Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 10:05 PM JST

PDB ID	:	7X32
Title	:	Crystal structure of E. coli NfsB in complex with berberine
Authors	:	Zhang, H.; Wen, H.Y.
Deposited on	:	2022-02-27
Resolution	:	1.83 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

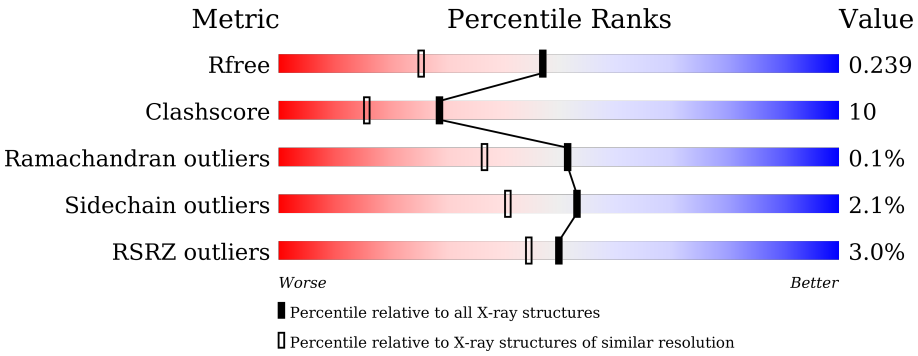
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.83 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	217	2% 91% 8%
1	B	217	3% 91% 8%
1	C	217	3% 88% 12%
1	D	217	4% 89% 10%
1	E	217	% 88% 11%
1	F	217	6% 88% 12%

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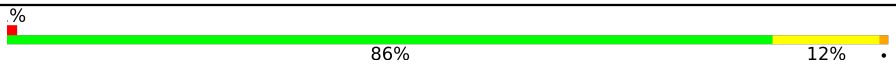
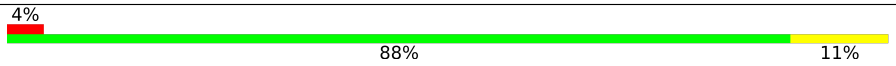
Mol	Chain	Length	Quality of chain
1	G	217	
1	H	217	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	C	301	-	-	X	-
2	FMN	F	301	-	X	X	-
5	BER	C	302	-	-	X	-
5	BER	D	302	-	-	X	-
5	BER	E	302	-	-	X	-
5	BER	G	302	-	-	X	-
5	BER	H	302	-	X	X	-

2 Entry composition (i)

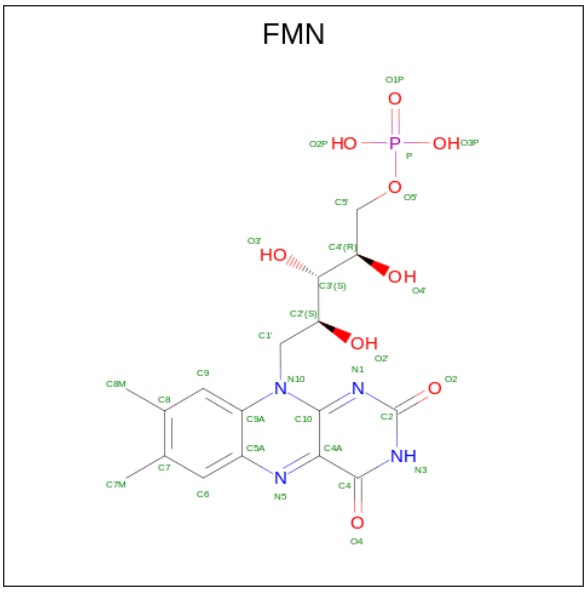
There are 6 unique types of molecules in this entry. The entry contains 14816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydropteridine reductase.

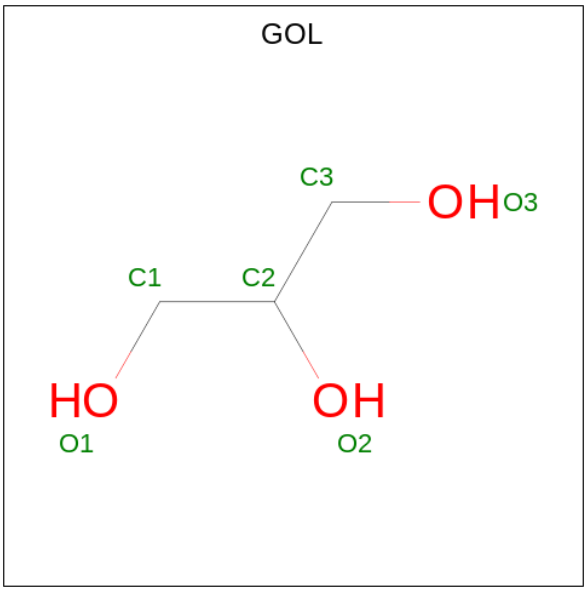
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1677	1065	287	320	5			
1	B	216	Total	C	N	O	S	0	0	0
			1677	1065	287	320	5			
1	C	216	Total	C	N	O	S	0	0	0
			1676	1065	286	320	5			
1	D	216	Total	C	N	O	S	0	0	0
			1677	1065	287	320	5			
1	E	217	Total	C	N	O	S	0	0	0
			1685	1070	288	321	6			
1	F	216	Total	C	N	O	S	0	0	0
			1677	1065	287	320	5			
1	G	217	Total	C	N	O	S	0	0	0
			1685	1070	288	321	6			
1	H	216	Total	C	N	O	S	0	0	0
			1677	1065	287	320	5			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



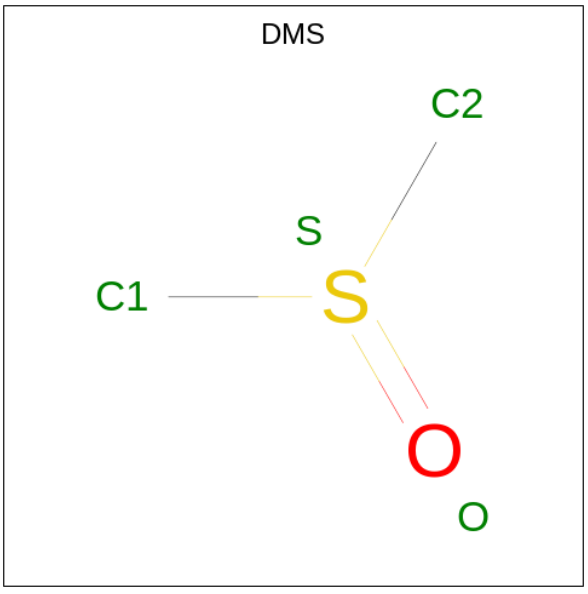
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



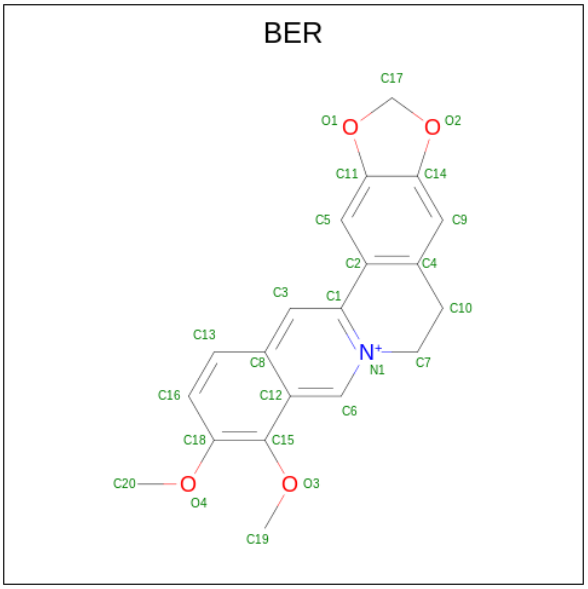
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	E	1	Total C O S 4 2 1 1	0	0
4	G	1	Total C O S 4 2 1 1	0	0
4	H	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is BERBERINE (three-letter code: BER) (formula: $C_{20}H_{18}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 25 20 1 4	0	0
5	D	1	Total C N O 25 20 1 4	0	0
5	E	1	Total C N O 25 20 1 4	0	0
5	G	1	Total C N O 25 20 1 4	0	0
5	H	1	Total C N O 25 20 1 4	0	0

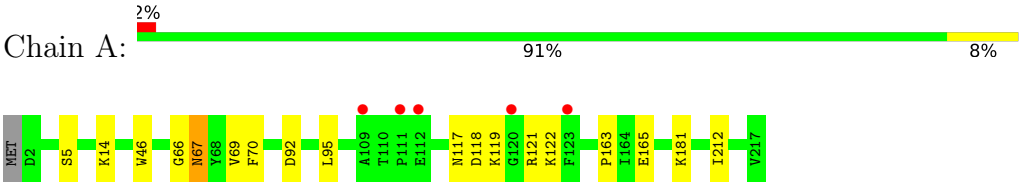
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	130	Total O 130 130	0	0
6	B	128	Total O 128 128	0	0
6	C	112	Total O 112 112	0	0
6	D	109	Total O 109 109	0	0
6	E	128	Total O 128 128	0	0
6	F	147	Total O 147 147	0	0
6	G	104	Total O 104 104	0	0
6	H	112	Total O 112 112	0	0

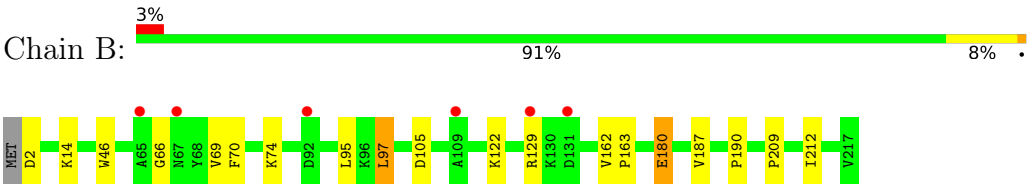
3 Residue-property plots (i)

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

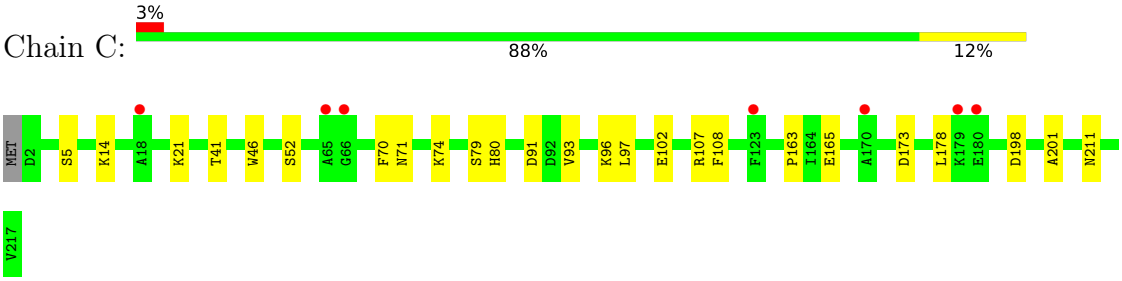
• Molecule 1: Dihydropteridine reductase



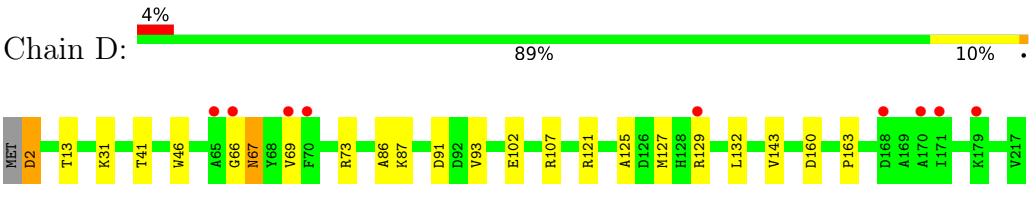
• Molecule 1: Dihydropteridine reductase



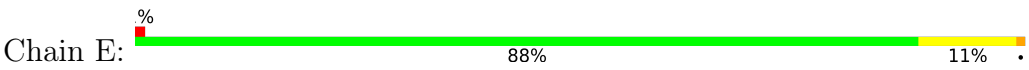
• Molecule 1: Dihydropteridine reductase

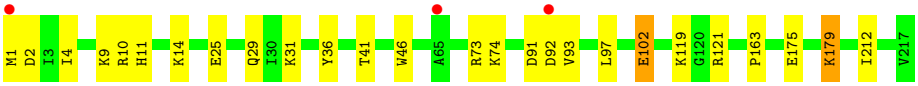


• Molecule 1: Dihydropteridine reductase

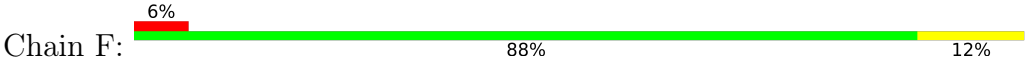


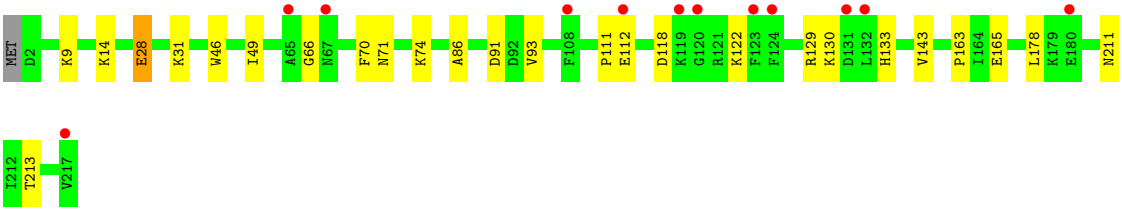
• Molecule 1: Dihydropteridine reductase



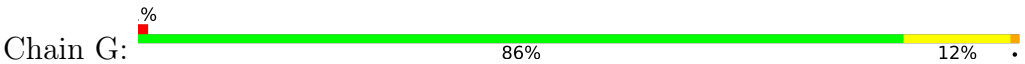


• Molecule 1: Dihydropteridine reductase

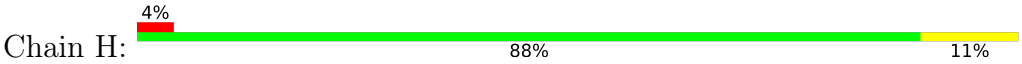




• Molecule 1: Dihydropteridine reductase



• Molecule 1: Dihydropteridine reductase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.47Å 77.94Å 116.13Å 74.05° 79.44° 74.26°	Depositor
Resolution (Å)	54.93 – 1.83 54.93 – 1.83	Depositor EDS
% Data completeness (in resolution range)	92.5 (54.93-1.83) 92.5 (54.93-1.83)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.205 , 0.241 0.205 , 0.239	Depositor DCC
R_{free} test set	7589 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14816	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GOL, FMN, DMS, BER

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	0.71	0/1712	0.75	0/2318
1	B	0.68	0/1712	0.77	1/2318 (0.0%)
1	C	0.65	0/1711	0.71	0/2316
1	D	0.65	0/1712	0.72	0/2318
1	E	0.71	0/1720	0.75	0/2328
1	F	0.71	0/1712	0.78	0/2318
1	G	0.71	0/1720	0.75	0/2328
1	H	0.70	0/1712	0.77	0/2318
All	All	0.69	0/13711	0.75	1/18562 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	97	LEU	CA-CB-CG	5.68	128.36	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1677	0	1661	15	0
1	B	1677	0	1661	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1676	0	1660	37	0
1	D	1677	0	1661	28	0
1	E	1685	0	1673	32	0
1	F	1677	0	1661	28	0
1	G	1685	0	1673	50	0
1	H	1677	0	1661	31	0
2	A	31	0	19	6	0
2	B	31	0	19	6	0
2	C	31	0	19	21	0
2	D	31	0	19	1	0
2	E	31	0	19	6	0
2	F	31	0	19	20	0
2	G	31	0	19	6	0
2	H	31	0	18	2	0
3	A	6	0	8	0	0
3	D	6	0	8	0	0
3	H	6	0	8	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
4	E	4	0	6	3	0
4	G	4	0	6	1	0
4	H	4	0	6	2	0
5	C	25	0	18	14	0
5	D	25	0	18	26	0
5	E	25	0	18	22	0
5	G	25	0	18	35	0
5	H	25	0	18	22	0
6	A	130	0	0	2	0
6	B	128	0	0	4	0
6	C	112	0	0	3	0
6	D	109	0	0	6	0
6	E	128	0	0	4	0
6	F	147	0	0	2	0
6	G	104	0	0	6	0
6	H	112	0	0	3	0
All	All	14816	0	13612	266	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.

