Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2025 – 10:13 AM JST

PDB ID	:	9VF7 / pdb_00009vf7
Title	:	Structure of Meiothermus ruber Mrub_1259 LOV domain with N- and C-terminal alpha helices (MrLOVe)
Authors	:	Semenov, O.; Nazarenko, V.; Yudenko, A.; Remeeva, A.; Borshchevskiy, V.; Yang, Y.; Gushchin, I.
Deposited on	:	2025-06-10
Resolution	:	2.40 Å(reported)

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

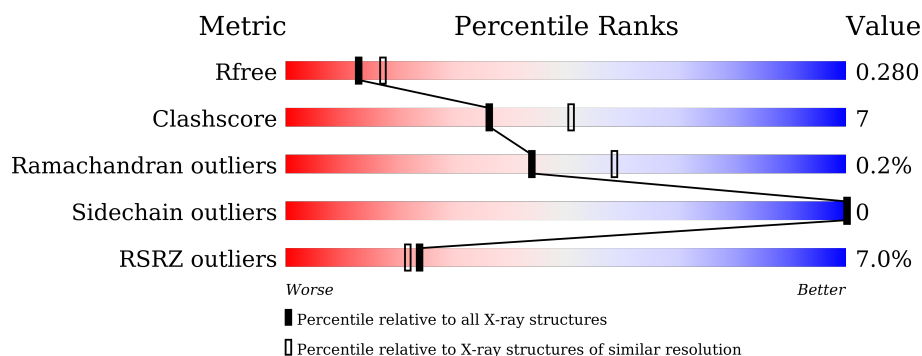|		
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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	Percentile Ranks	Value
Rfree		0.280
Clashscore		7
Ramachandran outliers		0.2%
Sidechain outliers		0
RSRZ outliers		7.0%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

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 <=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	148	5% — 71% / 24% / 5%
1	B	148	3% — 81% / 14% / 5%
1	C	148	14% — 80% / 12% / 7%
1	D	148	5% — 86% / 7% · 7%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4490 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 histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	3	0
			1104	709	191	201	3			
1	B	140	Total	C	N	O	S	0	2	0
			1077	689	190	195	3			
1	C	137	Total	C	N	O	S	0	2	0
			1042	672	180	186	4			
1	D	138	Total	C	N	O	S	0	4	0
			1094	700	198	193	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	HIS	-	expression tag	UNP D3PRD8
A	144	HIS	-	expression tag	UNP D3PRD8
A	145	HIS	-	expression tag	UNP D3PRD8
A	146	HIS	-	expression tag	UNP D3PRD8
A	147	HIS	-	expression tag	UNP D3PRD8
A	148	HIS	-	expression tag	UNP D3PRD8
B	143	HIS	-	expression tag	UNP D3PRD8
B	144	HIS	-	expression tag	UNP D3PRD8
B	145	HIS	-	expression tag	UNP D3PRD8
B	146	HIS	-	expression tag	UNP D3PRD8
B	147	HIS	-	expression tag	UNP D3PRD8
B	148	HIS	-	expression tag	UNP D3PRD8
C	143	HIS	-	expression tag	UNP D3PRD8
C	144	HIS	-	expression tag	UNP D3PRD8
C	145	HIS	-	expression tag	UNP D3PRD8
C	146	HIS	-	expression tag	UNP D3PRD8
C	147	HIS	-	expression tag	UNP D3PRD8
C	148	HIS	-	expression tag	UNP D3PRD8
D	143	HIS	-	expression tag	UNP D3PRD8
D	144	HIS	-	expression tag	UNP D3PRD8
D	145	HIS	-	expression tag	UNP D3PRD8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	146	HIS	-	expression tag	UNP D3PRD8
D	147	HIS	-	expression tag	UNP D3PRD8
D	148	HIS	-	expression tag	UNP D3PRD8

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).
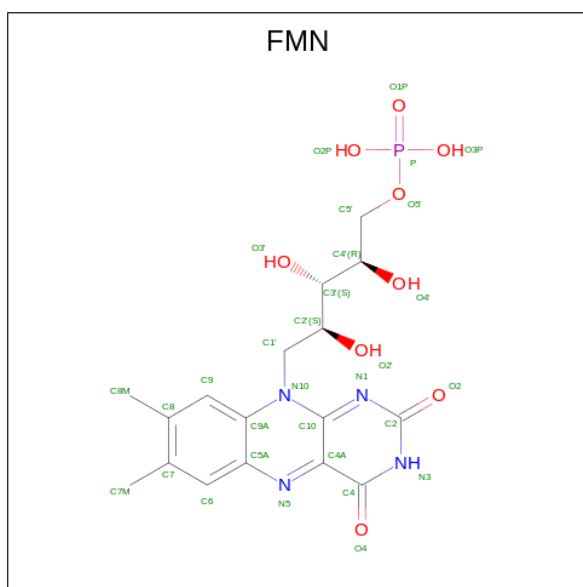
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	12	Total	O	0	0
			12	12		
3	C	9	Total	O	0	0
			9	9		

Continued on next page...

Continued from previous page...

