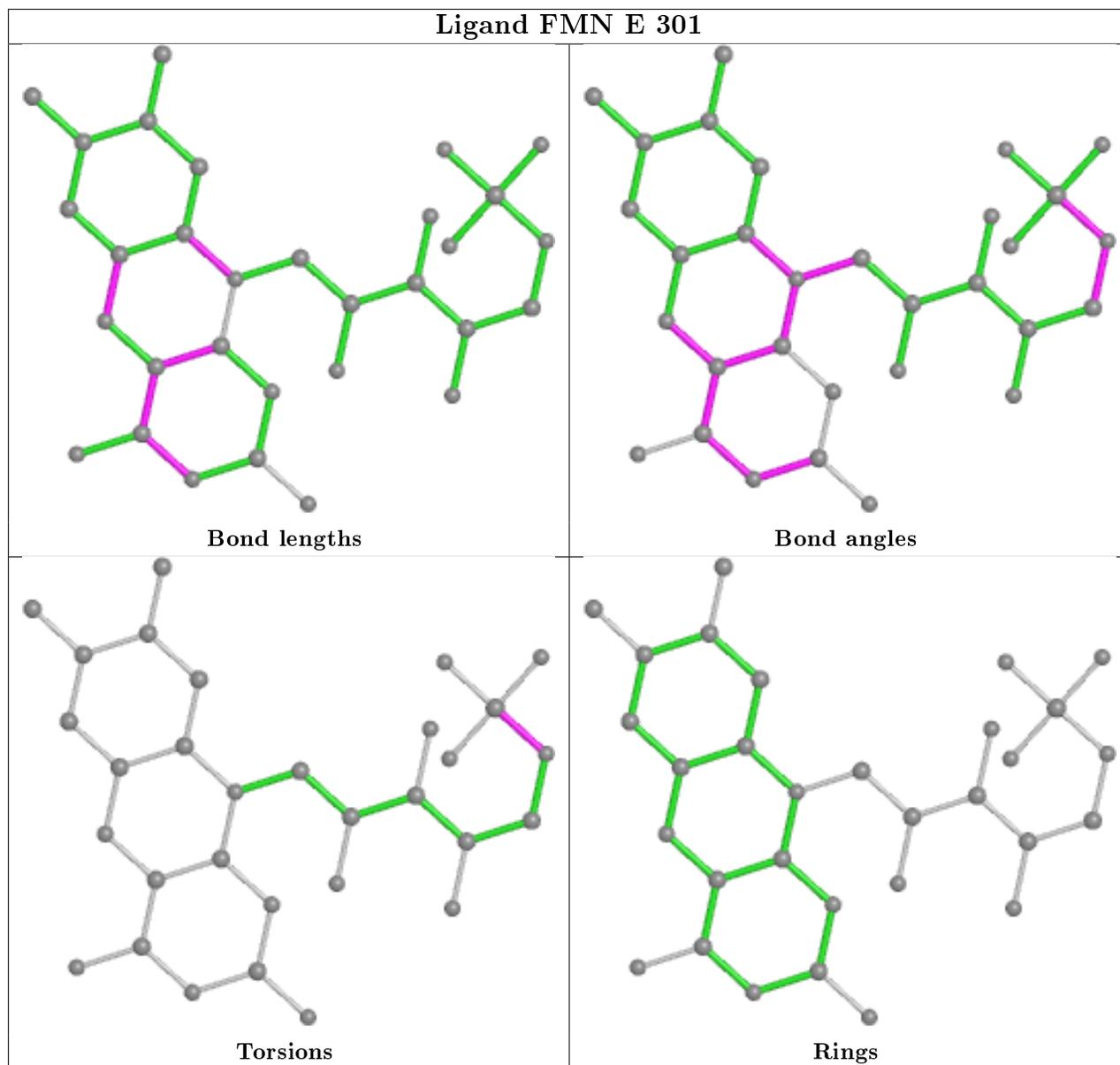


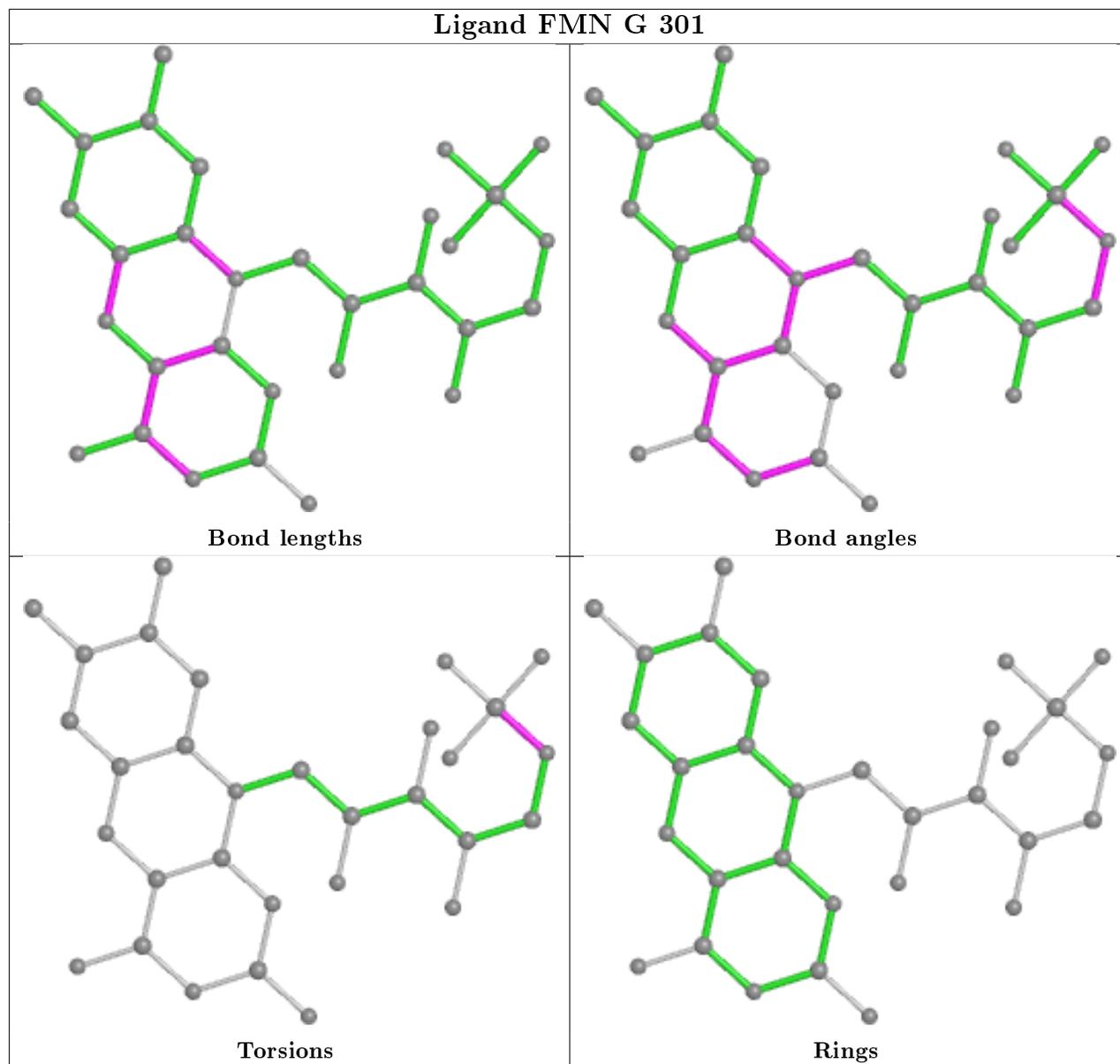












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