All (266) 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)
2:E:301:FMN:O2'	5:G:302:BER:H101	1.41	1.16
1:D:102:GLU:OE2	5:D:302:BER:H161	1.48	1.13
1:C:14:LYS:NZ	2:C:301:FMN:HM81	1.64	1.12
1:G:41:THR:HA	5:G:302:BER:H71	1.24	1.12
1:C:14:LYS:HZ3	2:C:301:FMN:HM81	1.07	1.11
1:F:71:ASN:OD1	2:F:301:FMN:HM73	1.52	1.10
1:H:41:THR:HA	5:H:302:BER:H131	1.39	1.05
1:C:102:GLU:OE2	5:C:302:BER:H161	1.56	1.04
1:G:41:THR:HA	5:G:302:BER:C7	1.90	1.01
1:B:70:PHE:CE2	5:H:302:BER:H102	1.95	1.01
1:D:41:THR:HA	5:D:302:BER:H31	1.43	1.00
1:H:41:THR:HA	5:H:302:BER:C13	1.98	0.94
1:B:70:PHE:CZ	5:H:302:BER:H102	2.02	0.94
1:E:29:GLN:HE21	1:G:1:MET:HG2	1.34	0.92
1:G:102:GLU:OE2	5:G:302:BER:H191	1.70	0.91
1:H:41:THR:CA	5:H:302:BER:H131	2.01	0.90
1:G:107:ARG:HH21	5:G:302:BER:C18	1.84	0.89
5:E:302:BER:H71	2:G:301:FMN:C2	2.03	0.88
1:F:74:LYS:HZ3	2:F:301:FMN:HM83	1.37	0.88
1:C:91:ASP:OD2	1:C:93:VAL:HG22	1.74	0.86
2:E:301:FMN:C2'	5:G:302:BER:H101	2.06	0.85
1:C:71:ASN:ND2	2:C:301:FMN:HM73	1.92	0.84
1:G:117:ASN:HD21	5:G:302:BER:H193	1.40	0.84
1:C:71:ASN:HD21	2:C:301:FMN:HM73	1.43	0.84
1:G:41:THR:N	5:G:302:BER:H102	1.95	0.82
1:G:41:THR:H	5:G:302:BER:H102	1.44	0.81
1:C:102:GLU:CD	5:C:302:BER:H161	2.00	0.81
5:E:302:BER:H71	2:G:301:FMN:O2	1.81	0.81
5:G:302:BER:C6	5:G:302:BER:H192	2.12	0.79
5:D:302:BER:H61	5:D:302:BER:H192	1.66	0.78
1:F:74:LYS:NZ	2:F:301:FMN:HM83	1.98	0.78
5:D:302:BER:H71	2:F:301:FMN:C8M	2.13	0.78
1:E:41:THR:HA	5:E:302:BER:H131	1.64	0.78
5:E:302:BER:H102	1:G:70:PHE:CE2	2.19	0.78
5:E:302:BER:H91	1:G:70:PHE:CZ	2.19	0.77
5:E:302:BER:H102	1:G:70:PHE:HE2	1.49	0.77
5:E:302:BER:H51	6:G:439:HOH:O	1.86	0.76
1:G:1:MET:HB3	1:G:4:ILE:HB	1.68	0.75
1:C:70:PHE:CE2	2:C:301:FMN:HM71	2.21	0.75
1:G:102:GLU:CD	5:G:302:BER:H191	2.07	0.75
1:F:70:PHE:HE2	2:F:301:FMN:HM72	1.51	0.74
5:G:302:BER:H192	5:G:302:BER:H61	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:302:BER:H172	6:H:401:HOH:O	1.86	0.74
1:C:71:ASN:OD1	2:C:301:FMN:HM73	1.89	0.73
1:C:71:ASN:HD21	2:C:301:FMN:C7M	2.02	0.72
1:F:71:ASN:CG	2:F:301:FMN:HM73	2.10	0.72
1:D:102:GLU:CD	5:D:302:BER:H161	2.10	0.72
5:E:302:BER:C5	6:G:439:HOH:O	2.38	0.72
1:G:41:THR:CA	5:G:302:BER:H71	2.14	0.71
1:G:107:ARG:NH2	5:G:302:BER:O4	2.24	0.71
1:F:14:LYS:HZ3	2:F:301:FMN:HM81	1.56	0.70
1:H:128:HIS:NE2	6:H:401:HOH:O	2.23	0.70
1:G:107:ARG:HB3	5:G:302:BER:H201	1.72	0.70
5:E:302:BER:C3	6:G:439:HOH:O	2.39	0.69
1:C:71:ASN:CG	2:C:301:FMN:HM73	2.11	0.69
2:E:301:FMN:O2'	5:G:302:BER:C10	2.33	0.69
1:E:29:GLN:NE2	1:G:1:MET:HG2	2.05	0.69
1:D:102:GLU:OE2	5:D:302:BER:C16	2.33	0.69
1:F:91:ASP:OD2	1:F:93:VAL:HB	1.93	0.68
1:C:70:PHE:CE2	2:C:301:FMN:C7M	2.78	0.67
6:D:409:HOH:O	1:G:119:LYS:HE3	1.95	0.67
5:E:302:BER:H91	1:G:70:PHE:HZ	1.59	0.67
1:F:71:ASN:OD1	2:F:301:FMN:C7M	2.38	0.67
1:C:74:LYS:HZ3	2:C:301:FMN:HM83	1.59	0.66
1:G:117:ASN:ND2	5:G:302:BER:H193	2.09	0.66
2:B:301:FMN:O2'	5:H:302:BER:C13	2.44	0.65
1:C:71:ASN:OD1	2:C:301:FMN:C7M	2.44	0.65
1:G:41:THR:H	5:G:302:BER:H91	1.61	0.65
1:E:41:THR:HA	5:E:302:BER:H31	1.77	0.65
1:G:41:THR:HA	5:G:302:BER:C10	2.25	0.65
1:D:41:THR:H	5:D:302:BER:H51	1.63	0.64
1:F:129:ARG:HH21	1:F:130:LYS:HG3	1.62	0.64
1:F:111:PRO:HG2	1:F:112:GLU:OE2	1.97	0.64
1:G:118:ASP:O	1:G:122:LYS:HG2	1.98	0.64
1:G:41:THR:CA	5:G:302:BER:C7	2.71	0.63
1:E:41:THR:CA	5:E:302:BER:H131	2.28	0.63
1:C:178:LEU:N	6:C:402:HOH:O	2.32	0.62
5:D:302:BER:H71	2:F:301:FMN:HM82	1.80	0.62
1:E:11:HIS:H	4:E:303:DMS:H13	1.65	0.62
1:F:70:PHE:CE2	2:F:301:FMN:HM72	2.34	0.62
1:A:163:PRO:HG2	2:A:301:FMN:C9	2.30	0.62
1:F:129:ARG:NH2	1:F:130:LYS:HG3	2.15	0.61
1:B:14:LYS:HE3	5:H:302:BER:H192	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:ASP:HA	1:H:95:LEU:HD12	1.83	0.60
1:F:14:LYS:NZ	2:F:301:FMN:HM81	2.15	0.60
1:A:117:ASN:ND2	6:A:404:HOH:O	2.35	0.59
1:G:102:GLU:OE1	5:G:302:BER:H191	2.00	0.59
1:E:11:HIS:H	4:E:303:DMS:C1	2.14	0.59
1:E:121:ARG:HH21	5:E:302:BER:H161	1.67	0.59
1:F:9:LYS:HE3	6:F:532:HOH:O	2.01	0.59
1:C:70:PHE:CZ	2:C:301:FMN:HM72	2.38	0.58
1:E:163:PRO:HG2	2:E:301:FMN:C9	2.33	0.58
1:C:96:LYS:NZ	6:C:405:HOH:O	2.37	0.58
1:G:14:LYS:NZ	2:G:301:FMN:O2	2.36	0.58
1:B:14:LYS:NZ	2:B:301:FMN:O2	2.35	0.57
1:A:14:LYS:NZ	2:A:301:FMN:O2	2.37	0.57
1:D:41:THR:HA	5:D:302:BER:H51	1.86	0.57
1:H:41:THR:H	5:H:302:BER:H31	1.69	0.57
1:A:92:ASP:HA	1:A:95:LEU:HD23	1.87	0.57
1:D:87:LYS:NZ	6:D:402:HOH:O	2.32	0.57
1:G:41:THR:H	5:G:302:BER:C9	2.18	0.56
1:D:163:PRO:HG2	2:D:301:FMN:C9	2.35	0.56
1:B:70:PHE:CE2	5:H:302:BER:C10	2.81	0.56
1:C:102:GLU:CD	5:C:302:BER:H202	2.26	0.56
5:G:302:BER:C6	5:G:302:BER:C19	2.82	0.55
1:G:117:ASN:O	4:G:303:DMS:H13	2.06	0.55
1:D:125:ALA:O	1:D:129:ARG:HG2	2.07	0.55
1:D:41:THR:CA	5:D:302:BER:H31	2.28	0.55
1:A:181:LYS:NZ	6:A:402:HOH:O	2.34	0.55
2:A:301:FMN:H9	2:A:301:FMN:H2'	1.89	0.55
1:E:41:THR:HA	5:E:302:BER:C13	2.33	0.55
5:E:302:BER:C1	6:G:439:HOH:O	2.53	0.54
2:F:301:FMN:C4'	2:F:301:FMN:O2P	2.55	0.54
1:H:117:ASN:HD21	5:H:302:BER:H203	1.71	0.54
2:B:301:FMN:H5'1	6:B:471:HOH:O	2.08	0.54
5:E:302:BER:H91	1:G:70:PHE:CE2	2.42	0.54
1:C:107:ARG:HE	5:C:302:BER:C20	2.20	0.54
1:H:102:GLU:OE2	5:H:302:BER:H201	2.08	0.54
5:D:302:BER:H192	5:D:302:BER:C6	2.37	0.54
1:H:163:PRO:HG2	2:H:301:FMN:C9	2.37	0.54
1:E:97:LEU:HD21	1:G:212:ILE:HD13	1.90	0.54
1:C:74:LYS:NZ	2:C:301:FMN:HM83	2.23	0.53
1:D:91:ASP:OD2	1:D:93:VAL:HB	2.09	0.53
2:A:301:FMN:C9	2:A:301:FMN:H2'	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PRO:HG2	2:B:301:FMN:C9	2.39	0.53
1:D:107:ARG:HE	5:D:302:BER:C20	2.21	0.53
1:D:73:ARG:HD2	6:D:480:HOH:O	2.09	0.52
1:B:129:ARG:O	1:B:129:ARG:NE	2.43	0.52
1:E:2:ASP:OD2	1:E:4:ILE:HB	2.10	0.52
1:H:14:LYS:NZ	2:H:301:FMN:O2	2.40	0.52
1:H:129:ARG:HE	1:H:130:LYS:HG2	1.74	0.52
1:A:14:LYS:HZ1	5:C:302:BER:H71	1.75	0.51
1:F:118:ASP:OD1	1:F:122:LYS:NZ	2.43	0.51
1:A:165:GLU:HG3	2:A:301:FMN:H6	1.92	0.51
1:E:212:ILE:HD13	1:G:97:LEU:HD21	1.91	0.51
1:G:124:PHE:CZ	5:G:302:BER:H172	2.45	0.51
1:H:41:THR:HA	5:H:302:BER:C3	2.41	0.51
1:D:107:ARG:HH21	5:D:302:BER:C19	2.24	0.51
1:C:102:GLU:OE2	5:C:302:BER:C16	2.44	0.51
2:G:301:FMN:H9	2:G:301:FMN:O2'	2.11	0.51
1:G:163:PRO:HG2	2:G:301:FMN:C9	2.40	0.51
1:H:102:GLU:OE1	5:H:302:BER:H201	2.11	0.50
1:C:14:LYS:HZ2	2:C:301:FMN:HM81	1.70	0.50
1:F:71:ASN:ND2	2:F:301:FMN:HM73	2.26	0.50
1:A:14:LYS:NZ	5:C:302:BER:H71	2.27	0.50
1:F:129:ARG:O	1:F:133:HIS:ND1	2.45	0.50
1:H:41:THR:C	5:H:302:BER:H131	2.32	0.49
1:H:124:PHE:CZ	5:H:302:BER:C9	2.95	0.49
1:C:70:PHE:HE2	2:C:301:FMN:HM71	1.74	0.49
1:G:46:TRP:HB3	1:G:143:VAL:HG22	1.95	0.49
1:B:66:GLY:O	1:B:69:VAL:HG23	2.12	0.49
1:E:14:LYS:NZ	2:E:301:FMN:O2	2.46	0.49
1:F:165:GLU:HG3	2:F:301:FMN:O4	2.13	0.49
1:A:118:ASP:OD2	1:A:122:LYS:HE3	2.13	0.48
1:C:41:THR:HA	5:C:302:BER:H51	1.94	0.48
1:D:86:ALA:HB2	1:D:143:VAL:HG21	1.94	0.48
2:F:301:FMN:H9	2:F:301:FMN:H1'1	1.56	0.48
1:H:129:ARG:HG3	1:H:129:ARG:HH11	1.77	0.48
1:G:211:ASN:ND2	6:G:406:HOH:O	2.42	0.48
2:A:301:FMN:O2'	5:C:302:BER:H51	2.14	0.48
1:G:41:THR:CA	5:G:302:BER:H102	2.44	0.48
1:B:95:LEU:HD13	1:B:122:LYS:HG2	1.95	0.48
1:F:66:GLY:N	6:F:402:HOH:O	2.23	0.48
1:G:41:THR:CA	5:G:302:BER:C10	2.91	0.48
1:C:108:PHE:CZ	5:C:302:BER:H203	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:THR:HA	5:E:302:BER:C3	2.42	0.47
1:H:162:VAL:O	1:H:190:PRO:HD2	2.14	0.47
5:H:302:BER:H161	5:H:302:BER:H202	1.51	0.47
1:E:9:LYS:NZ	6:E:411:HOH:O	2.48	0.47
1:E:91:ASP:OD2	1:E:93:VAL:CG1	2.63	0.47
1:E:73:ARG:NE	6:E:410:HOH:O	2.47	0.47
1:D:41:THR:N	5:D:302:BER:H51	2.28	0.46
1:H:121:ARG:HB2	4:H:304:DMS:C1	2.46	0.46
1:C:21:LYS:HA	1:C:79:SER:HB2	1.97	0.46
1:C:165:GLU:HG3	2:C:301:FMN:O4	2.15	0.46
5:E:302:BER:H202	6:G:404:HOH:O	2.16	0.46
1:A:212:ILE:HD13	1:C:97:LEU:HD21	1.97	0.46
1:E:31:LYS:NZ	1:G:216:GLU:OE2	2.41	0.46
1:H:91:ASP:OD1	1:H:91:ASP:N	2.48	0.46
1:D:41:THR:HA	5:D:302:BER:C5	2.46	0.46
1:B:180:GLU:H	1:B:180:GLU:CD	2.19	0.46
2:B:301:FMN:C5'	6:B:471:HOH:O	2.64	0.46
1:E:102:GLU:OE2	5:E:302:BER:H201	2.16	0.45
1:D:127:MET:HG2	1:D:132:LEU:HD12	1.97	0.45
1:E:121:ARG:NH2	5:E:302:BER:H161	2.31	0.45
1:G:107:ARG:NE	5:G:302:BER:O4	2.49	0.45
1:C:173:ASP:OD1	1:C:178:LEU:HD12	2.15	0.45
1:A:70:PHE:CE2	5:C:302:BER:H91	2.51	0.45
1:D:107:ARG:NH2	5:D:302:BER:C19	2.79	0.45
1:E:10:ARG:HA	4:E:303:DMS:H11	1.98	0.45
1:H:54:GLU:OE1	1:H:54:GLU:N	2.36	0.45
1:D:41:THR:O	5:D:302:BER:H131	2.17	0.45
2:E:301:FMN:C2'	5:G:302:BER:C10	2.88	0.45
1:A:5:SER:OG	1:F:28:GLU:OE1	2.30	0.45
5:D:302:BER:H71	2:F:301:FMN:HM81	1.94	0.45
1:H:133:HIS:CD2	6:H:415:HOH:O	2.69	0.45
6:C:479:HOH:O	1:D:2:ASP:HB2	2.17	0.44
1:D:13:THR:OG1	1:D:160:ASP:HB3	2.17	0.44
1:E:41:THR:HG22	5:E:302:BER:H51	1.99	0.44
6:D:458:HOH:O	1:F:31:LYS:HE3	2.17	0.44
1:H:2:ASP:O	1:H:6:VAL:HG23	2.17	0.44
5:E:302:BER:H161	5:E:302:BER:H203	1.36	0.44
1:C:163:PRO:HG2	2:C:301:FMN:N1	2.33	0.44
1:B:70:PHE:HZ	5:H:302:BER:H91	1.83	0.44
5:G:302:BER:H61	5:G:302:BER:C19	2.40	0.44
1:A:67:ASN:OD1	1:A:67:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:PHE:CE2	2:C:301:FMN:HM72	2.51	0.43
5:D:302:BER:C7	2:F:301:FMN:HM82	2.45	0.43
1:H:41:THR:HA	5:H:302:BER:C8	2.47	0.43
1:F:163:PRO:HG2	2:F:301:FMN:N1	2.33	0.43
1:H:102:GLU:CD	5:H:302:BER:H201	2.39	0.43
1:G:49:ILE:HB	1:G:83:VAL:HB	2.01	0.43
1:H:168:ASP:OD2	1:H:171:ILE:HD12	2.19	0.43
1:C:71:ASN:ND2	2:C:301:FMN:C7M	2.67	0.43
1:E:74:LYS:HG3	6:E:431:HOH:O	2.18	0.43
1:D:66:GLY:O	1:D:69:VAL:HG23	2.19	0.43
1:F:49:ILE:HD11	1:F:178:LEU:HD21	1.99	0.43
5:C:302:BER:H51	5:C:302:BER:H31	1.76	0.43
1:G:124:PHE:CE1	5:G:302:BER:H172	2.53	0.43
2:G:301:FMN:H9	2:G:301:FMN:C2'	2.49	0.43
1:B:162:VAL:O	1:B:190:PRO:HD2	2.19	0.43
5:D:302:BER:H61	5:D:302:BER:C19	2.42	0.43
1:B:74:LYS:HG3	6:B:453:HOH:O	2.19	0.42
5:D:302:BER:H91	2:F:301:FMN:HM72	2.01	0.42
1:H:117:ASN:O	4:H:304:DMS:H13	2.18	0.42
1:C:52:SER:HB3	1:C:80:HIS:CD2	2.53	0.42
1:A:66:GLY:O	1:A:69:VAL:HG23	2.20	0.42
2:B:301:FMN:O4'	1:H:42:ASN:HB2	2.19	0.42
1:G:41:THR:H	5:G:302:BER:C10	2.22	0.42
1:G:117:ASN:HD21	5:G:302:BER:C19	2.20	0.42
1:B:105:ASP:OD2	1:H:206:SER:OG	2.21	0.42
1:G:130:LYS:HB2	1:G:130:LYS:HE2	1.71	0.42
1:D:129:ARG:NH2	6:D:412:HOH:O	2.50	0.42
1:E:179:LYS:HD2	1:E:179:LYS:HA	1.76	0.42
1:H:91:ASP:O	1:H:95:LEU:HD12	2.20	0.42
1:A:95:LEU:HD12	1:A:121:ARG:HG2	2.02	0.42
1:C:198:ASP:OD2	1:C:201:ALA:HB2	2.20	0.42
1:E:14:LYS:HZ2	5:G:302:BER:H31	1.85	0.42
1:E:91:ASP:OD1	1:E:91:ASP:N	2.50	0.41
1:D:31:LYS:HB2	1:D:31:LYS:HE2	1.87	0.41
1:D:41:THR:CA	5:D:302:BER:H51	2.49	0.41
1:F:86:ALA:HB2	1:F:143:VAL:HG21	2.02	0.41
1:G:209:PRO:HB2	1:G:211:ASN:OD1	2.21	0.41
5:D:302:BER:O3	5:D:302:BER:H203	2.21	0.41
6:D:430:HOH:O	1:F:213:THR:HA	2.20	0.41
1:F:70:PHE:CE2	2:F:301:FMN:C7M	3.03	0.41
1:C:108:PHE:CE1	5:C:302:BER:H203	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ARG:HH21	5:D:302:BER:H131	1.85	0.41
1:G:41:THR:N	5:G:302:BER:C10	2.77	0.41
1:H:41:THR:HA	5:H:302:BER:H31	2.03	0.41
1:E:14:LYS:NZ	5:G:302:BER:C3	2.84	0.41
1:H:102:GLU:OE2	5:H:302:BER:C20	2.69	0.41
2:C:301:FMN:H9	2:C:301:FMN:H1'1	1.66	0.41
1:G:2:ASP:HB3	1:G:3:ILE:H	1.67	0.41
1:B:2:ASP:N	6:B:418:HOH:O	2.54	0.41
1:B:209:PRO:HD2	1:B:212:ILE:HD12	2.03	0.41
1:E:36:TYR:CD1	1:G:205:LYS:HD2	2.56	0.41
1:C:102:GLU:OE1	5:C:302:BER:H161	2.19	0.40
5:D:302:BER:H172	1:F:165:GLU:HB2	2.03	0.40
1:G:92:ASP:HA	1:G:95:LEU:HD12	2.03	0.40
1:C:165:GLU:CG	2:C:301:FMN:O4	2.69	0.40
1:D:67:ASN:OD1	1:D:67:ASN:N	2.55	0.40
1:E:91:ASP:OD2	1:E:93:VAL:HG13	2.21	0.40
1:E:175:GLU:HB2	6:E:458:HOH:O	2.21	0.40
5:D:302:BER:C7	1:F:14:LYS:NZ	2.85	0.40
1:E:29:GLN:HE21	1:G:1:MET:CG	2.17	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	214/217 (99%)	210 (98%)	4 (2%)	0	100	100
1	B	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
1	C	214/217 (99%)	212 (99%)	2 (1%)	0	100	100
1	D	214/217 (99%)	212 (99%)	2 (1%)	0	100	100
1	E	215/217 (99%)	212 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	214/217 (99%)	210 (98%)	4 (2%)	0	100 100
1	G	215/217 (99%)	210 (98%)	4 (2%)	1 (0%)	29 15
1	H	214/217 (99%)	211 (99%)	3 (1%)	0	100 100
All	All	1714/1736 (99%)	1688 (98%)	25 (2%)	1 (0%)	51 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	2	ASP