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	10	Total 10	O 10	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.
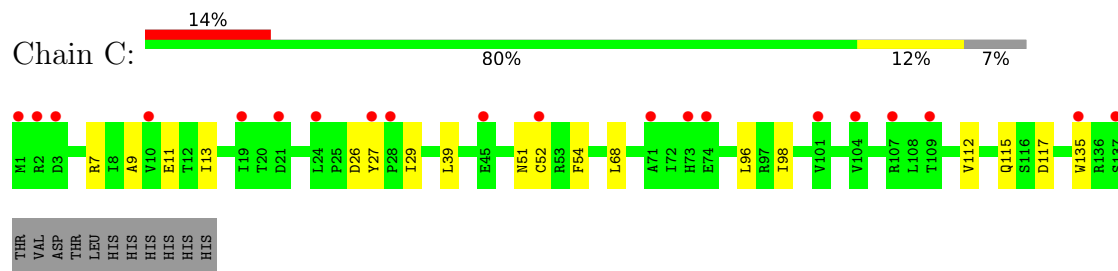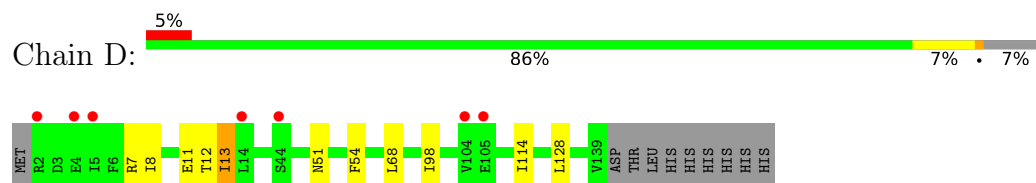
- Molecule 1: histidine kinase
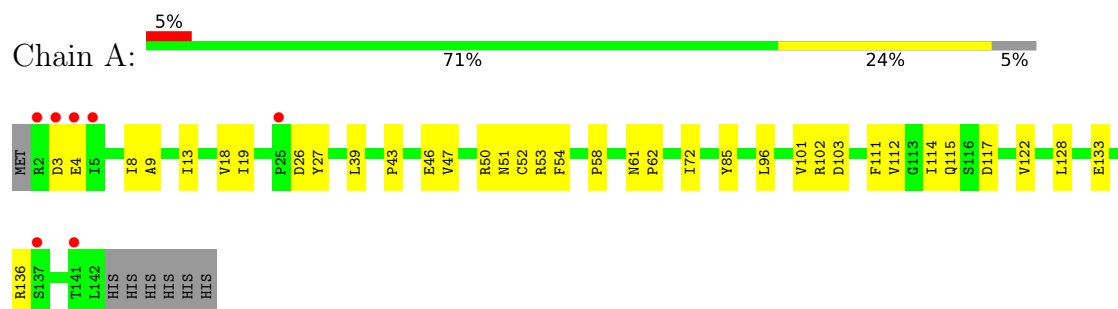
Chain A:

- Molecule 1: histidine kinase

Chain B:

- Molecule 1: histidine kinase

Chain C:

- Molecule 1: histidine kinase

Chain D:
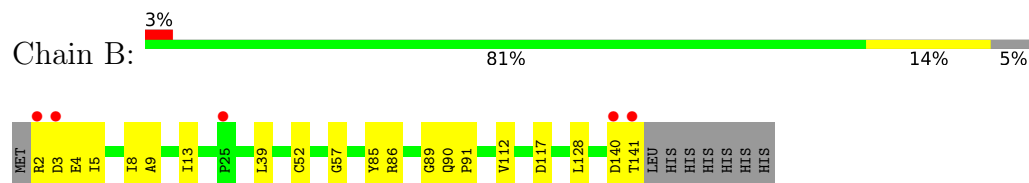
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.29Å 77.02Å 103.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.28 – 2.40 47.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.9 (47.28-2.40) 87.9 (47.28-2.40)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.230 , 0.279 0.233 , 0.280	Depositor DCC
R_{free} test set	1183 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4490	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.31 % 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 8.9302e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FMN

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	0.53	0/1137	0.95	0/1553
1	B	0.53	0/1100	0.93	0/1503
1	C	0.50	0/1071	0.92	0/1465
1	D	0.52	0/1130	0.99	0/1540
All	All	0.52	0/4438	0.95	0/6061

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	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.

WORLD WIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1104	0	1091	29	0
1	B	1077	0	1044	20	0
1	C	1042	0	1022	17	0
1	D	1094	0	1097	13	0
2	A	31	0	19	4	0
2	B	31	0	19	3	0
2	C	31	0	19	2	0
2	D	31	0	19	1	0
3	A	18	0	0	1	0
3	B	12	0	0	0	0
3	C	9	0	0	0	0
3	D	10	0	0	0	0
All	All	4490	0	4330	62	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 7.