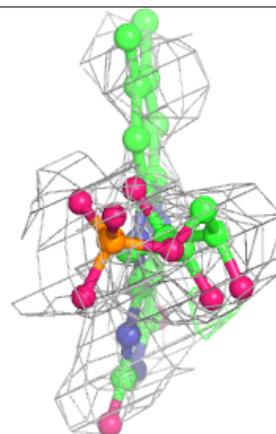
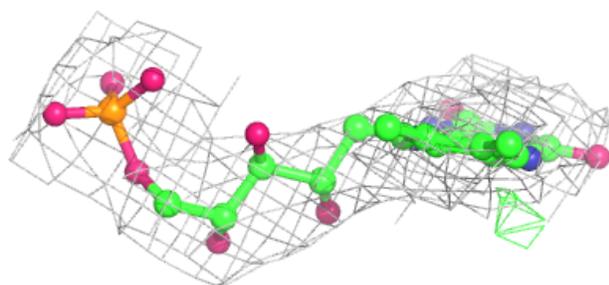
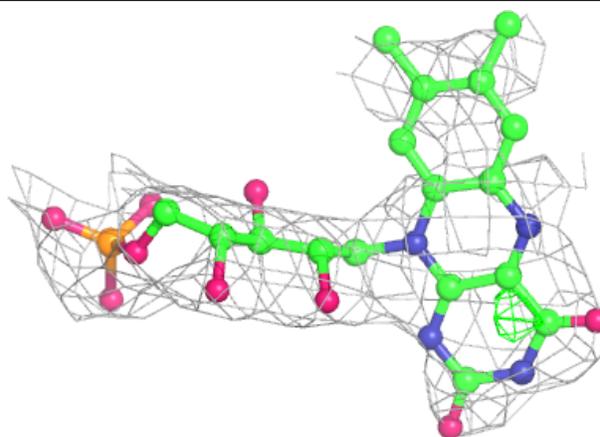
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