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	178/179 (99%)	175 (98%)	3 (2%)	60 50
1	B	178/179 (99%)	174 (98%)	4 (2%)	52 39
1	C	177/179 (99%)	174 (98%)	3 (2%)	60 50
1	D	178/179 (99%)	175 (98%)	3 (2%)	60 50
1	E	179/179 (100%)	172 (96%)	7 (4%)	32 17
1	F	178/179 (99%)	175 (98%)	3 (2%)	60 50
1	G	179/179 (100%)	175 (98%)	4 (2%)	52 39
1	H	178/179 (99%)	175 (98%)	3 (2%)	60 50
All	All	1425/1432 (100%)	1395 (98%)	30 (2%)	53 41

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	TRP
1	A	67	ASN
1	A	119	LYS
1	B	46	TRP
1	B	97	LEU

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Mol	Chain	Res	Type
1	B	180	GLU
1	B	187	VAL
1	C	5	SER
1	C	46	TRP
1	C	211	ASN
1	D	2	ASP
1	D	46	TRP
1	D	67	ASN
1	E	1	MET
1	E	25	GLU
1	E	46	TRP
1	E	92	ASP
1	E	102	GLU
1	E	119	LYS
1	E	179	LYS
1	F	28	GLU
1	F	46	TRP
1	F	211	ASN
1	G	46	TRP
1	G	92	ASP
1	G	129	ARG
1	G	187	VAL
1	H	46	TRP
1	H	73	ARG
1	H	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	29	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

22 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	GOL	H	303	-	5,5,5	0.49	0	5,5,5	1.09	0
2	FMN	G	301	-	33,33,33	1.58	6 (18%)	48,50,50	2.35	17 (35%)
5	BER	D	302	-	29,29,29	1.98	9 (31%)	40,43,43	3.32	22 (55%)
2	FMN	B	301	-	33,33,33	1.39	3 (9%)	48,50,50	2.75	15 (31%)
2	FMN	C	301	-	33,33,33	1.85	10 (30%)	48,50,50	1.55	10 (20%)
4	DMS	G	303	-	3,3,3	0.69	0	3,3,3	0.97	0
5	BER	G	302	-	29,29,29	2.92	11 (37%)	40,43,43	4.58	22 (55%)
4	DMS	B	302	-	3,3,3	0.62	0	3,3,3	0.36	0
5	BER	C	302	-	29,29,29	1.22	2 (6%)	40,43,43	4.31	24 (60%)
4	DMS	C	303	-	3,3,3	0.75	0	3,3,3	1.08	0
2	FMN	D	301	-	33,33,33	1.48	5 (15%)	48,50,50	1.37	4 (8%)
5	BER	H	302	-	29,29,29	1.87	9 (31%)	40,43,43	5.13	28 (70%)
3	GOL	A	302	-	5,5,5	0.72	0	5,5,5	0.56	0
2	FMN	A	301	-	33,33,33	1.24	4 (12%)	48,50,50	1.93	15 (31%)
3	GOL	D	303	-	5,5,5	0.34	0	5,5,5	0.63	0
2	FMN	E	301	-	33,33,33	1.25	3 (9%)	48,50,50	1.79	12 (25%)
4	DMS	H	304	-	3,3,3	0.73	0	3,3,3	1.01	0
2	FMN	H	301	-	33,33,33	1.59	4 (12%)	48,50,50	2.82	21 (43%)
4	DMS	D	304	-	3,3,3	0.82	0	3,3,3	0.57	0
4	DMS	E	303	-	3,3,3	0.66	0	3,3,3	1.10	0
5	BER	E	302	-	29,29,29	2.14	13 (44%)	40,43,43	4.17	23 (57%)
2	FMN	F	301	-	33,33,33	3.08	14 (42%)	48,50,50	3.54	24 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	H	303	-	-	4/4/4/4	-
5	BER	G	302	-	-	3/4/19/19	0/5/5/5
2	FMN	A	301	-	-	2/18/18/18	0/3/3/3
2	FMN	H	301	-	-	10/18/18/18	0/3/3/3
3	GOL	D	303	-	-	2/4/4/4	-
5	BER	C	302	-	-	4/4/19/19	0/5/5/5
2	FMN	D	301	-	-	0/18/18/18	0/3/3/3
5	BER	E	302	-	-	1/4/19/19	0/5/5/5
2	FMN	G	301	-	-	8/18/18/18	0/3/3/3
2	FMN	F	301	-	-	9/18/18/18	0/3/3/3
5	BER	D	302	-	-	4/4/19/19	0/5/5/5
2	FMN	B	301	-	-	9/18/18/18	0/3/3/3
2	FMN	C	301	-	-	2/18/18/18	0/3/3/3
2	FMN	E	301	-	-	4/18/18/18	0/3/3/3
5	BER	H	302	-	-	2/4/19/19	0/5/5/5

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	302	BER	C10-C4	-9.46	1.43	1.50
2	F	301	FMN	C1'-C2'	8.53	1.64	1.52
2	F	301	FMN	C4A-N5	6.71	1.43	1.30
2	F	301	FMN	C4'-C3'	-6.47	1.41	1.53
2	H	301	FMN	C1'-C2'	5.92	1.61	1.52
5	G	302	BER	C2-C1	5.89	1.51	1.42
2	F	301	FMN	C10-N1	5.78	1.45	1.33
5	E	302	BER	C2-C1	5.53	1.51	1.42
5	G	302	BER	C7-N1	-5.29	1.37	1.48
5	D	302	BER	C12-C8	-4.70	1.34	1.43
2	B	301	FMN	C4A-N5	4.69	1.39	1.30
2	G	301	FMN	C5'-C4'	4.55	1.58	1.51
5	E	302	BER	C6-N1	4.52	1.39	1.33
2	D	301	FMN	C9A-C5A	4.48	1.48	1.41
2	F	301	FMN	C7M-C7	-4.40	1.42	1.51
2	C	301	FMN	C4-N3	-4.14	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	302	BER	C1-N1	-3.88	1.33	1.39
5	H	302	BER	C5-C11	3.86	1.43	1.36
5	H	302	BER	C7-C10	-3.79	1.46	1.51
2	C	301	FMN	C5A-N5	-3.77	1.32	1.39
2	G	301	FMN	C4A-N5	3.75	1.38	1.30
2	D	301	FMN	C4-N3	-3.66	1.32	1.38
5	G	302	BER	C7-C10	-3.65	1.46	1.51
5	G	302	BER	C5-C11	3.53	1.42	1.36
5	G	302	BER	C6-N1	-3.51	1.28	1.33
5	D	302	BER	O2-C14	3.50	1.43	1.38
2	F	301	FMN	O2-C2	3.47	1.30	1.24
5	E	302	BER	C12-C8	-3.45	1.36	1.43
5	G	302	BER	C12-C8	-3.39	1.36	1.43
5	D	302	BER	C15-C12	-3.33	1.36	1.43
5	H	302	BER	O3-C15	3.30	1.43	1.38
2	C	301	FMN	C2-N3	-3.26	1.31	1.39
2	H	301	FMN	C1'-N10	3.15	1.56	1.48
2	H	301	FMN	C4A-N5	3.15	1.36	1.30
2	C	301	FMN	C9A-C5A	3.12	1.46	1.41
5	D	302	BER	O4-C18	3.08	1.42	1.37
2	E	301	FMN	C4A-N5	3.08	1.36	1.30
2	A	301	FMN	C4A-N5	3.02	1.36	1.30
2	F	301	FMN	C2'-C3'	3.01	1.59	1.53
2	C	301	FMN	C6-C7	-3.00	1.35	1.39
5	G	302	BER	C15-C12	-2.96	1.37	1.43
5	H	302	BER	C12-C8	-2.94	1.37	1.43
5	C	302	BER	O3-C15	2.94	1.43	1.38
2	B	301	FMN	O2'-C2'	-2.86	1.37	1.43
2	F	301	FMN	O3'-C3'	2.86	1.49	1.43
2	F	301	FMN	C9-C8	-2.86	1.35	1.39
2	F	301	FMN	O2'-C2'	-2.85	1.37	1.43
5	E	302	BER	O3-C15	2.72	1.42	1.38
5	E	302	BER	O1-C11	2.69	1.42	1.38
2	C	301	FMN	C8-C7	2.68	1.47	1.40
5	D	302	BER	C2-C1	2.67	1.46	1.42
2	F	301	FMN	C6-C5A	2.67	1.44	1.40
5	H	302	BER	C2-C1	2.66	1.46	1.42
2	C	301	FMN	P-O2P	-2.65	1.44	1.54
2	F	301	FMN	O4-C4	-2.64	1.18	1.23
2	C	301	FMN	P-O3P	-2.63	1.44	1.54
5	G	302	BER	O4-C18	2.61	1.41	1.37
2	A	301	FMN	C1'-C2'	2.60	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	302	BER	C1-N1	2.56	1.42	1.39
5	C	302	BER	C7-C10	-2.53	1.47	1.51
2	D	301	FMN	C5A-N5	-2.51	1.34	1.39
2	A	301	FMN	C10-N10	2.46	1.42	1.37
2	E	301	FMN	C9A-C5A	-2.40	1.37	1.41
2	D	301	FMN	C2-N3	-2.39	1.33	1.39
2	C	301	FMN	P-O1P	-2.39	1.42	1.50
2	G	301	FMN	C1'-C2'	2.33	1.55	1.52
2	G	301	FMN	C4'-C3'	2.33	1.57	1.53
2	G	301	FMN	C1'-N10	2.32	1.54	1.48
5	G	302	BER	O1-C11	2.30	1.41	1.38
5	H	302	BER	C16-C18	-2.29	1.34	1.39
5	D	302	BER	O1-C11	2.29	1.41	1.38
5	E	302	BER	C9-C4	2.26	1.41	1.37
5	H	302	BER	O2-C14	2.25	1.41	1.38
2	C	301	FMN	P-O5'	-2.22	1.53	1.60
5	E	302	BER	C5-C11	2.21	1.40	1.36
2	A	301	FMN	O2'-C2'	-2.20	1.38	1.43
2	F	301	FMN	C9-C9A	-2.20	1.36	1.39
5	E	302	BER	C7-C10	-2.18	1.48	1.51
2	G	301	FMN	C2'-C3'	-2.18	1.49	1.53
5	E	302	BER	C13-C8	-2.18	1.36	1.41
5	E	302	BER	C16-C18	-2.17	1.35	1.39
2	D	301	FMN	C8-C7	2.15	1.46	1.40
5	E	302	BER	O4-C20	-2.14	1.36	1.42
5	D	302	BER	C13-C8	-2.13	1.36	1.41
2	E	301	FMN	C2'-C3'	-2.09	1.49	1.53
5	E	302	BER	C9-C14	2.08	1.42	1.38
5	H	302	BER	C6-N1	2.08	1.35	1.33
5	G	302	BER	C4-C2	-2.07	1.37	1.42
2	H	301	FMN	C10-N1	2.05	1.37	1.33
2	F	301	FMN	C6-C7	-2.04	1.36	1.39
5	D	302	BER	C7-C10	-2.03	1.48	1.51
5	E	302	BER	O2-C14	2.01	1.41	1.38
2	B	301	FMN	C6-C7	-2.00	1.36	1.39