All (62) 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:86:ARG:NH2	1:B:90:GLN:HG2	2.07	0.69
1:B:86:ARG:CZ	1:B:90:GLN:HG2	2.23	0.69
1:A:112:VAL:HG11	1:B:9:ALA:HA	1.75	0.69
1:B:52[B]:CYS:SG	2:B:201:FMN:C4A	2.84	0.65
1:B:140:ASP:O	1:B:141:THR:CB	2.43	0.65
1:C:29:ILE:HD11	1:C:52[A]:CYS:SG	2.36	0.65
1:C:39:LEU:CD1	1:C:117:ASP:HB2	2.31	0.60
1:B:4:GLU:O	1:B:8:ILE:HG12	2.03	0.57
1:C:13:ILE:CG1	1:D:114:ILE:HD13	2.36	0.55
1:A:114[B]:ILE:HD12	1:B:13[B]:ILE:HD11	1.90	0.53
1:A:128:LEU:CD2	1:D:128:LEU:HD22	2.40	0.52
1:C:52[B]:CYS:SG	2:C:201:FMN:C4A	2.99	0.51
1:A:19:ILE:HD13	1:B:5:ILE:HG22	1.92	0.51
1:C:13:ILE:HG12	1:D:114:ILE:HD13	1.92	0.51
1:A:114[B]:ILE:HD12	1:B:13[B]:ILE:CD1	2.41	0.50
1:A:101:VAL:HG22	1:B:8:ILE:HG21	1.94	0.49
1:A:9:ALA:O	1:A:13:ILE:HG13	2.12	0.49
1:A:52[B]:CYS:HG	2:A:201:FMN:C4A	2.26	0.48
1:A:103:ASP:HB2	3:A:305:HOH:O	2.13	0.48
1:A:128:LEU:HD22	1:D:128:LEU:HD22	1.95	0.48
1:B:57:GLY:HA3	1:B:85:TYR:CE1	2.47	0.48
1:C:96:LEU:HG	1:C:98[A]:ILE:CD1	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:HG23	1:A:111:PHE:CE2	2.49	0.48
1:A:4:GLU:O	1:A:8:ILE:HG13	2.14	0.47
1:D:68:LEU:HD11	1:D:98[A]:ILE:HD12	1.97	0.47
1:A:52[B]:CYS:SG	2:A:201:FMN:C4A	3.03	0.46
1:A:26:ASP:O	1:A:27:TYR:C	2.58	0.46
1:A:122:VAL:HG12	1:C:135:TRP:CZ3	2.50	0.46
1:C:96:LEU:CG	1:C:98[A]:ILE:HD11	2.46	0.46
1:D:7:ARG:O	1:D:11:GLU:HG2	2.16	0.46
1:A:3:ASP:CB	1:B:3:ASP:CB	2.93	0.46
1:A:9:ALA:HA	1:B:112:VAL:HG11	1.98	0.46
1:B:52[B]:CYS:SG	2:B:201:FMN:C4	3.04	0.46
1:B:52[B]:CYS:HG	2:B:201:FMN:C4A	2.28	0.45
1:D:12:THR:O	1:D:13:ILE:C	2.60	0.45
1:C:68:LEU:HD11	1:C:98[A]:ILE:HD13	1.98	0.44
1:A:133:GLU:HA	1:A:136:ARG:HG2	1.98	0.44
1:C:26:ASP:O	1:C:27:TYR:C	2.60	0.44
1:A:96:LEU:HD13	1:A:115:GLN:HG3	1.99	0.44
1:D:8:ILE:O	1:D:12:THR:HG23	2.18	0.43
1:B:89:GLY:O	1:B:91:PRO:HD3	2.18	0.43
1:B:2:ARG:HD2	1:B:5:ILE:HD12	2.01	0.42
1:C:13:ILE:HG13	1:D:114:ILE:HD13	2.01	0.42
1:C:96:LEU:HD13	1:C:115:GLN:HG3	2.02	0.42
1:A:53:ARG:NE	2:A:201:FMN:O1P	2.53	0.42
1:A:51:ASN:O	1:A:54:PHE:HD2	2.01	0.42
1:A:43:PRO:O	1:A:47:VAL:HG23	2.20	0.42
1:A:128:LEU:HD21	1:B:128:LEU:HD11	2.02	0.42
1:C:51:ASN:O	1:C:54:PHE:HD2	2.02	0.42
1:B:39:LEU:CD1	1:B:117:ASP:HB2	2.50	0.42
1:C:9:ALA:O	1:D:114:ILE:HD11	2.20	0.41
1:C:7:ARG:O	1:C:11:GLU:HG3	2.20	0.41
1:A:128:LEU:HD21	1:B:128:LEU:CD1	2.50	0.41
1:D:51:ASN:O	1:D:54:PHE:HD2	2.03	0.41
1:A:61:ASN:HA	1:A:62:PRO:HD3	1.97	0.41
1:C:52[B]:CYS:HG	2:C:201:FMN:C4A	2.33	0.41
1:A:46:GLU:O	1:A:50:ARG:HD3	2.20	0.41
1:A:58:PRO:HD2	1:A:85:TYR:CZ	2.56	0.41
1:C:112:VAL:HG11	1:D:12:THR:OG1	2.21	0.41
1:D:98[A]:ILE:HD13	2:D:201:FMN:C8	2.50	0.40
1:A:39:LEU:CD1	1:A:117:ASP:HB2	2.50	0.40
1:A:18:VAL:HG23	2:A:201:FMN:HM71	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	142/148 (96%)	141 (99%)	1 (1%)	0	100	100
1	B	139/148 (94%)	136 (98%)	3 (2%)	0	100	100
1	C	137/148 (93%)	131 (96%)	6 (4%)	0	100	100
1	D	140/148 (95%)	138 (99%)	1 (1%)	1 (1%)	19	29
All	All	558/592 (94%)	546 (98%)	11 (2%)	1 (0%)	44	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	13	ILE

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	115/128 (90%)	115 (100%)	0	100	100
1	B	109/128 (85%)	109 (100%)	0	100	100
1	C	105/128 (82%)	105 (100%)	0	100	100
1	D	115/128 (90%)	115 (100%)	0	100	100
All	All	444/512 (87%)	444 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	94	ASN
1	C	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\#|Z| > 2$
2	FMN	A	201	-	33,33,33	0.62	0	48,50,50	0.76	1 (2%)
2	FMN	B	201	-	33,33,33	0.63	0	48,50,50	0.84	2 (4%)
2	FMN	D	201	-	33,33,33	0.60	0	48,50,50	0.81	1 (2%)
2	FMN	C	201	-	33,33,33	0.63	0	48,50,50	0.78	1 (2%)