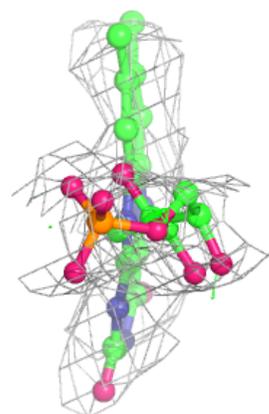
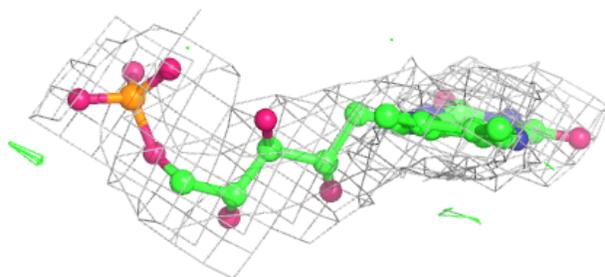
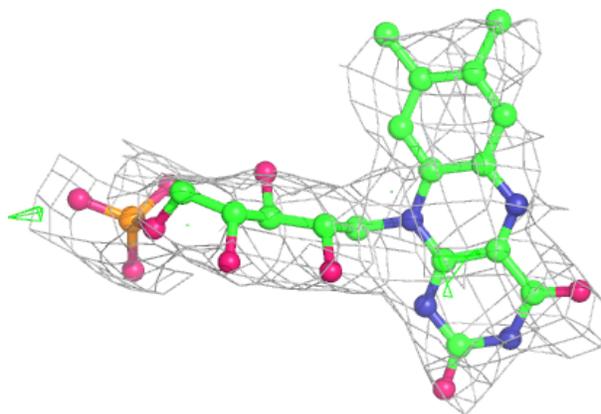
Electron density around FMN B 301:

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



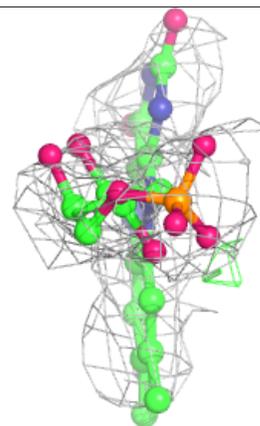
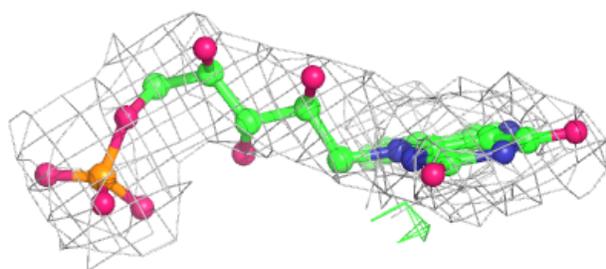
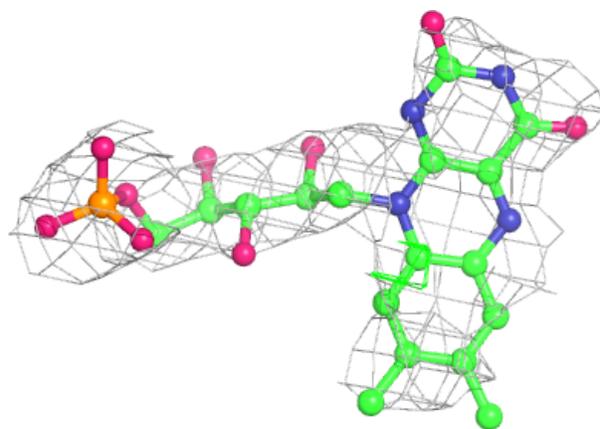
Electron density around FMN D 301:

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



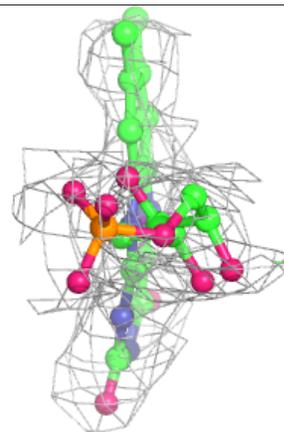
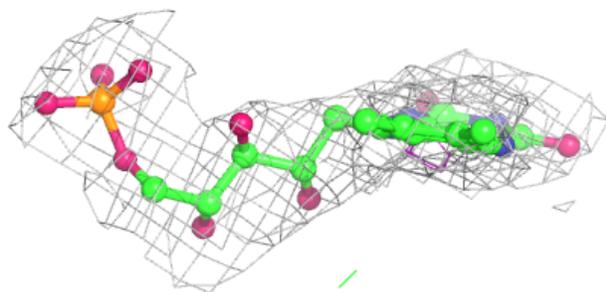
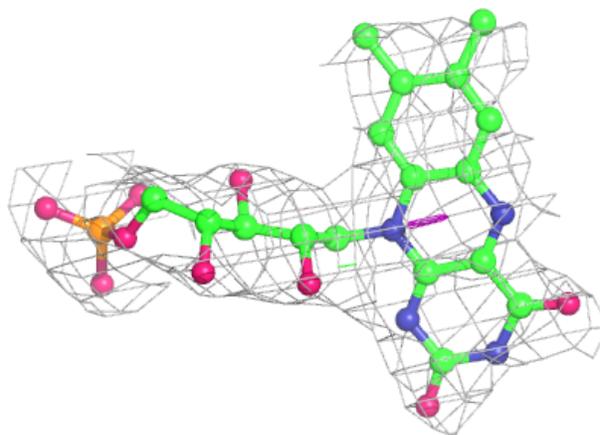
Electron density around FMN F 301:

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



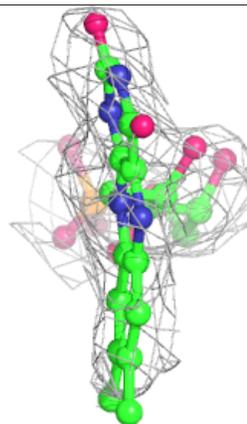
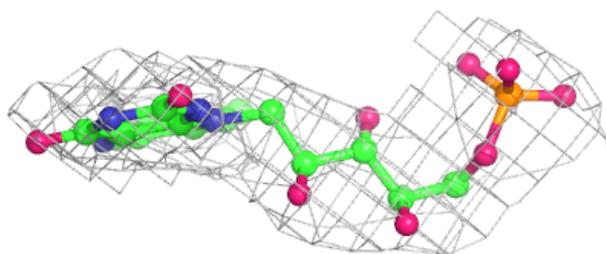
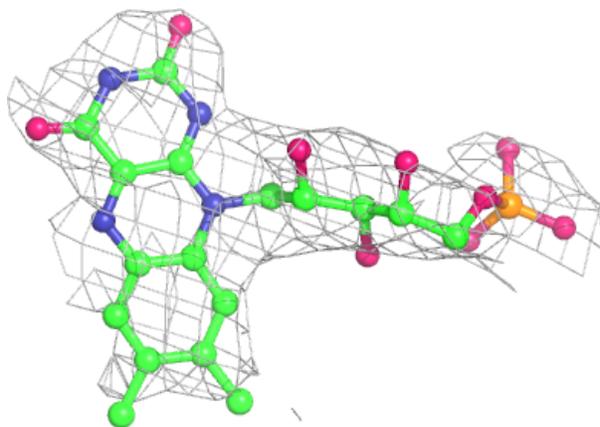
Electron density around FMN H 301:

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

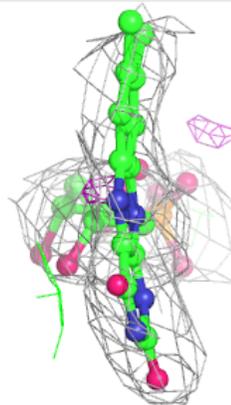
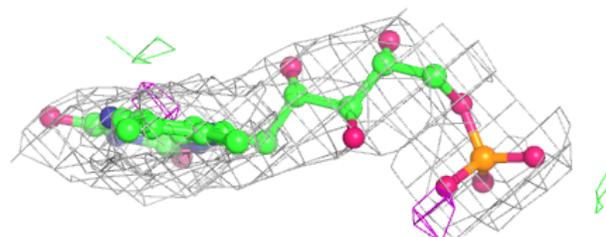
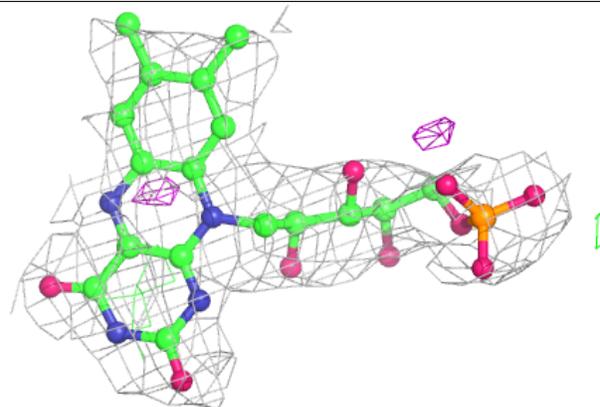


Electron density around FMN A 301:

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

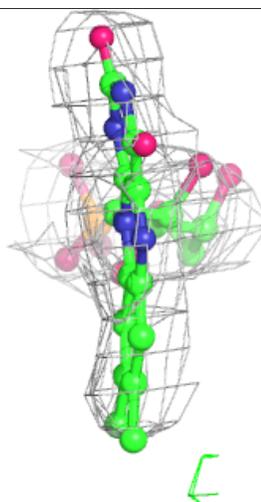
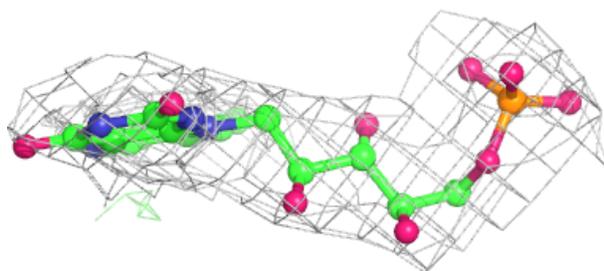
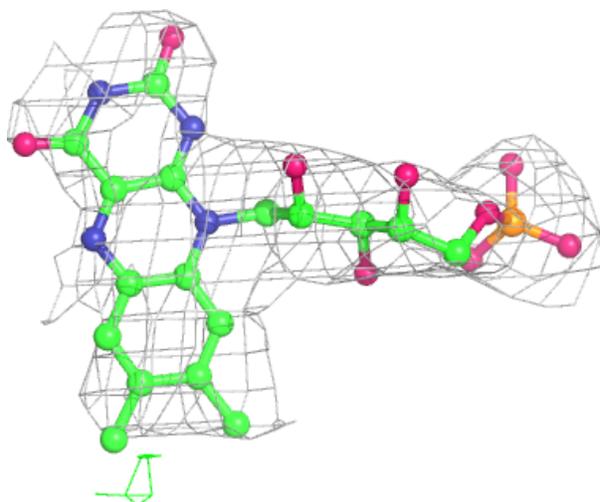
**Electron density around FMN C 301:**