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	302	BER	O3-C15-C12	13.39	143.91	117.27
5	G	302	BER	C6-C12-C15	-12.62	112.57	121.62
5	H	302	BER	O3-C15-C12	11.53	140.22	117.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	302	BER	O3-C15-C12	11.34	139.84	117.27
5	H	302	BER	C7-C10-C4	11.33	122.74	109.79
2	B	301	FMN	C5'-C4'-C3'	-11.25	90.46	112.20
5	G	302	BER	C12-C6-N1	-11.11	114.70	121.82
5	H	302	BER	C20-O4-C18	-10.98	100.96	117.53
5	E	302	BER	C20-O4-C18	-10.43	101.78	117.53
2	B	301	FMN	O4'-C4'-C5'	-10.41	86.52	109.92
5	G	302	BER	C7-N1-C6	-10.39	106.88	118.67
5	C	302	BER	C6-C12-C15	-9.61	114.73	121.62
5	H	302	BER	C12-C6-N1	-9.29	115.87	121.82
5	G	302	BER	C2-C1-N1	-9.25	112.14	118.76
5	D	302	BER	C6-C12-C15	-9.08	115.11	121.62
5	C	302	BER	O3-C15-C18	-8.57	100.38	120.84
5	D	302	BER	O3-C15-C12	8.54	134.26	117.27
2	G	301	FMN	C5'-C4'-C3'	8.47	128.57	112.20
5	C	302	BER	C20-O4-C18	-8.27	105.05	117.53
2	F	301	FMN	O3'-C3'-C2'	8.22	128.67	108.81
5	H	302	BER	C8-C3-C1	-8.11	112.15	120.86
5	E	302	BER	C12-C6-N1	-8.04	116.67	121.82
5	H	302	BER	C2-C1-N1	8.04	124.50	118.76
2	F	301	FMN	O2'-C2'-C3'	-7.98	89.70	109.10
2	H	301	FMN	C1'-C2'-C3'	7.88	131.81	109.79
5	H	302	BER	C3-C8-C12	7.80	127.60	119.26
5	H	302	BER	O3-C15-C18	-7.54	102.85	120.84
2	F	301	FMN	C1'-C2'-C3'	7.39	130.45	109.79
2	F	301	FMN	C5A-C6-C7	-7.11	107.66	120.71
2	H	301	FMN	C4'-C3'-C2'	-7.05	98.71	113.36
5	H	302	BER	O1-C11-C5	7.04	133.74	128.11
5	E	302	BER	O3-C15-C18	-6.93	104.30	120.84
5	G	302	BER	O3-C15-C12	6.90	131.01	117.27
2	F	301	FMN	C5'-C4'-C3'	-6.75	99.17	112.20
2	F	301	FMN	C9-C9A-N10	-6.65	112.85	121.84
2	H	301	FMN	O3'-C3'-C2'	6.57	124.69	108.81
2	F	301	FMN	C6-C7-C8	6.46	128.92	119.67
5	G	302	BER	C9-C4-C2	6.43	127.25	118.70
5	E	302	BER	C16-C18-C15	6.41	124.29	119.76
5	H	302	BER	O1-C11-C14	-6.40	102.49	109.78
5	E	302	BER	C3-C8-C12	6.34	126.04	119.26
5	C	302	BER	C12-C6-N1	-6.23	117.83	121.82
5	E	302	BER	C13-C8-C3	-6.18	111.87	122.00
5	D	302	BER	C16-C18-C15	-5.99	115.53	119.76
5	D	302	BER	C7-C10-C4	-5.94	103.00	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	FMN	C7M-C7-C8	-5.93	108.58	120.74
5	H	302	BER	O4-C18-C16	-5.84	114.36	124.37
5	G	302	BER	C10-C4-C2	-5.83	112.15	119.08
2	F	301	FMN	C5A-C9A-N10	5.80	123.95	117.95
2	H	301	FMN	C4A-C10-N10	5.80	124.96	116.48
5	H	302	BER	C3-C1-C2	-5.77	113.11	122.51
5	E	302	BER	O1-C11-C5	5.66	132.63	128.11
5	C	302	BER	C5-C2-C1	-5.52	115.81	120.80
5	C	302	BER	C8-C3-C1	-5.48	114.97	120.86
5	C	302	BER	C16-C13-C8	-5.44	112.40	120.82
5	D	302	BER	O3-C15-C18	-5.29	108.22	120.84
5	G	302	BER	C19-O3-C15	-5.28	101.26	114.88
2	G	301	FMN	C4A-C10-N10	5.28	124.20	116.48
5	E	302	BER	C2-C1-N1	5.27	122.52	118.76
2	G	301	FMN	O2'-C2'-C1'	5.25	122.49	109.80
5	D	302	BER	C2-C1-N1	-5.24	115.01	118.76
5	G	302	BER	C3-C1-C2	5.23	131.03	122.51
5	G	302	BER	C6-N1-C1	5.05	129.05	121.27
5	C	302	BER	C6-C12-C8	5.02	122.91	117.67
2	H	301	FMN	C1'-N10-C9A	4.92	128.72	120.51
5	H	302	BER	O4-C18-C15	4.89	123.34	116.49
5	C	302	BER	O4-C18-C15	-4.87	109.66	116.49
2	A	301	FMN	C4A-C10-N10	4.63	123.26	116.48
2	H	301	FMN	O3'-C3'-C4'	-4.59	97.72	108.81
5	D	302	BER	O1-C11-C5	4.57	131.76	128.11
5	G	302	BER	C6-C12-C8	4.54	122.41	117.67
5	G	302	BER	O3-C15-C18	-4.52	110.06	120.84
5	D	302	BER	C13-C16-C18	4.52	127.66	119.95
2	G	301	FMN	C4-N3-C2	-4.50	117.33	125.64
2	E	301	FMN	C4A-C10-N10	4.46	123.00	116.48
5	G	302	BER	C7-N1-C1	4.41	122.79	117.91
2	E	301	FMN	O2'-C2'-C3'	-4.37	98.48	109.10
5	E	302	BER	O4-C18-C16	-4.33	116.94	124.37
5	C	302	BER	C13-C16-C18	4.32	127.33	119.95
2	F	301	FMN	C4A-C4-N3	4.31	124.13	113.19
5	H	302	BER	O2-C17-O1	-4.26	101.27	108.08
2	A	301	FMN	O3'-C3'-C2'	-4.25	98.55	108.81
5	E	302	BER	C7-N1-C1	-4.15	113.31	117.91
5	C	302	BER	C3-C1-C2	-4.11	115.81	122.51
2	H	301	FMN	C9A-N10-C10	-4.08	114.41	120.77
2	B	301	FMN	C4A-C10-N10	4.06	122.42	116.48
2	F	301	FMN	O5'-C5'-C4'	-4.00	98.68	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	302	BER	C16-C13-C8	-3.87	114.83	120.82
2	G	301	FMN	O3'-C3'-C4'	3.85	118.10	108.81
5	G	302	BER	C20-O4-C18	-3.84	111.73	117.53
5	C	302	BER	O4-C18-C16	3.78	130.85	124.37
5	C	302	BER	C18-C15-C12	-3.75	115.69	120.06
2	A	301	FMN	C10-C4A-N5	-3.72	116.97	124.86
5	E	302	BER	C6-C12-C15	3.70	124.27	121.62
5	H	302	BER	C11-C5-C2	-3.69	113.72	120.58
2	E	301	FMN	C1'-C2'-C3'	3.69	120.09	109.79
5	H	302	BER	C13-C8-C3	-3.61	116.08	122.00
5	E	302	BER	C18-C15-C12	-3.60	115.86	120.06
5	E	302	BER	C10-C4-C2	-3.58	114.83	119.08
2	F	301	FMN	C4'-C3'-C2'	-3.57	105.93	113.36
5	G	302	BER	C8-C3-C1	-3.57	117.03	120.86
2	H	301	FMN	C5'-C4'-C3'	3.56	119.09	112.20
2	C	301	FMN	C4A-C10-N1	-3.53	116.53	124.73
5	G	302	BER	C15-C12-C8	3.48	125.00	118.63
2	H	301	FMN	O2'-C2'-C3'	-3.46	100.68	109.10
2	H	301	FMN	C4-N3-C2	-3.43	119.30	125.64
5	E	302	BER	C7-N1-C6	3.43	122.57	118.67
2	A	301	FMN	C9-C8-C7	3.42	124.58	119.67
2	B	301	FMN	O4'-C4'-C3'	3.41	117.39	109.10
5	C	302	BER	C7-N1-C1	3.38	121.64	117.91
2	G	301	FMN	C9A-N10-C10	-3.33	115.58	120.77
2	F	301	FMN	C9A-C5A-N5	-3.32	118.83	122.43
2	F	301	FMN	C6-C5A-C9A	3.32	123.63	118.94
5	H	302	BER	C16-C18-C15	3.31	122.10	119.76
5	H	302	BER	C7-N1-C1	3.29	121.55	117.91
5	E	302	BER	C17-O2-C14	3.21	109.52	105.34
2	C	301	FMN	C4A-C4-N3	3.20	121.32	113.19
2	G	301	FMN	O5'-C5'-C4'	3.20	117.89	109.36
2	H	301	FMN	C4-C4A-C10	3.18	122.14	116.79
5	C	302	BER	C4-C2-C5	3.16	125.17	119.21
5	D	302	BER	C17-O1-C11	3.14	109.42	105.34
5	H	302	BER	C7-N1-C6	-3.11	115.14	118.67
5	D	302	BER	C6-C12-C8	3.09	120.90	117.67
2	F	301	FMN	O4-C4-C4A	-3.07	118.45	126.60
5	E	302	BER	O2-C14-C9	3.07	131.96	127.85
2	A	301	FMN	C4-N3-C2	-3.06	119.98	125.64
5	E	302	BER	C8-C3-C1	-3.05	117.58	120.86
2	B	301	FMN	O2P-P-O5'	-3.04	98.63	106.73
5	C	302	BER	C13-C8-C3	-3.04	117.01	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	FMN	C10-C4A-N5	-3.04	118.40	124.86
2	F	301	FMN	C10-N1-C2	3.00	122.91	116.90
2	G	301	FMN	C1'-N10-C9A	2.98	125.47	120.51
2	C	301	FMN	C10-N1-C2	2.96	122.82	116.90
5	H	302	BER	C17-O2-C14	-2.95	101.51	105.34
2	H	301	FMN	P-O5'-C5'	2.94	126.40	118.30
2	F	301	FMN	C4-N3-C2	-2.94	120.20	125.64
2	H	301	FMN	C4A-C10-N1	-2.92	117.95	124.73
5	D	302	BER	C15-C12-C8	2.89	123.91	118.63
2	G	301	FMN	C4A-C10-N1	-2.87	118.08	124.73
2	C	301	FMN	O3P-P-O2P	2.84	118.51	107.64
5	H	302	BER	C16-C13-C8	2.84	125.22	120.82
2	A	301	FMN	C9A-C5A-N5	-2.82	119.37	122.43
2	G	301	FMN	C4A-C4-N3	2.81	120.33	113.19
2	C	301	FMN	C4-N3-C2	-2.81	120.45	125.64
2	F	301	FMN	C9A-C9-C8	-2.79	113.69	119.30
2	D	301	FMN	C4A-C10-N1	-2.78	118.27	124.73
2	E	301	FMN	C1'-N10-C9A	2.78	125.15	120.51
5	H	302	BER	C5-C2-C1	2.76	123.30	120.80
5	H	302	BER	C10-C7-N1	-2.74	106.00	109.47
2	H	301	FMN	O3P-P-O5'	-2.73	99.48	106.73
5	H	302	BER	C18-C15-C12	-2.71	116.90	120.06
2	C	301	FMN	C9A-C5A-N5	-2.71	119.49	122.43
2	B	301	FMN	C10-C4A-N5	-2.70	119.12	124.86
2	D	301	FMN	N3-C2-N1	2.70	124.68	119.38
5	C	302	BER	C13-C8-C12	2.66	122.63	119.12
2	G	301	FMN	C4-C4A-C10	2.64	121.23	116.79
2	A	301	FMN	C5A-N5-C4A	2.64	122.46	118.07
5	G	302	BER	O1-C11-C14	-2.63	106.79	109.78
5	H	302	BER	C6-C12-C15	-2.62	119.74	121.62
5	G	302	BER	O4-C18-C15	-2.61	112.83	116.49
2	C	301	FMN	C4-C4A-N5	2.59	121.92	118.23
2	F	301	FMN	C4A-C10-N1	-2.58	118.73	124.73
2	F	301	FMN	O3'-C3'-C4'	-2.58	102.57	108.81
2	B	301	FMN	C5A-C9A-N10	2.58	120.62	117.95
2	A	301	FMN	C4-C4A-N5	2.58	121.90	118.23
2	A	301	FMN	C4-C4A-C10	2.57	121.11	116.79
2	F	301	FMN	O4'-C4'-C5'	2.57	115.70	109.92
5	D	302	BER	C4-C2-C5	2.57	124.05	119.21
2	B	301	FMN	O5'-C5'-C4'	2.56	116.21	109.36
2	B	301	FMN	C4-N3-C2	-2.55	120.93	125.64
5	G	302	BER	C14-C9-C4	-2.55	115.25	119.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	FMN	O2P-P-O5'	2.53	113.46	106.73
2	H	301	FMN	C5A-C9A-N10	2.52	120.55	117.95
2	B	301	FMN	C4'-C3'-C2'	2.51	118.58	113.36
5	C	302	BER	C11-C5-C2	-2.50	115.94	120.58
5	D	302	BER	C12-C6-N1	-2.49	120.22	121.82
2	C	301	FMN	O4-C4-C4A	-2.48	120.01	126.60
5	D	302	BER	C11-C5-C2	-2.46	116.01	120.58
2	H	301	FMN	O3P-P-O1P	2.46	120.30	110.68
2	C	301	FMN	C5A-N5-C4A	2.44	122.13	118.07
2	E	301	FMN	P-O5'-C5'	2.43	124.99	118.30
2	A	301	FMN	C5'-C4'-C3'	-2.42	107.53	112.20
2	G	301	FMN	C5A-C9A-N10	2.41	120.44	117.95
2	E	301	FMN	C4-N3-C2	-2.40	121.22	125.64
5	D	302	BER	C8-C3-C1	-2.38	118.31	120.86
5	D	302	BER	C5-C2-C1	-2.36	118.66	120.80
2	H	301	FMN	C10-C4A-N5	-2.34	119.89	124.86
5	C	302	BER	O2-C14-C11	-2.33	107.12	109.78
2	A	301	FMN	C8M-C8-C9	-2.32	115.19	119.49
2	B	301	FMN	O3P-P-O1P	2.32	119.77	110.68
2	F	301	FMN	O3P-P-O2P	2.32	116.49	107.64
5	D	302	BER	C7-N1-C1	2.31	120.46	117.91
5	E	302	BER	C17-O1-C11	2.30	108.32	105.34
2	A	301	FMN	C4A-C10-N1	-2.29	119.42	124.73
2	E	301	FMN	O2'-C2'-C1'	-2.28	104.28	109.80
2	A	301	FMN	O2-C2-N1	-2.28	118.05	121.83
2	C	301	FMN	N10-C10-N1	2.28	124.90	118.35
5	E	302	BER	C7-C10-C4	2.26	112.37	109.79
2	E	301	FMN	C4-C4A-C10	2.26	120.58	116.79
5	E	302	BER	C13-C8-C12	2.25	122.09	119.12
5	H	302	BER	C9-C4-C2	2.25	121.69	118.70
5	C	302	BER	C7-C10-C4	2.25	112.36	109.79
5	C	302	BER	C6-N1-C1	-2.24	117.81	121.27
2	H	301	FMN	C4A-C4-N3	2.23	118.86	113.19
5	G	302	BER	C11-C5-C2	-2.22	116.45	120.58
2	G	301	FMN	C10-C4A-N5	-2.22	120.15	124.86
2	B	301	FMN	C4A-C4-N3	2.21	118.81	113.19
5	G	302	BER	O4-C18-C16	2.21	128.16	124.37
2	F	301	FMN	C9-C8-C7	2.21	122.83	119.67
2	F	301	FMN	C9A-N10-C10	-2.21	117.33	120.77
5	D	302	BER	C18-C15-C12	-2.17	117.53	120.06
5	H	302	BER	C19-O3-C15	2.17	120.48	114.88
2	A	301	FMN	O4'-C4'-C3'	2.16	114.35	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	302	BER	C13-C8-C12	-2.15	116.29	119.12
5	D	302	BER	O1-C11-C14	-2.15	107.33	109.78
2	E	301	FMN	C6-C7-C8	-2.15	116.59	119.67
5	D	302	BER	C17-O2-C14	2.14	108.13	105.34
2	E	301	FMN	C9A-N10-C10	-2.13	117.44	120.77
5	E	302	BER	C10-C7-N1	2.13	112.17	109.47
5	E	302	BER	C3-C1-C2	-2.13	119.03	122.51
5	H	302	BER	C13-C8-C12	-2.13	116.32	119.12
2	B	301	FMN	C9A-N10-C10	-2.12	117.46	120.77
2	D	301	FMN	O3P-P-O2P	2.12	115.72	107.64
2	H	301	FMN	O4-C4-C4A	-2.11	120.99	126.60
2	A	301	FMN	C1'-N10-C9A	2.09	124.00	120.51
2	B	301	FMN	C4-C4A-N5	2.09	121.21	118.23
2	H	301	FMN	O5'-P-O1P	2.08	112.31	106.47
2	H	301	FMN	C6-C5A-C9A	2.08	121.88	118.94
2	G	301	FMN	N3-C2-N1	2.07	123.45	119.38
2	G	301	FMN	O4'-C4'-C5'	-2.06	105.29	109.92
2	B	301	FMN	C4A-C10-N1	-2.05	119.98	124.73
5	C	302	BER	C15-C12-C8	2.04	122.36	118.63
2	E	301	FMN	C4A-C10-N1	-2.04	120.01	124.73
2	D	301	FMN	C4-N3-C2	-2.03	121.89	125.64
5	C	302	BER	C14-C9-C4	-2.03	116.16	119.72
5	D	302	BER	C20-O4-C18	-2.01	114.50	117.53
2	G	301	FMN	O4-C4-C4A	-2.01	121.27	126.60