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	A	201	-	-	5/18/18/18	0/3/3/3
2	FMN	B	201	-	-	3/18/18/18	0/3/3/3
2	FMN	D	201	-	-	3/18/18/18	0/3/3/3
2	FMN	C	201	-	-	3/18/18/18	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	FMN	C4'-C3'-C2'	2.20	117.94	113.36
2	C	201	FMN	C4-N3-C2	-2.13	121.72	125.64
2	A	201	FMN	C4-N3-C2	-2.11	121.74	125.64
2	B	201	FMN	C4-N3-C2	-2.09	121.79	125.64
2	D	201	FMN	C4-N3-C2	-2.05	121.86	125.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	FMN	C3'-C4'-C5'-O5'
2	A	201	FMN	O4'-C4'-C5'-O5'
2	A	201	FMN	C5'-O5'-P-O1P
2	A	201	FMN	C5'-O5'-P-O2P
2	A	201	FMN	C5'-O5'-P-O3P
2	B	201	FMN	C3'-C4'-C5'-O5'
2	B	201	FMN	O4'-C4'-C5'-O5'
2	C	201	FMN	C3'-C4'-C5'-O5'
2	C	201	FMN	O4'-C4'-C5'-O5'
2	D	201	FMN	C3'-C4'-C5'-O5'
2	D	201	FMN	O4'-C4'-C5'-O5'
2	C	201	FMN	C4'-C5'-O5'-P
2	B	201	FMN	C4'-C5'-O5'-P
2	D	201	FMN	C4'-C5'-O5'-P

There are no ring outliers.
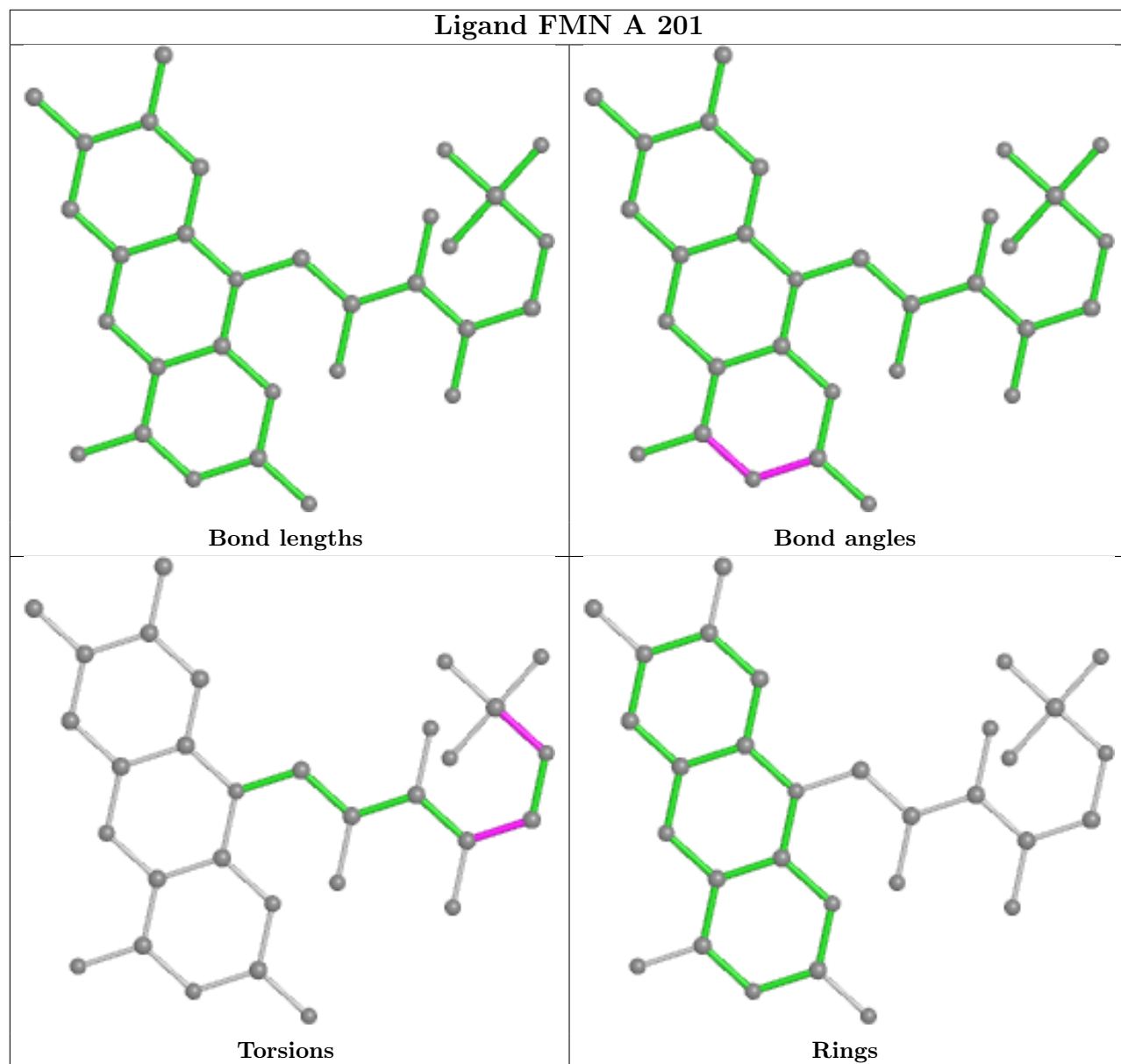
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	FMN	4	0
2	B	201	FMN	3	0
2	D	201	FMN	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	FMN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 A 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN C 201