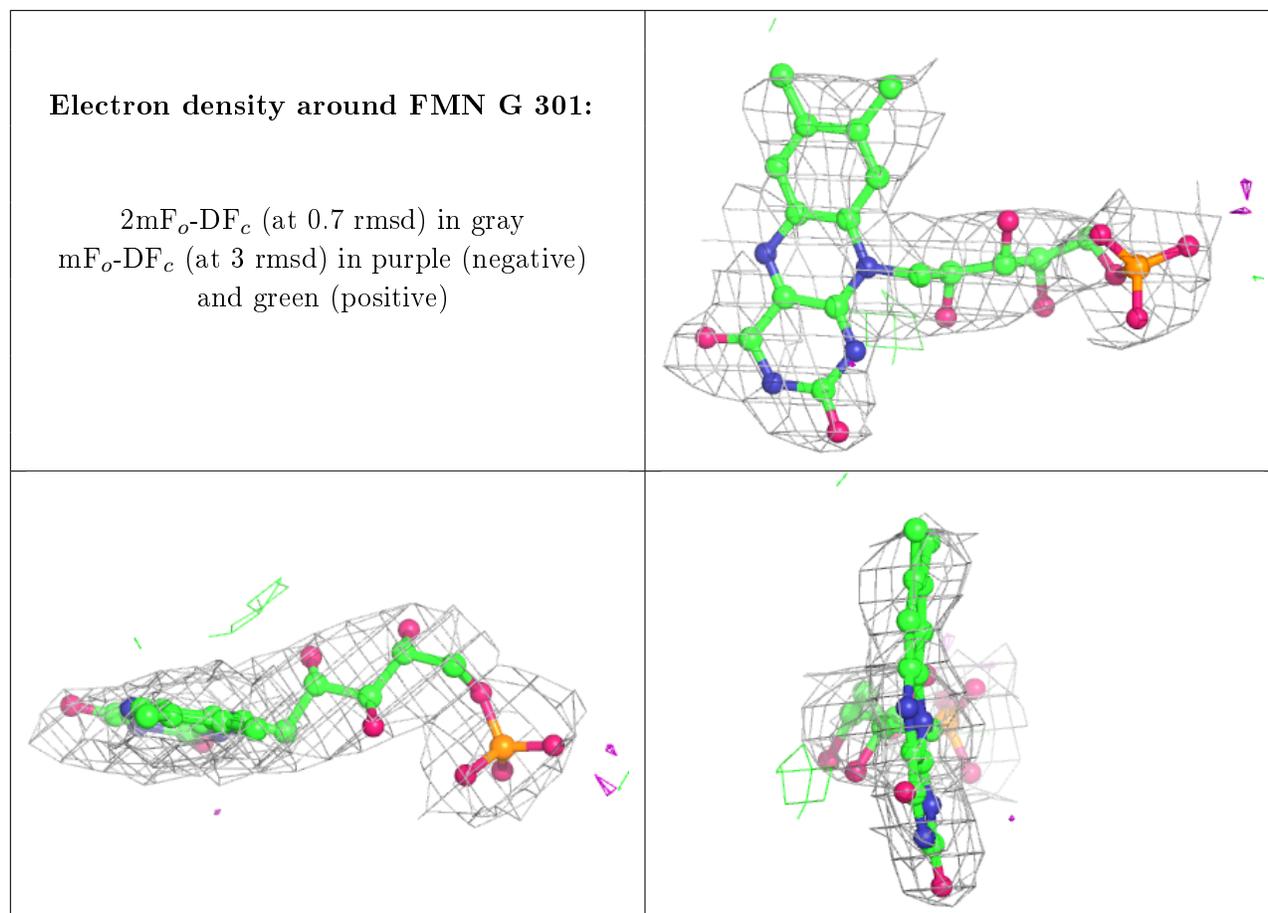
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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)





6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.