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	FMN	C2'-C1'-N10-C10
2	B	301	FMN	N10-C1'-C2'-O2'
2	B	301	FMN	C3'-C4'-C5'-O5'
2	B	301	FMN	O4'-C4'-C5'-O5'
2	B	301	FMN	C5'-O5'-P-O1P
2	E	301	FMN	C2'-C1'-N10-C10
2	E	301	FMN	N10-C1'-C2'-O2'
2	E	301	FMN	N10-C1'-C2'-C3'
2	F	301	FMN	N10-C1'-C2'-O2'
2	F	301	FMN	C1'-C2'-C3'-O3'
2	F	301	FMN	C1'-C2'-C3'-C4'
2	F	301	FMN	O2'-C2'-C3'-O3'
2	F	301	FMN	O2'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
2	F	301	FMN	C3'-C4'-C5'-O5'
2	F	301	FMN	O4'-C4'-C5'-O5'
2	F	301	FMN	C5'-O5'-P-O1P
2	G	301	FMN	C2'-C1'-N10-C9A
2	G	301	FMN	C2'-C1'-N10-C10
2	G	301	FMN	C2'-C3'-C4'-O4'
2	G	301	FMN	C2'-C3'-C4'-C5'
2	G	301	FMN	O3'-C3'-C4'-O4'
2	H	301	FMN	C2'-C1'-N10-C9A
2	H	301	FMN	C2'-C1'-N10-C10
2	H	301	FMN	C1'-C2'-C3'-O3'
2	H	301	FMN	O2'-C2'-C3'-O3'
2	H	301	FMN	C2'-C3'-C4'-O4'
2	H	301	FMN	C2'-C3'-C4'-C5'
2	H	301	FMN	O3'-C3'-C4'-O4'
2	H	301	FMN	O3'-C3'-C4'-C5'
3	A	302	GOL	O1-C1-C2-C3
3	D	303	GOL	O1-C1-C2-C3
3	H	303	GOL	O1-C1-C2-C3
3	H	303	GOL	C1-C2-C3-O3
5	C	302	BER	C12-C15-O3-C19
5	H	302	BER	C15-C18-O4-C20
5	G	302	BER	C15-C18-O4-C20
5	G	302	BER	C16-C18-O4-C20
2	B	301	FMN	O3'-C3'-C4'-C5'
2	G	301	FMN	O3'-C3'-C4'-C5'
2	B	301	FMN	C2'-C3'-C4'-C5'
5	D	302	BER	C12-C15-O3-C19
2	H	301	FMN	O2'-C2'-C3'-C4'
5	H	302	BER	C16-C18-O4-C20
5	D	302	BER	C16-C18-O4-C20
2	F	301	FMN	C4'-C5'-O5'-P
5	C	302	BER	C18-C15-O3-C19
3	A	302	GOL	O1-C1-C2-O2
3	D	303	GOL	O1-C1-C2-O2
5	D	302	BER	C15-C18-O4-C20
5	D	302	BER	C18-C15-O3-C19
2	H	301	FMN	C4'-C5'-O5'-P
2	B	301	FMN	C2'-C1'-N10-C10
5	C	302	BER	C15-C18-O4-C20
5	G	302	BER	C12-C15-O3-C19
3	H	303	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	G	301	FMN	C3'-C4'-C5'-O5'
2	A	301	FMN	O2'-C2'-C3'-O3'
2	B	301	FMN	C4'-C5'-O5'-P
5	C	302	BER	C16-C18-O4-C20
2	E	301	FMN	C4'-C5'-O5'-P
2	B	301	FMN	C5'-O5'-P-O2P
3	H	303	GOL	O2-C2-C3-O3
2	G	301	FMN	C1'-C2'-C3'-O3'
5	E	302	BER	C15-C18-O4-C20
2	C	301	FMN	N10-C1'-C2'-O2'
2	C	301	FMN	C2'-C1'-N10-C10

There are no ring outliers.

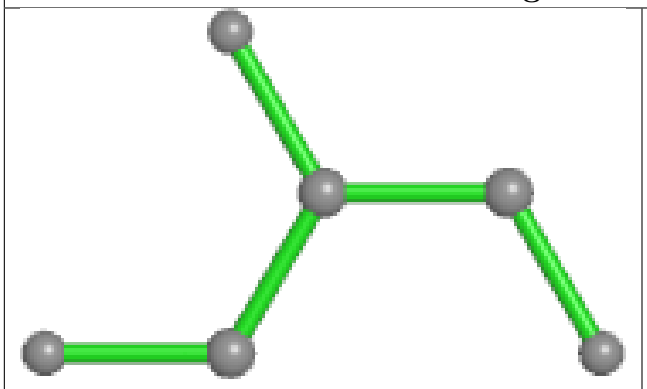
16 monomers are involved in 180 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	FMN	6	0
5	D	302	BER	26	0
2	B	301	FMN	6	0
2	C	301	FMN	21	0
4	G	303	DMS	1	0
5	G	302	BER	35	0
5	C	302	BER	14	0
2	D	301	FMN	1	0
5	H	302	BER	22	0
2	A	301	FMN	6	0
2	E	301	FMN	6	0
4	H	304	DMS	2	0
2	H	301	FMN	2	0
4	E	303	DMS	3	0
5	E	302	BER	22	0
2	F	301	FMN	20	0

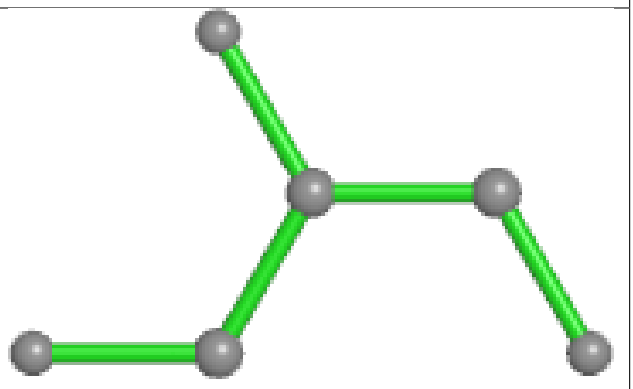
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

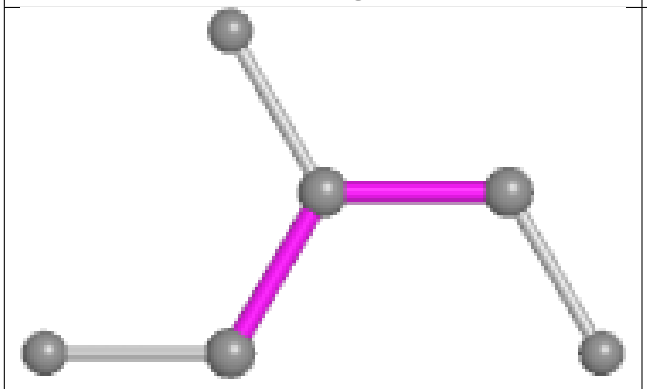
Ligand GOL H 303



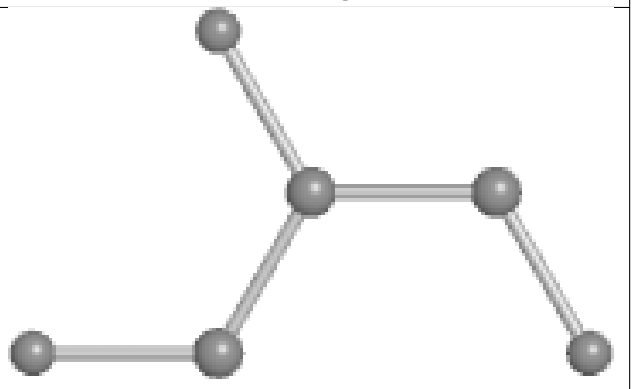
Bond lengths



Bond angles

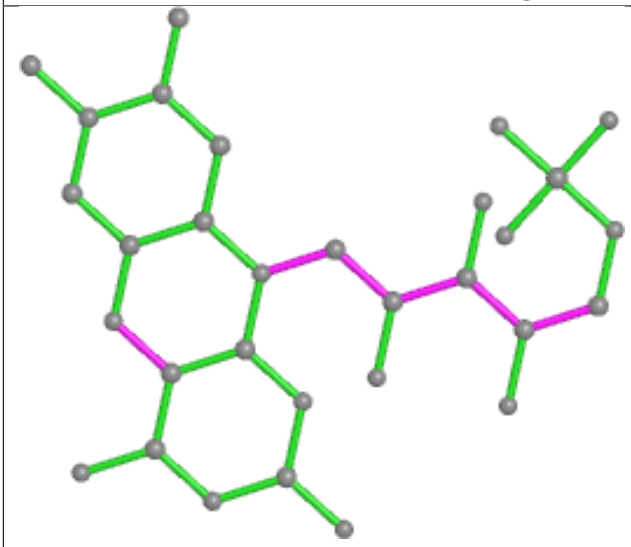


Torsions

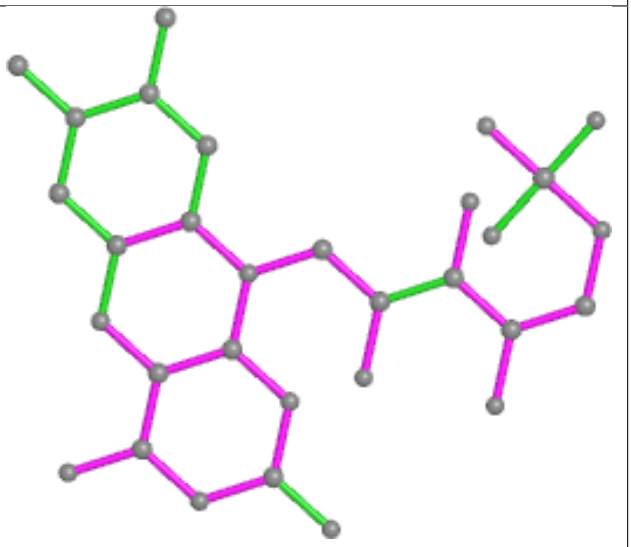


Rings

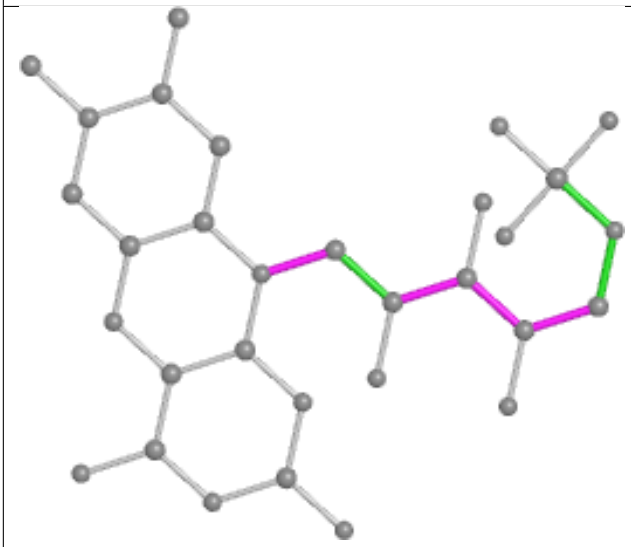
Ligand FMN G 301



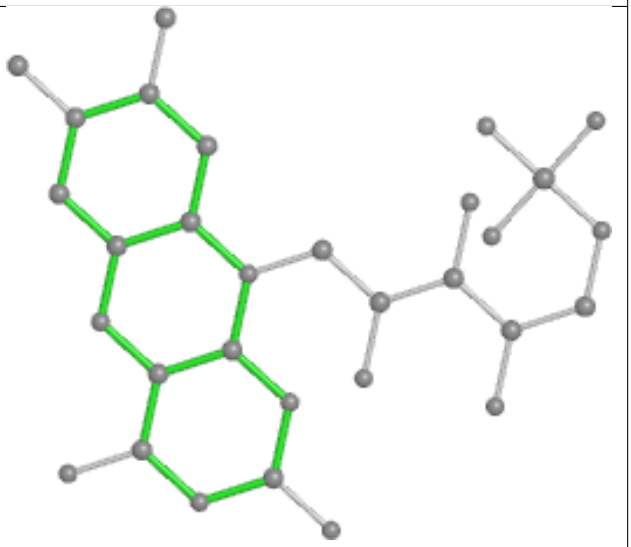
Bond lengths



Bond angles

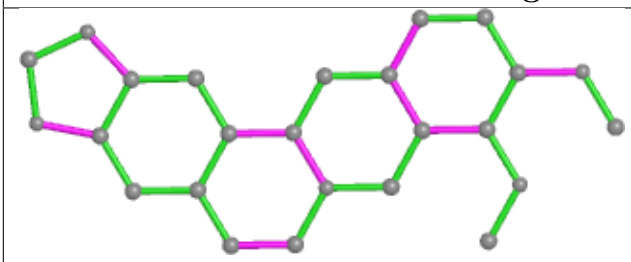


Torsions

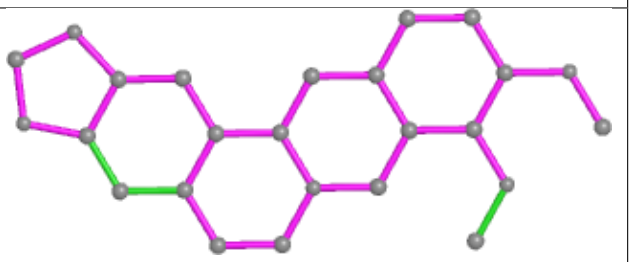


Rings

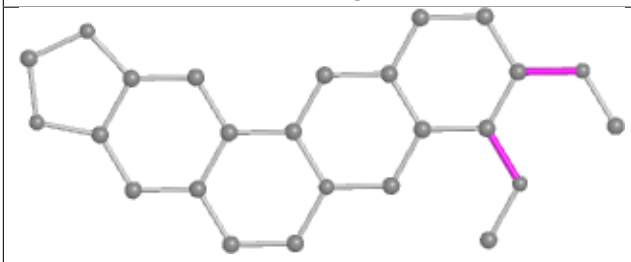
Ligand BER D 302



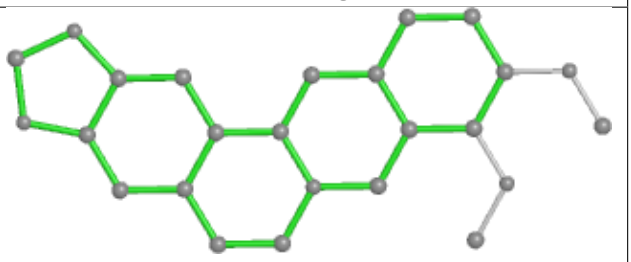
Bond lengths



Bond angles

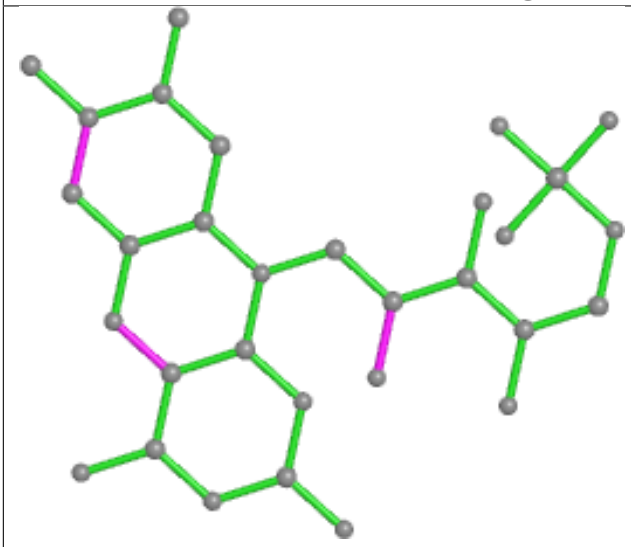


Torsions



Rings

Ligand FMN B 301



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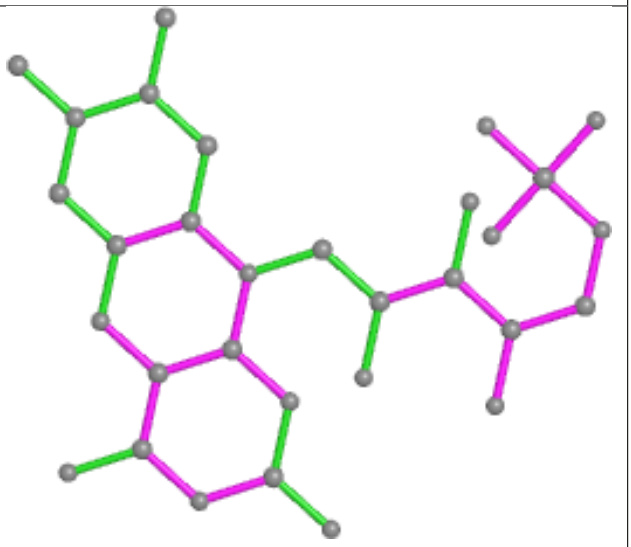
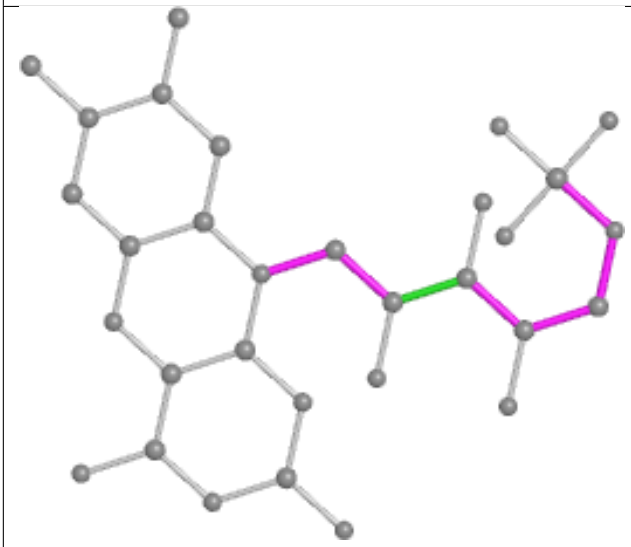