Bond lengths

Bond angles

Torsions

Rings
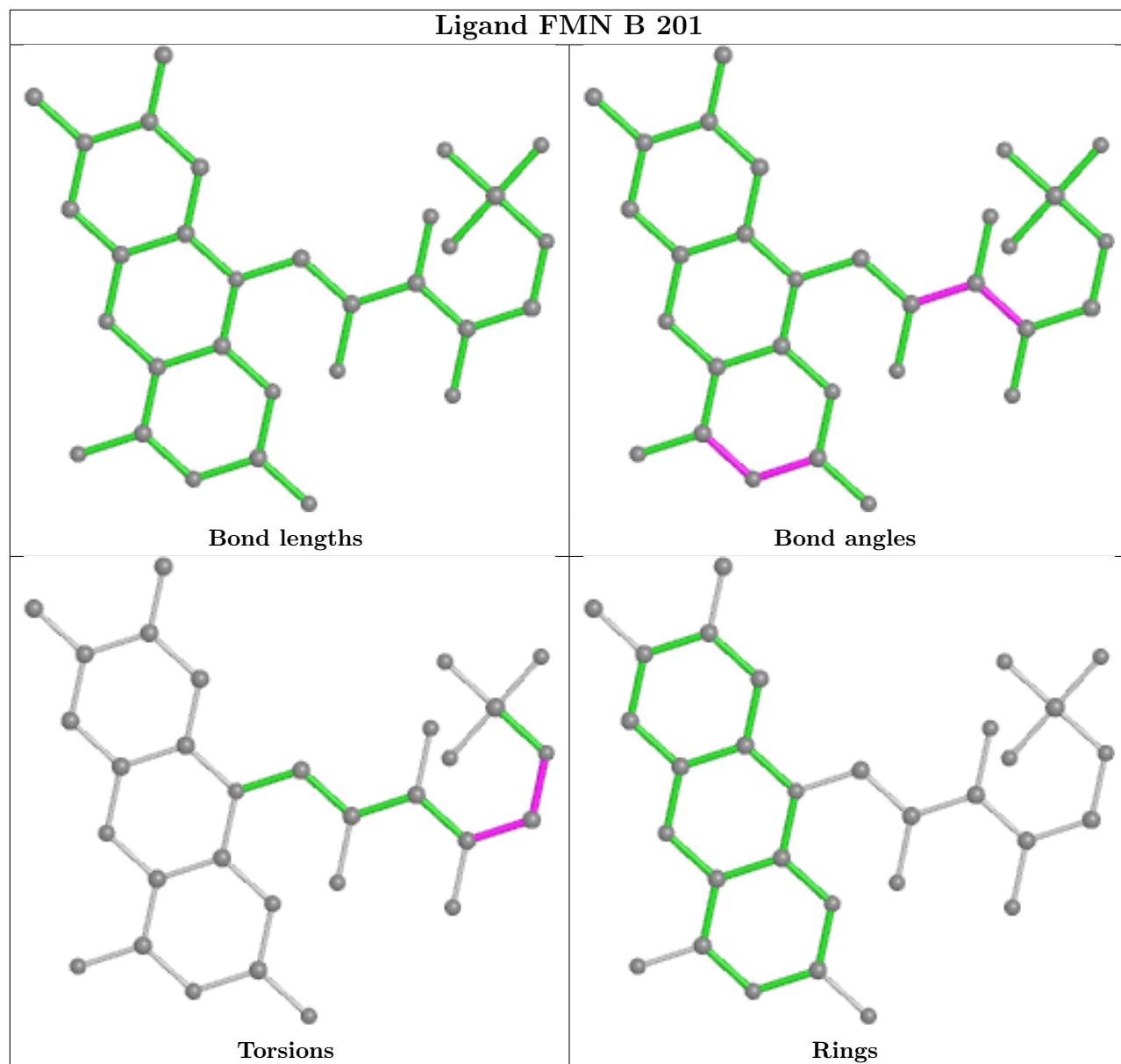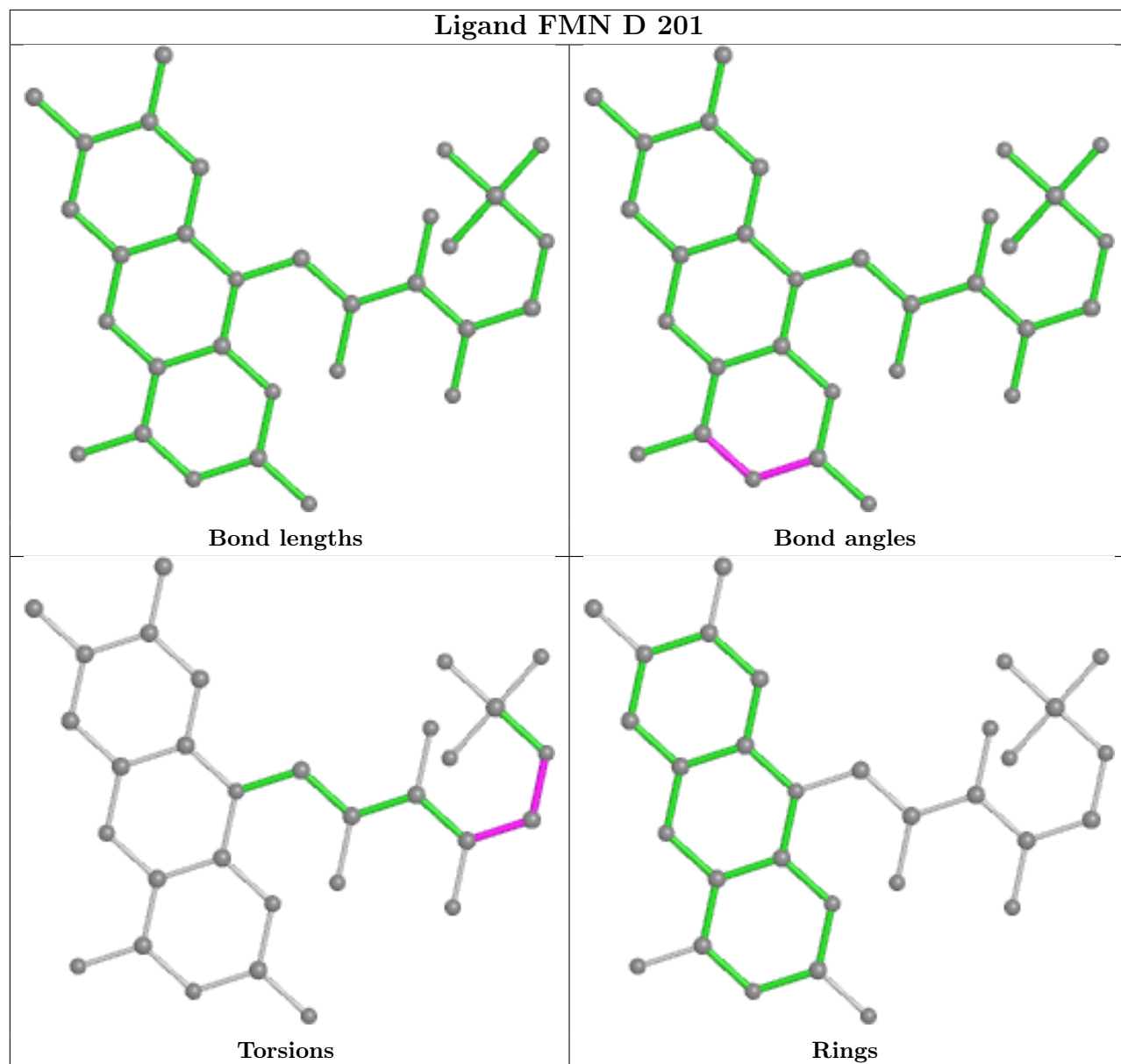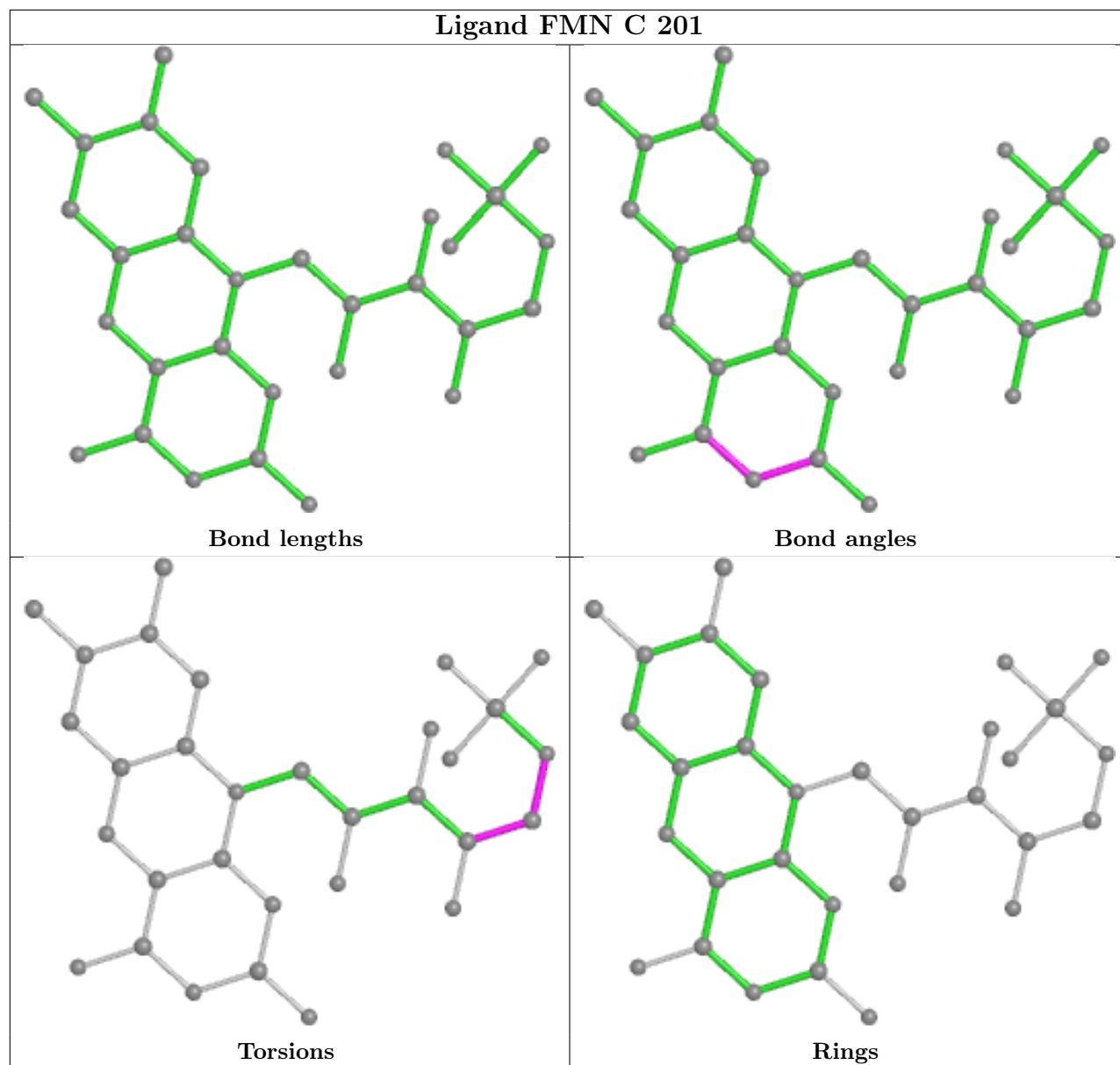
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	141/148 (95%)	-0.02	7 (4%)	35	32	11, 23, 48, 69	3 (2%)
1	B	140/148 (94%)	-0.10	5 (3%)	46	43	14, 22, 41, 61	1 (0%)
1	C	137/148 (92%)	0.74	20 (14%)	7	6	17, 36, 63, 83	2 (1%)
1	D	138/148 (93%)	0.23	7 (5%)	34	32	16, 28, 53, 72	4 (2%)
All	All	556/592 (93%)	0.21	39 (7%)	24	22	11, 27, 59, 83	10 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ARG	4.5
1	C	2	ARG	4.4
1	C	1	MET	4.1
1	D	105	GLU	3.9
1	D	5	ILE	3.9
1	D	104	VAL	3.4
1	B	141	THR	3.4
1	B	3	ASP	3.3
1	A	3	ASP	3.1
1	A	5	ILE	3.1
1	C	137	SER	3.0
1	C	135	TRP	2.9
1	C	27	TYR	2.9
1	C	73	HIS	2.9
1	A	4	GLU	2.8
1	C	104	VAL	2.8
1	C	74	GLU	2.6
1	C	71	ALA	2.6
1	A	25	PRO	2.6
1	C	19	ILE	2.5
1	B	2	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	109	THR	2.5
1	D	2	ARG	2.4
1	B	140	ASP	2.4
1	D	14	LEU	2.4
1	C	52[A]	CYS	2.4
1	D	4	GLU	2.4
1	C	3	ASP	2.3
1	C	24	LEU	2.3
1	C	107	ARG	2.3
1	D	44	SER	2.3
1	A	141	THR	2.2
1	B	25	PRO	2.2
1	C	21	ASP	2.1
1	A	137	SER	2.1
1	C	45	GLU	2.1
1	C	10	VAL	2.0
1	C	101	VAL	2.0
1	C	28	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

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
2	FMN	C	201	31/31	0.83	0.14	29,43,53,55	4
2	FMN	A	201	31/31	0.84	0.12	25,28,36,38	4
2	FMN	D	201	31/31	0.86	0.10	21,31,33,34	4
2	FMN	B	201	31/31	0.89	0.10	21,27,32,34	4

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.
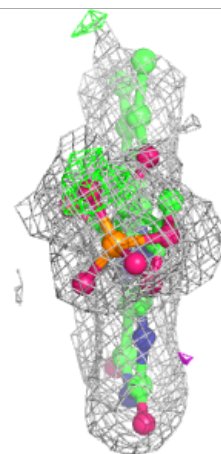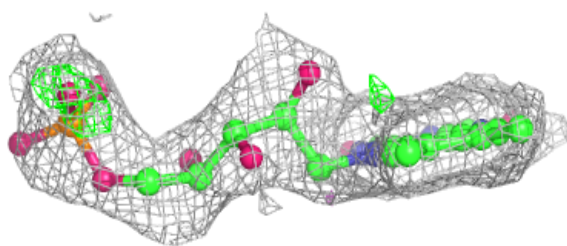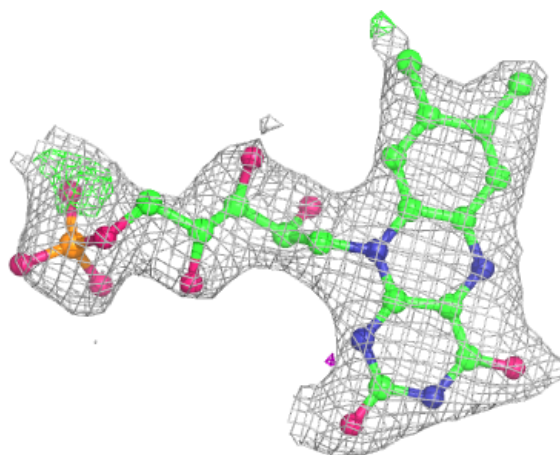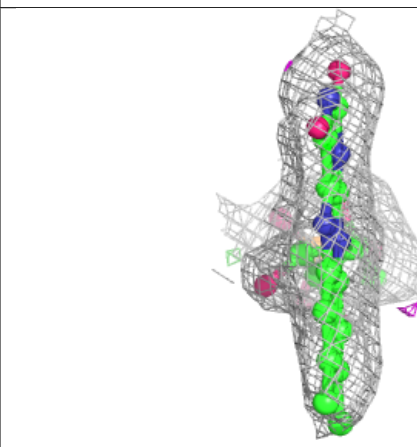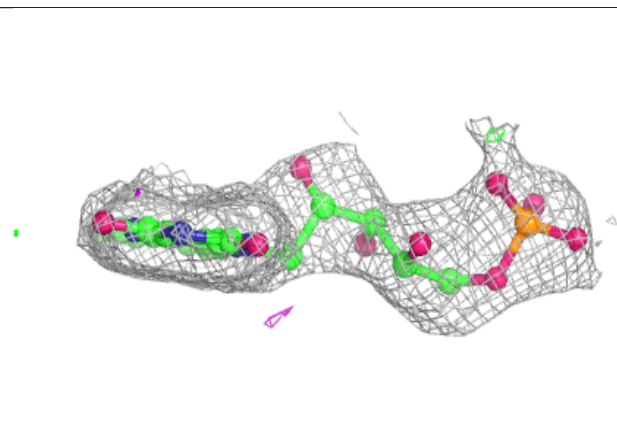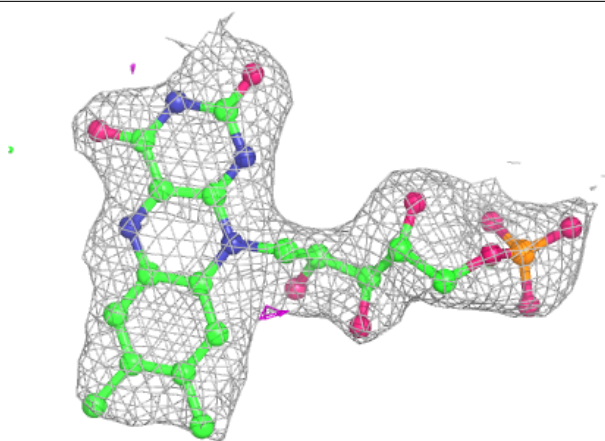