Bond angles



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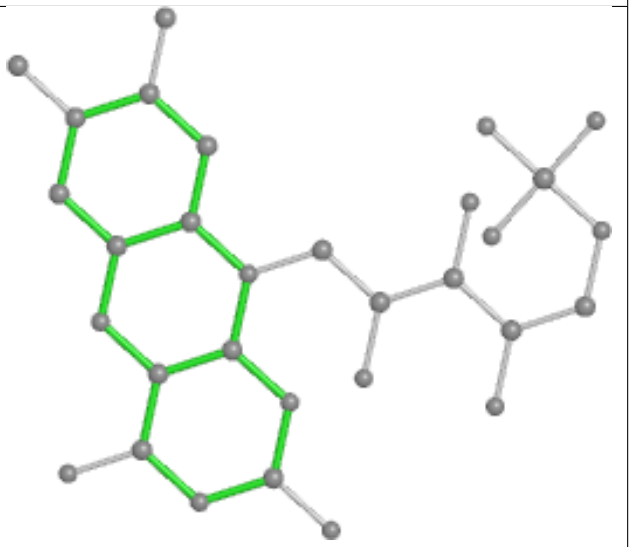
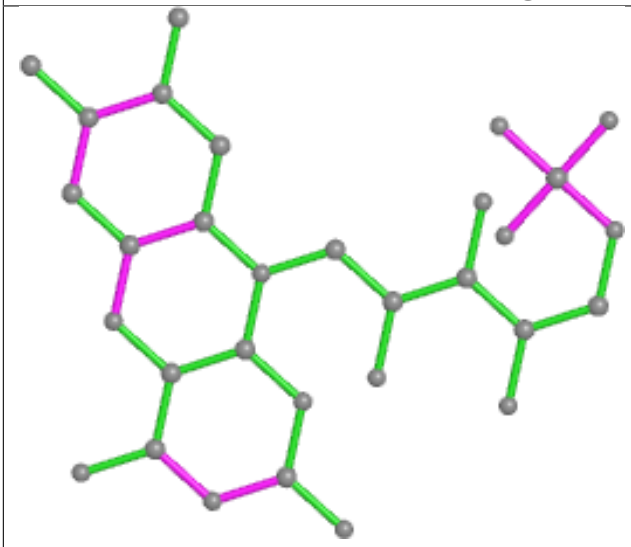


Rings

Ligand FMN C 301



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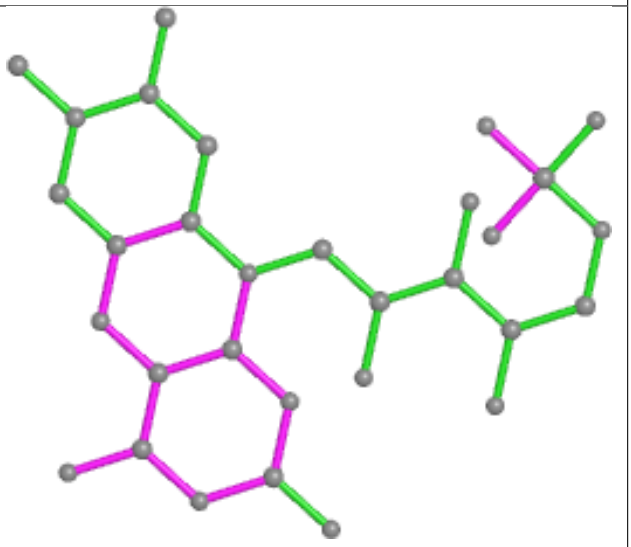
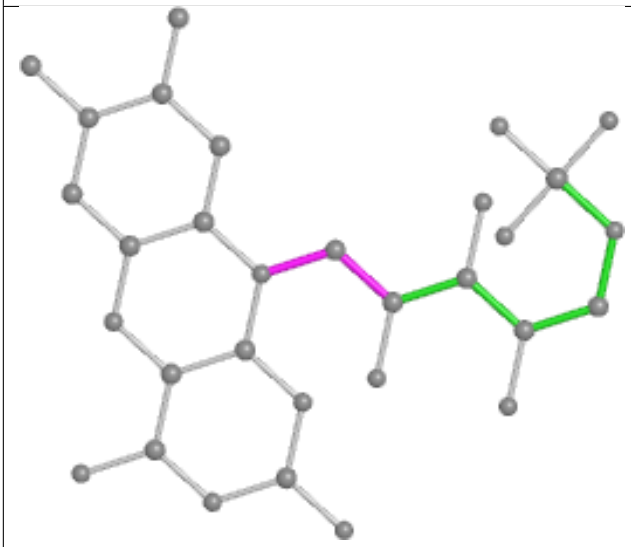


Bond angles



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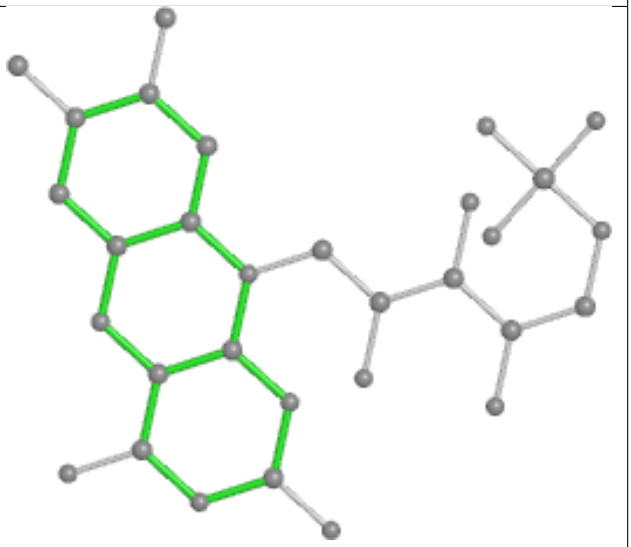
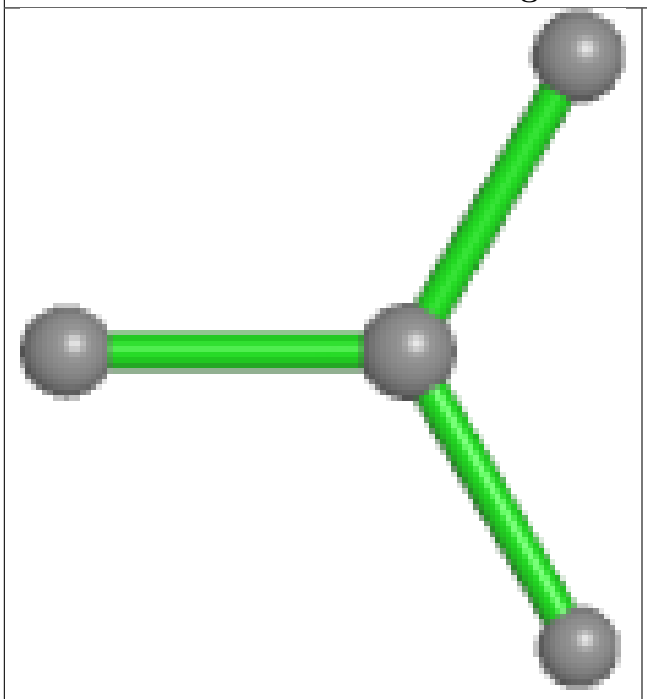


Rings

Ligand DMS G 303



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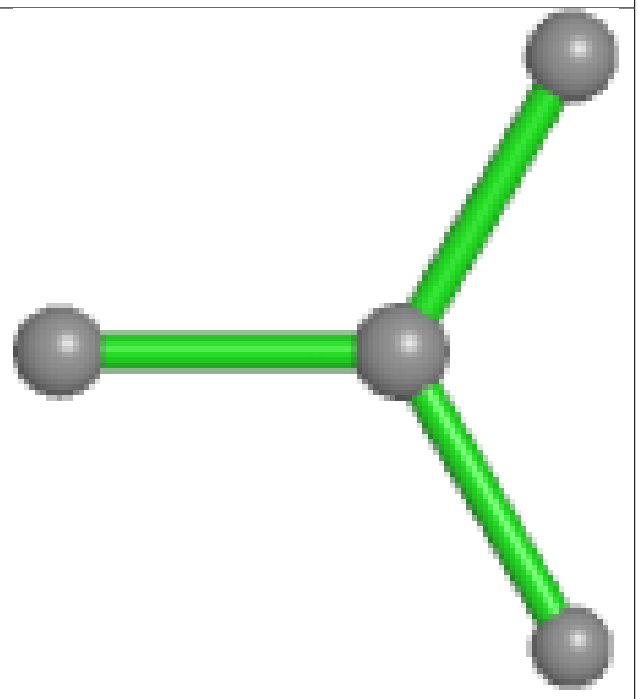
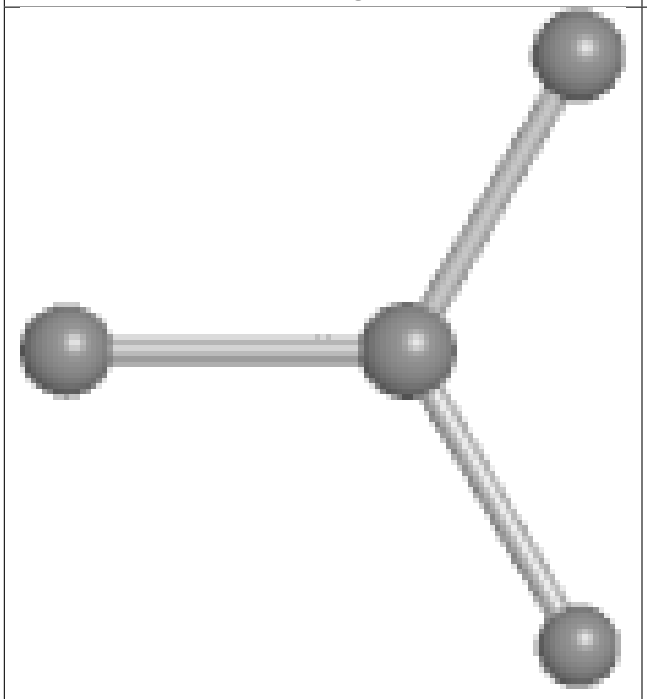


Bond angles



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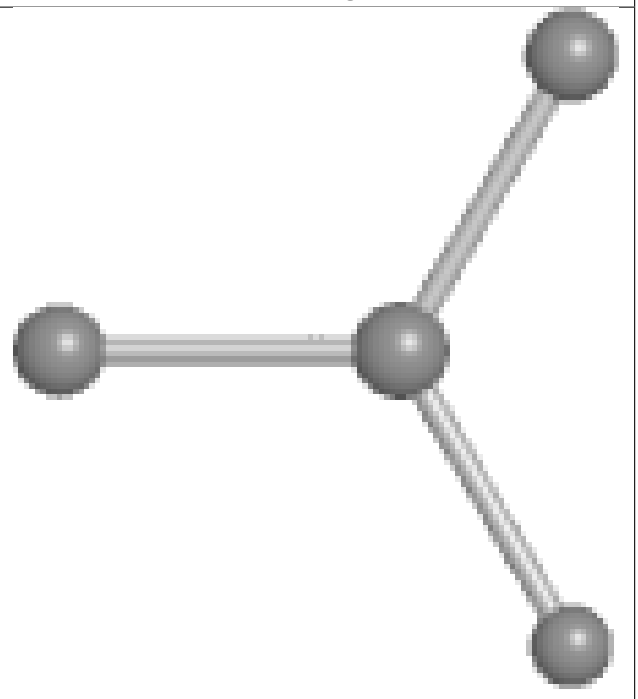
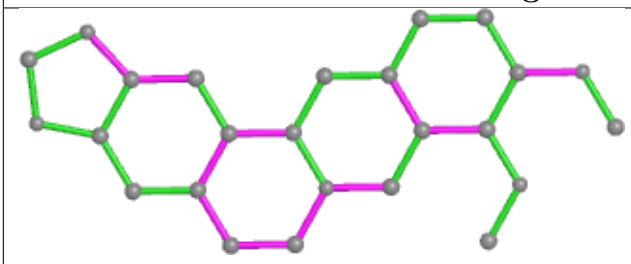


Rings

Ligand BER G 302



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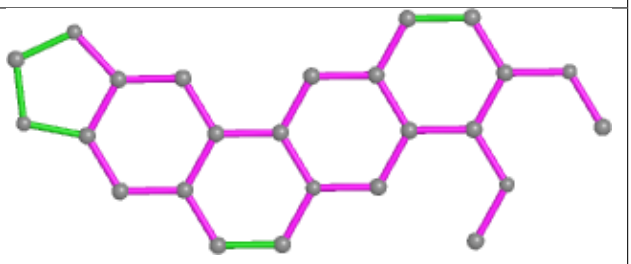
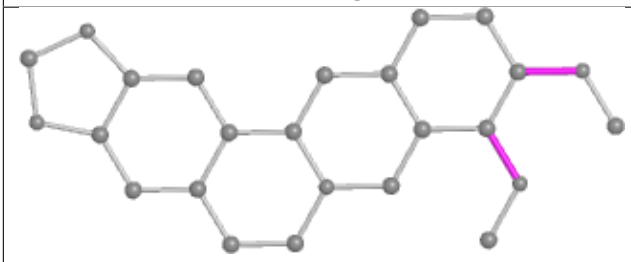


Bond angles



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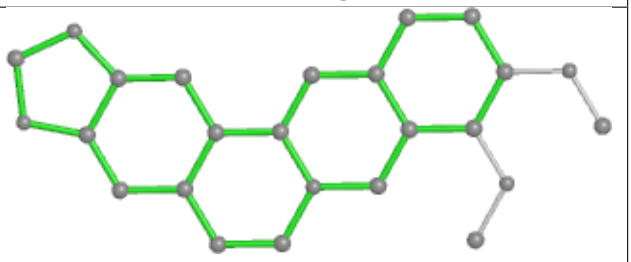
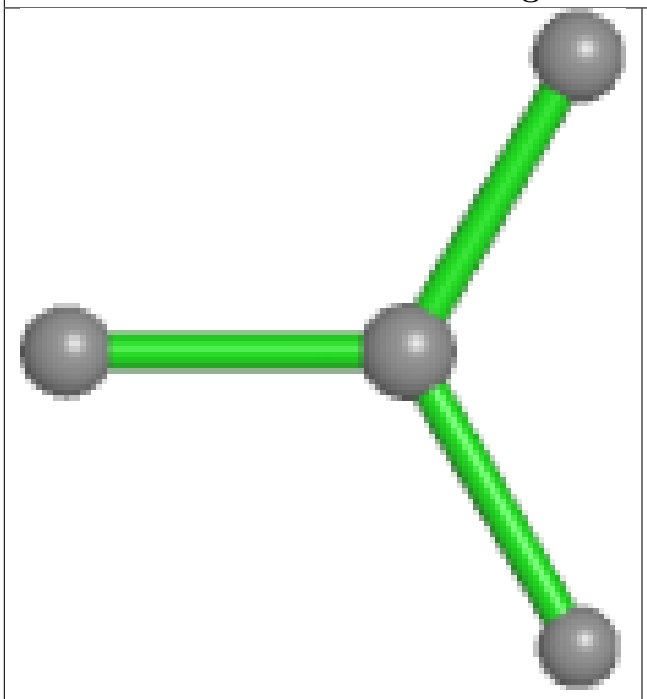