Electron density around FMN C 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
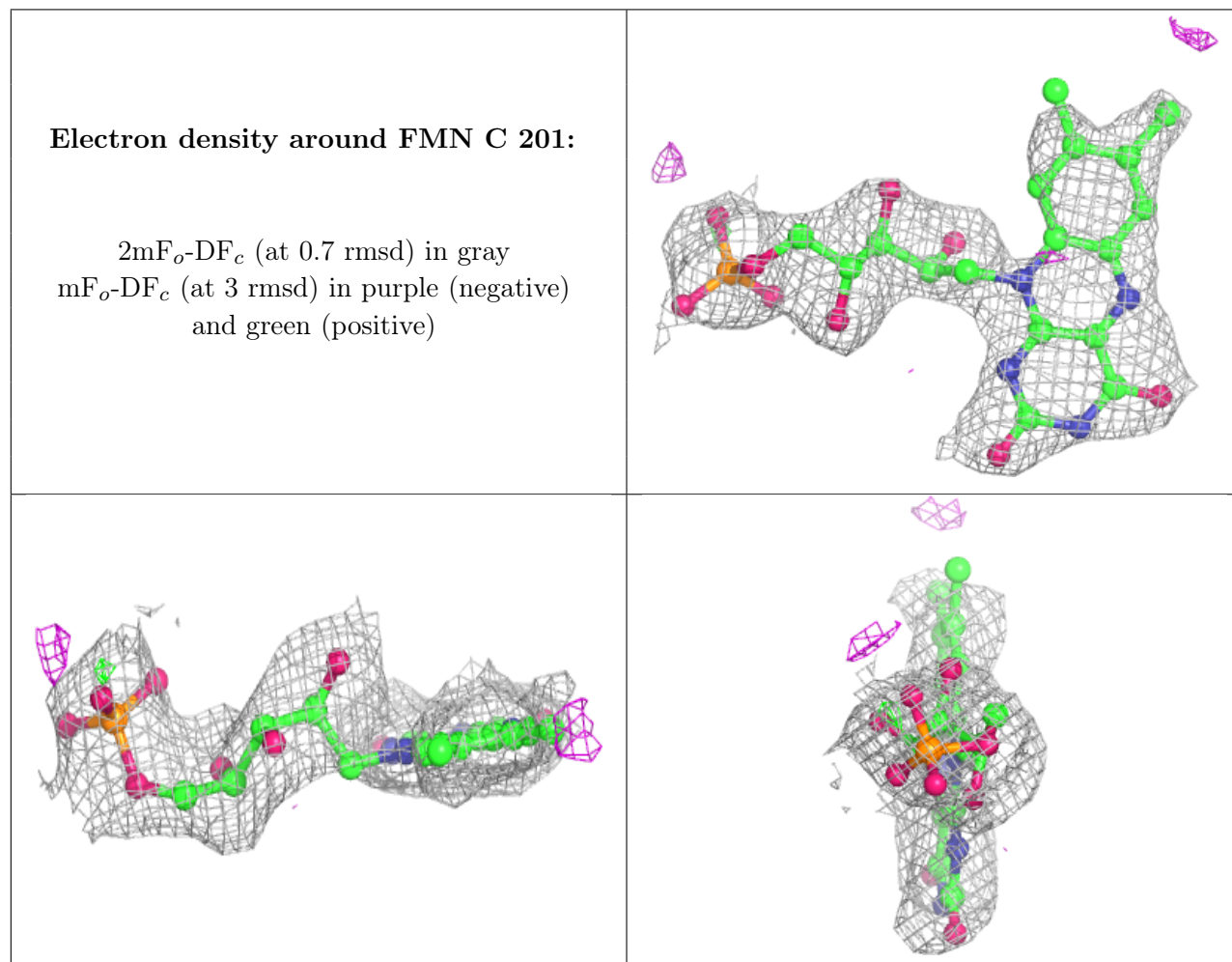
Electron density around FMN A 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
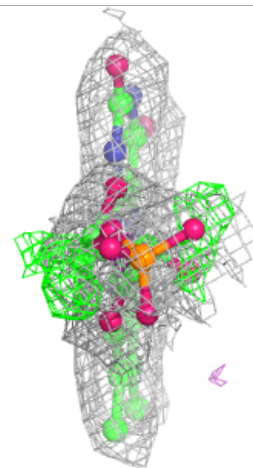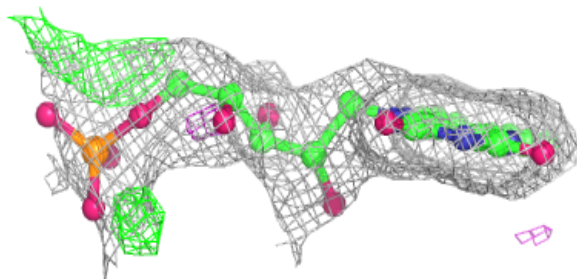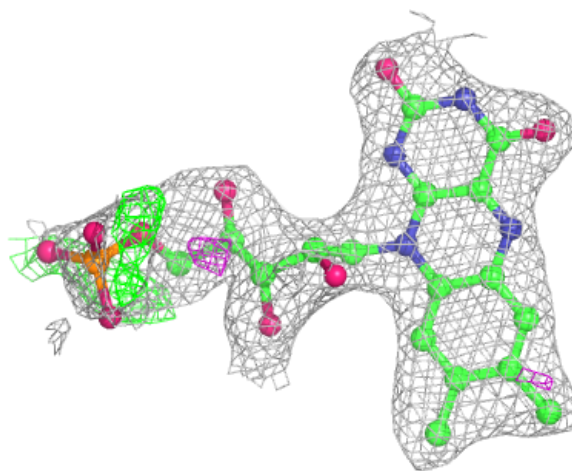
Electron density around FMN D 201:

$2mF_o$-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 201:

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.