Rings

Ligand DMS B 302



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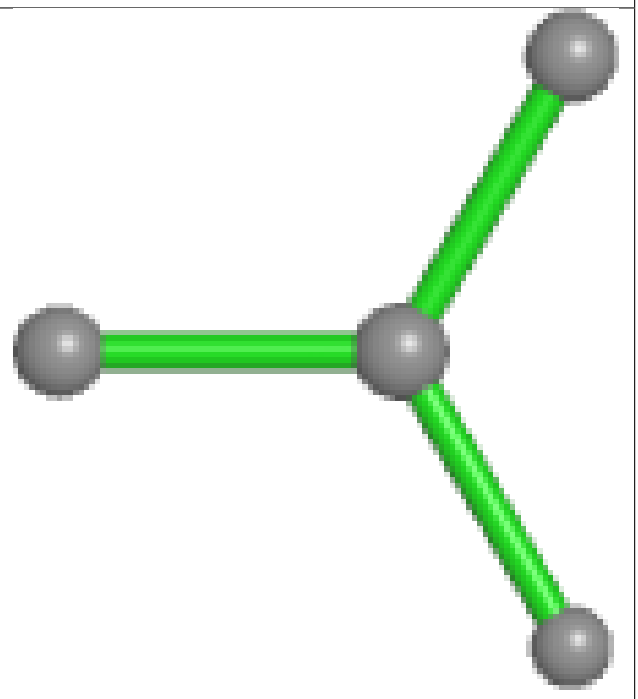

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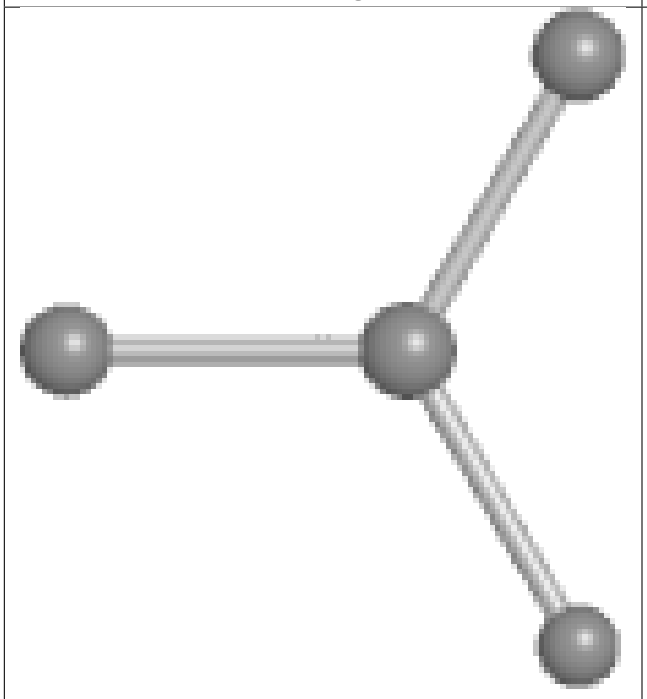

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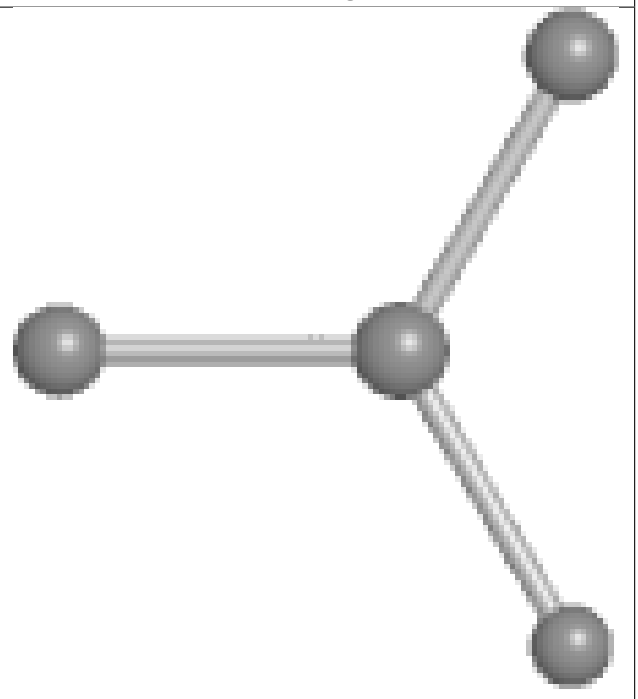
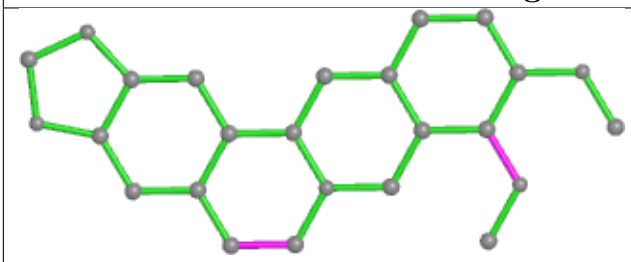
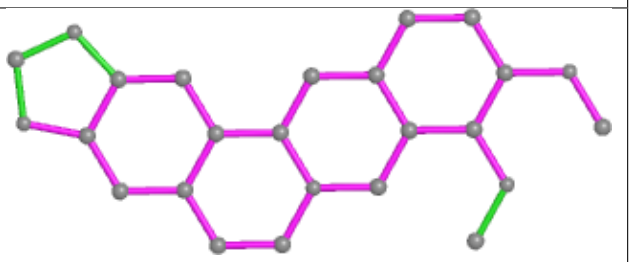


Rings

Ligand BER C 302



Bond lengths



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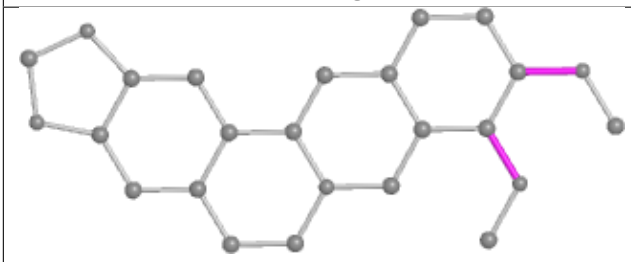

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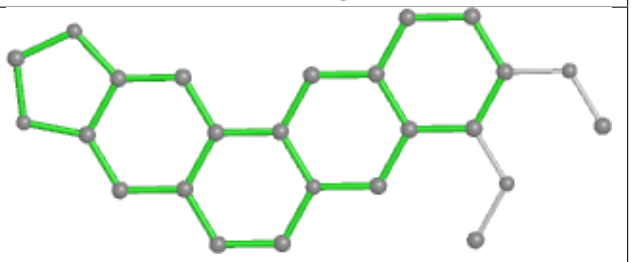
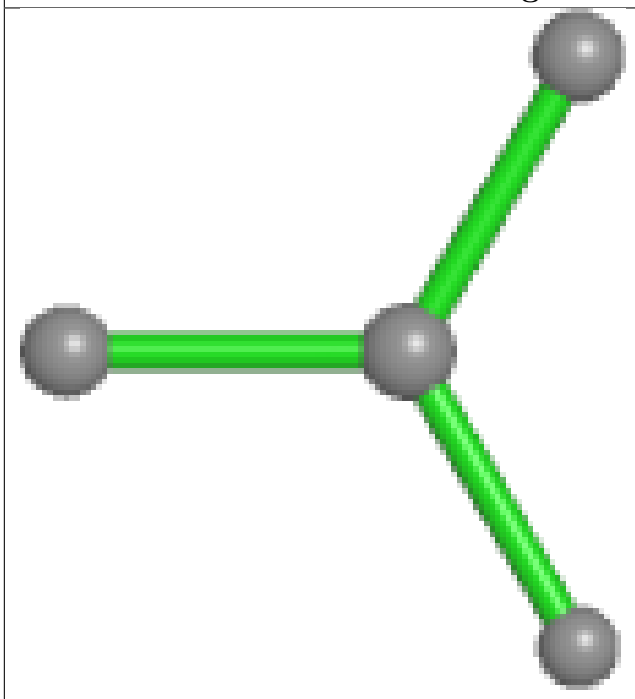


Rings

Ligand DMS C 303



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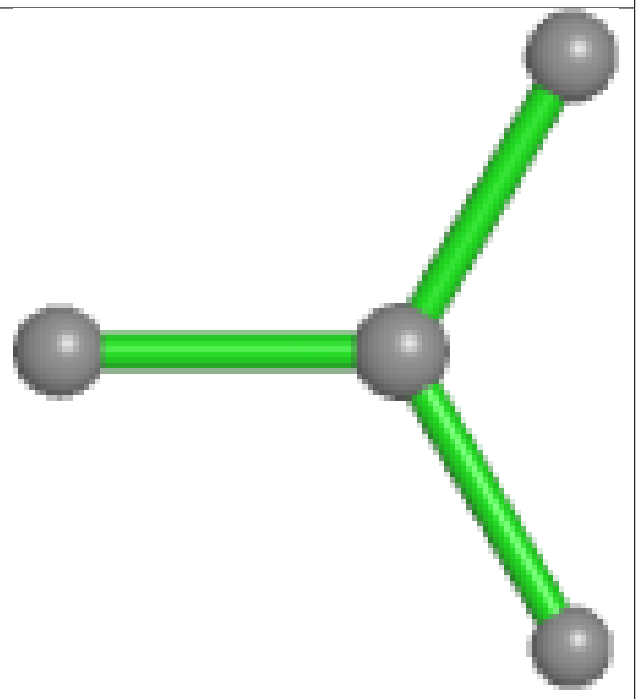
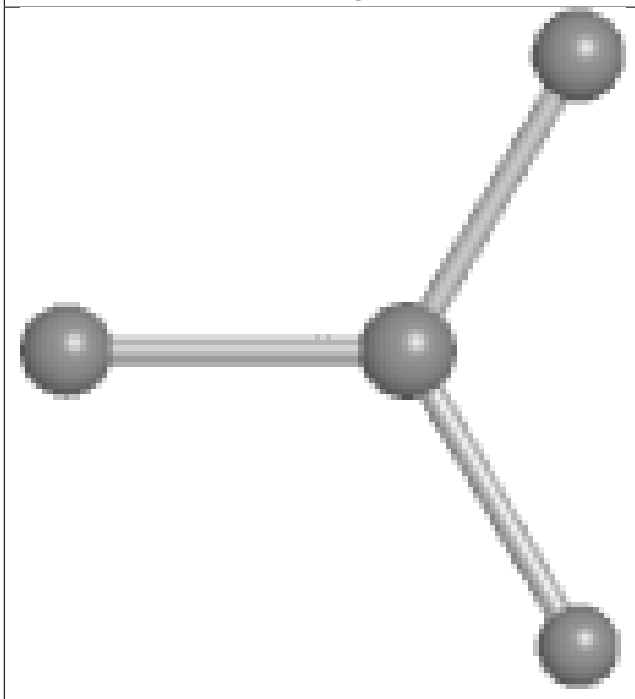
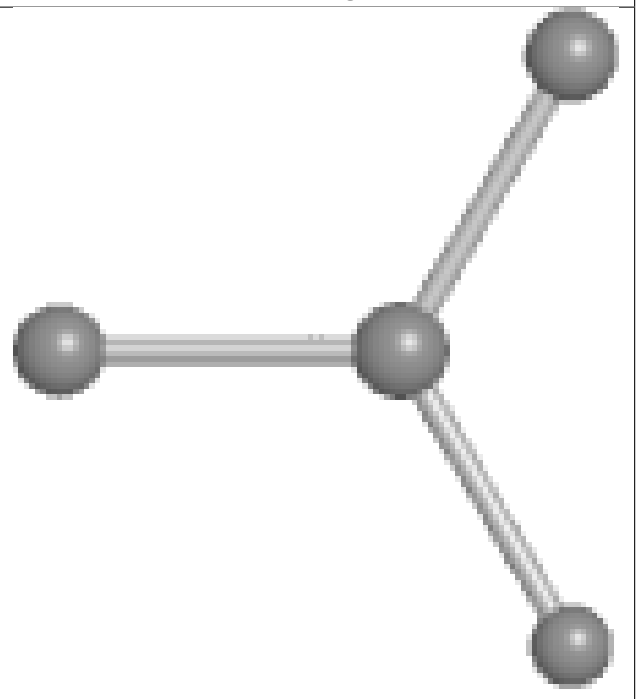


Bond angles

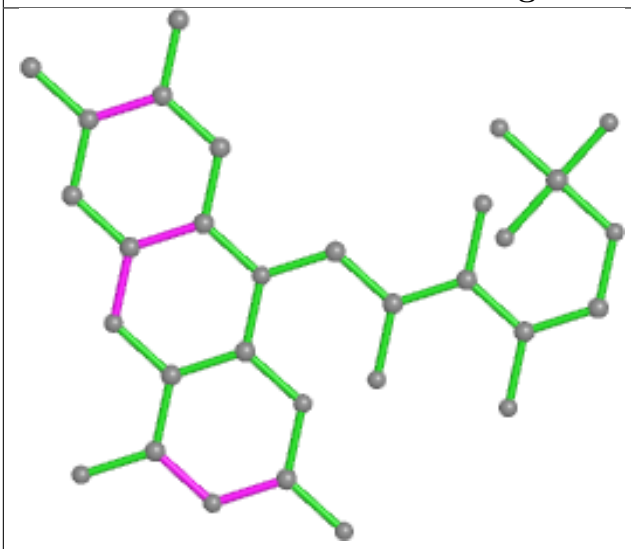


Torsions

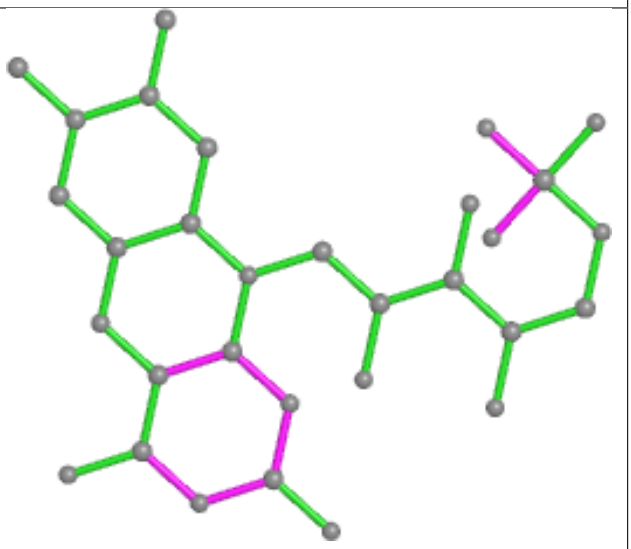


Rings

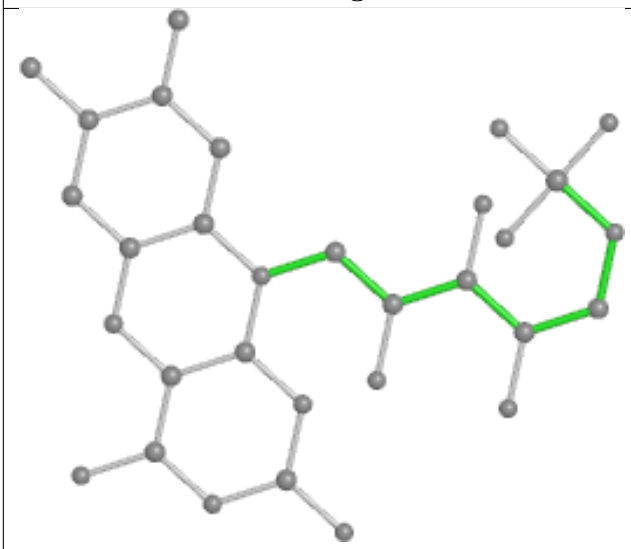
Ligand FMN D 301



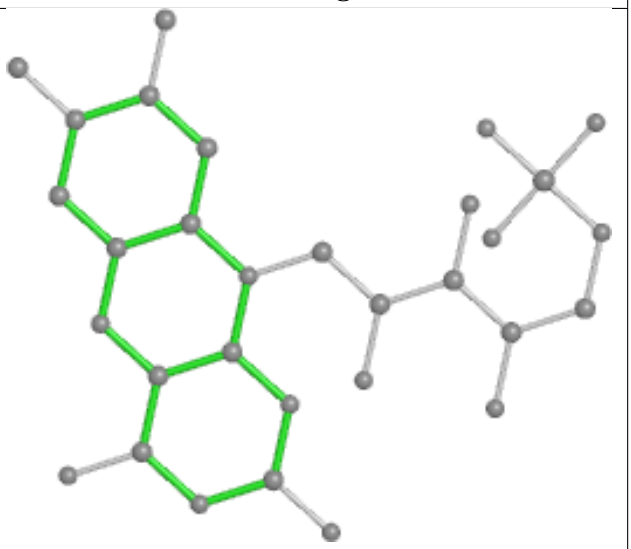
Bond lengths



Bond angles

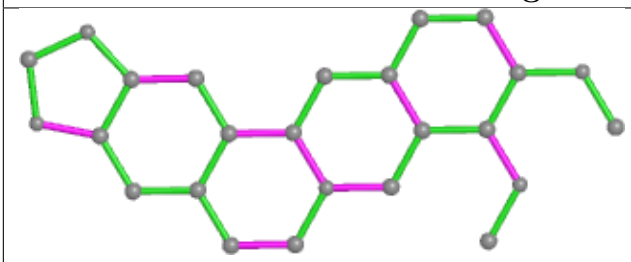


Torsions



Rings

Ligand BER H 302



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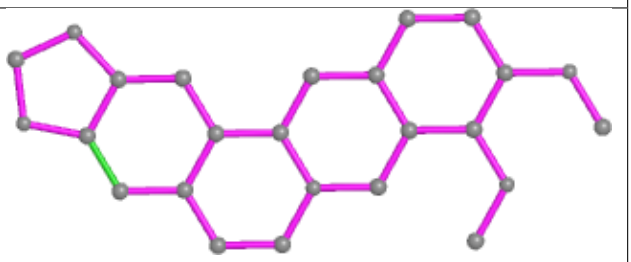
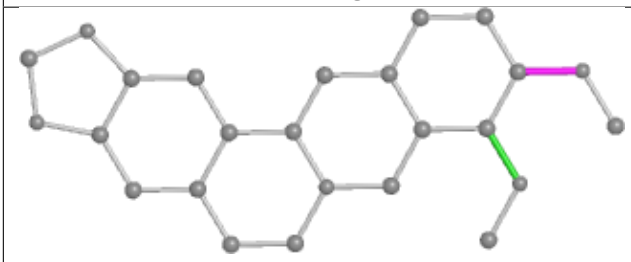


Bond angles



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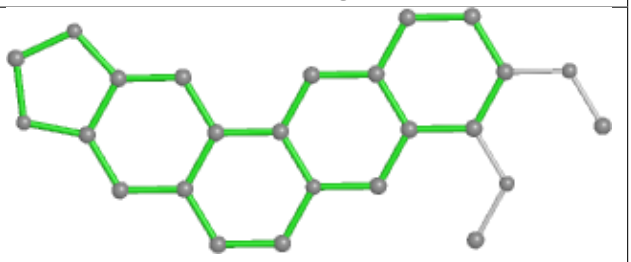
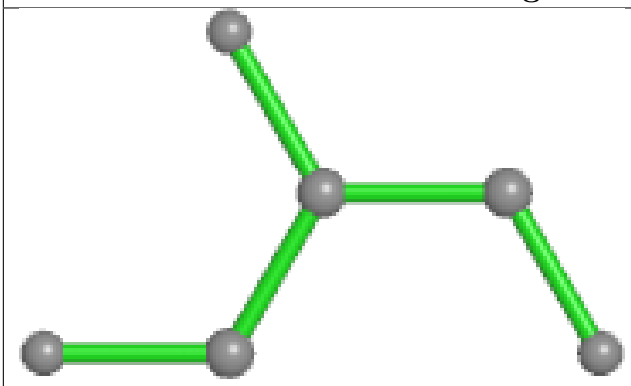


Rings

Ligand GOL A 302



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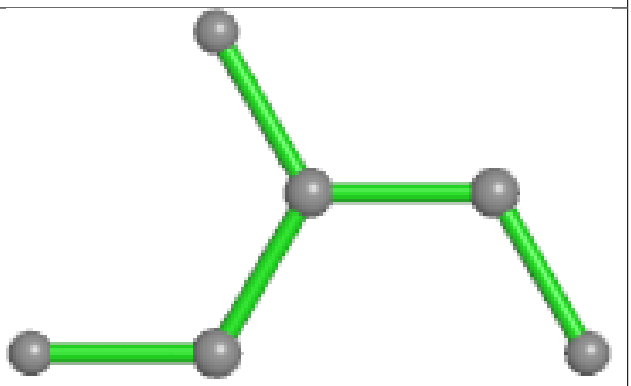
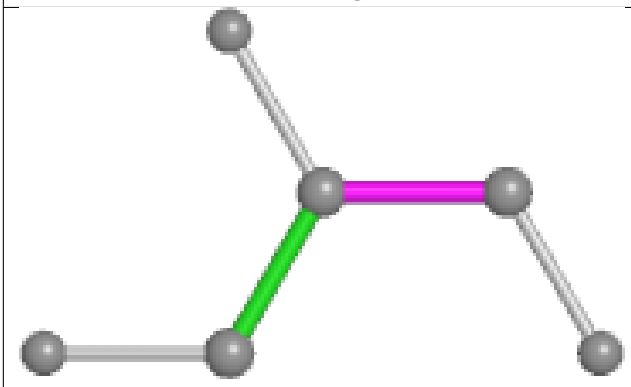


Bond angles



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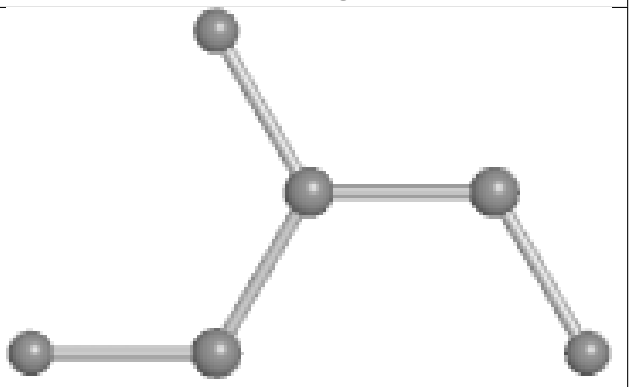
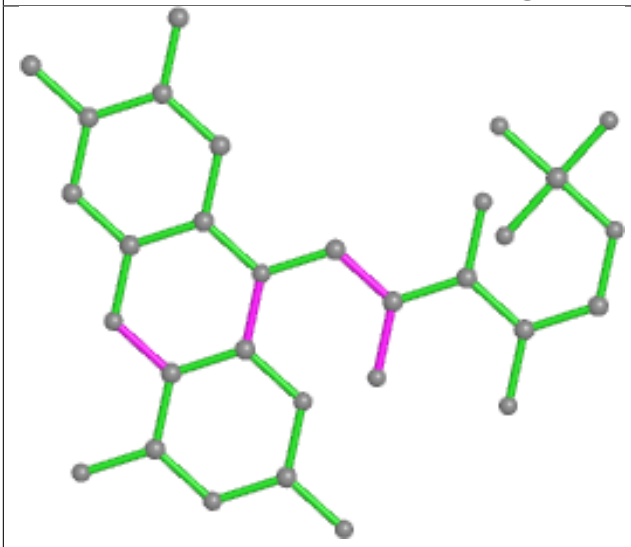


Rings

Ligand FMN A 301



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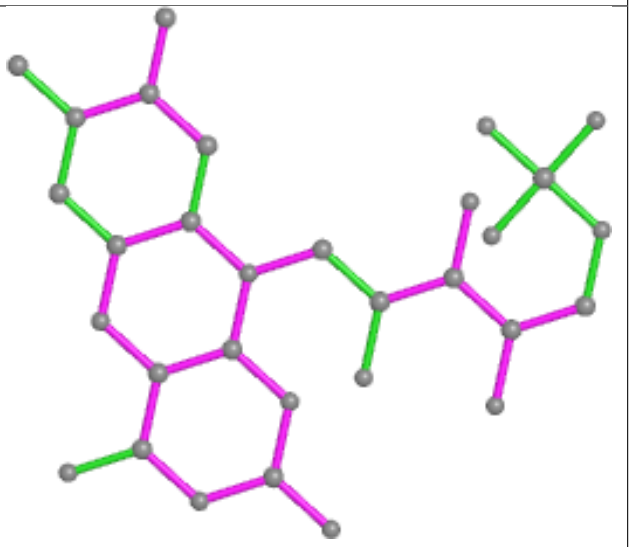
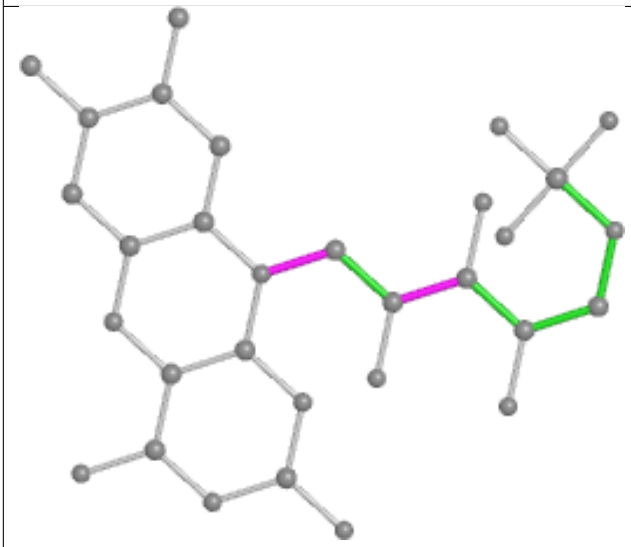


Bond angles



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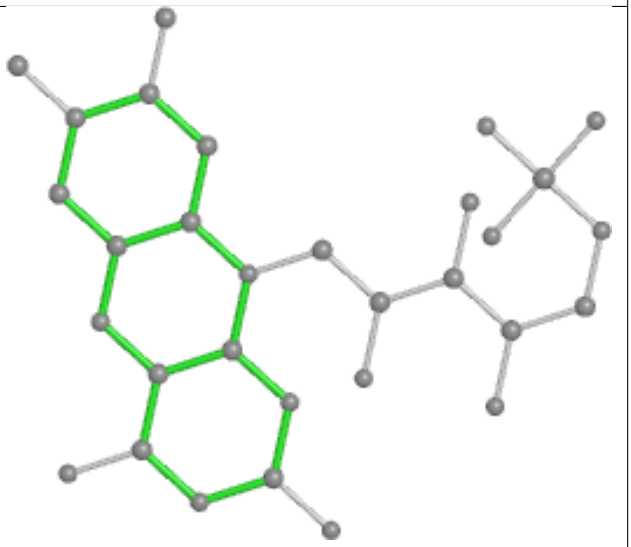
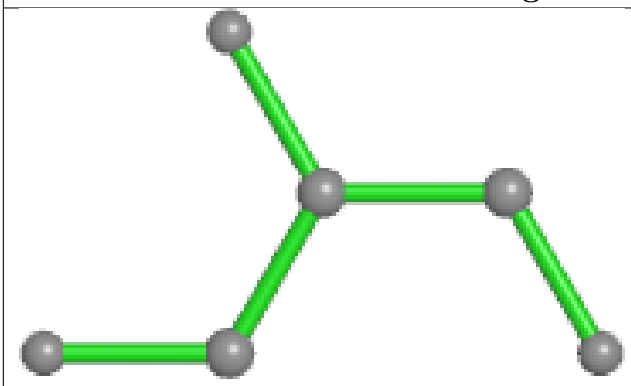


Rings

Ligand GOL D 303



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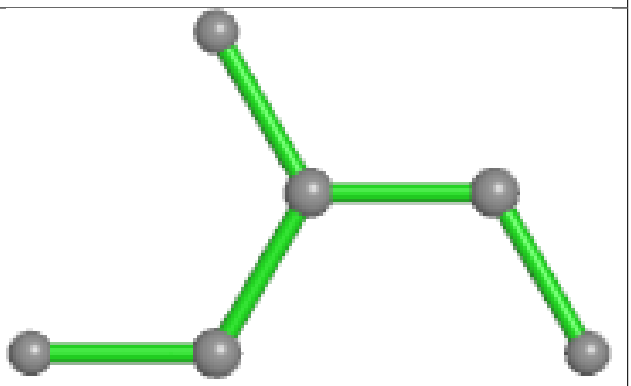
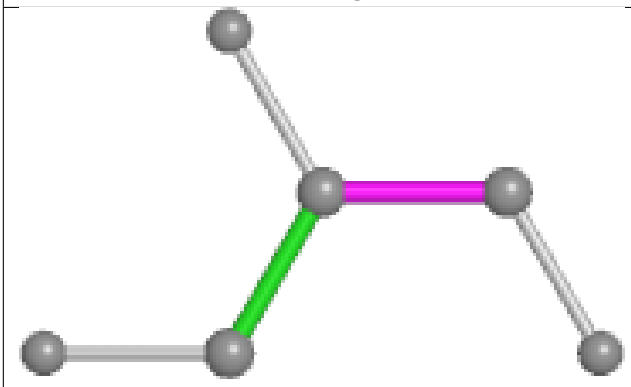
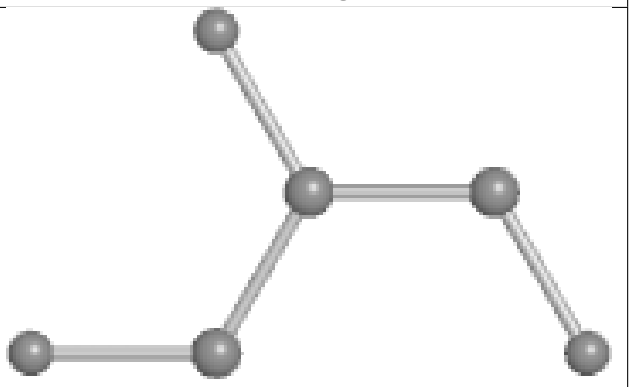


Bond angles

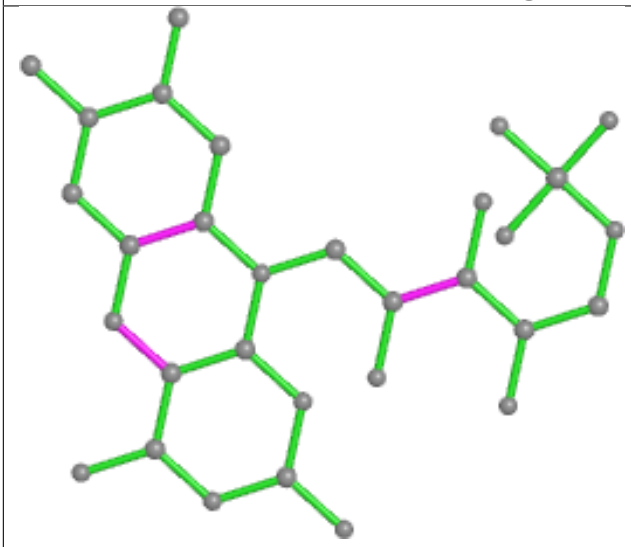


Torsions

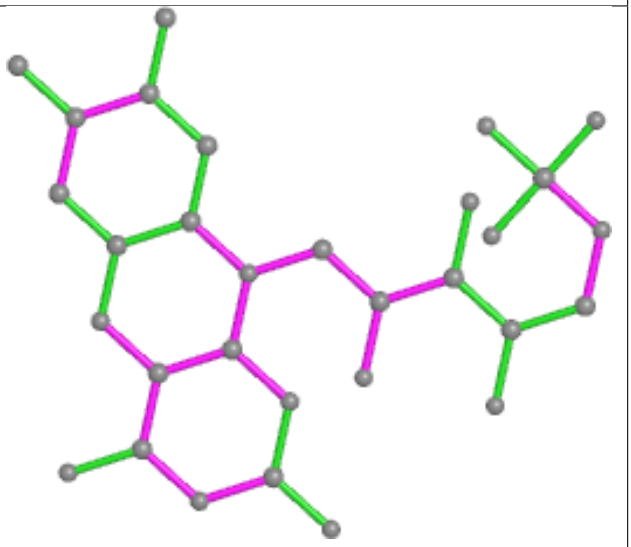


Rings

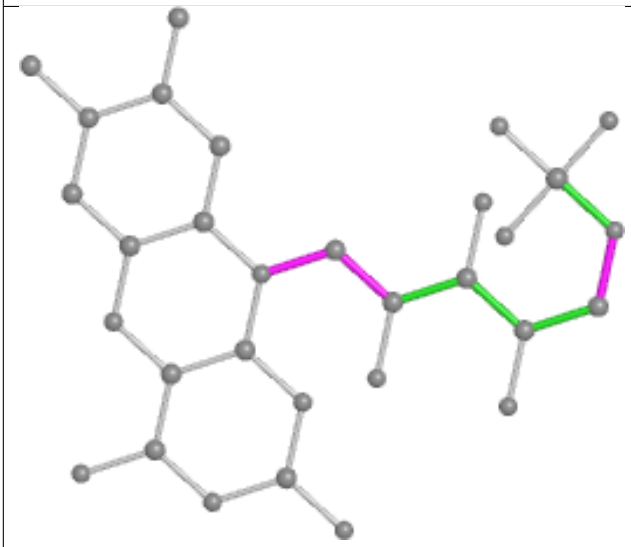
Ligand FMN E 301



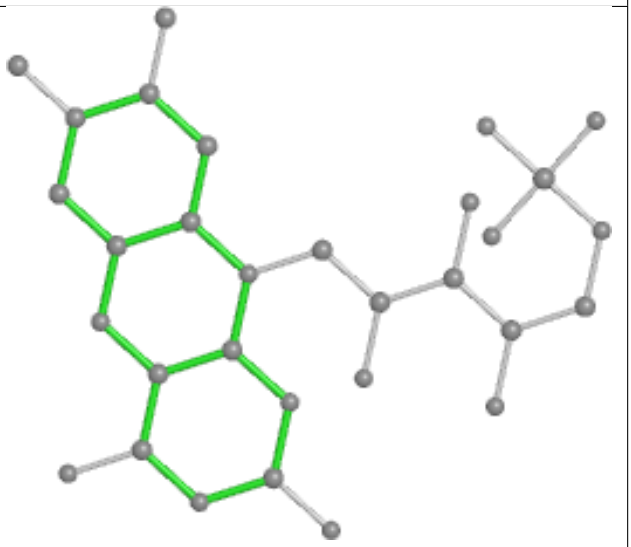
Bond lengths



Bond angles

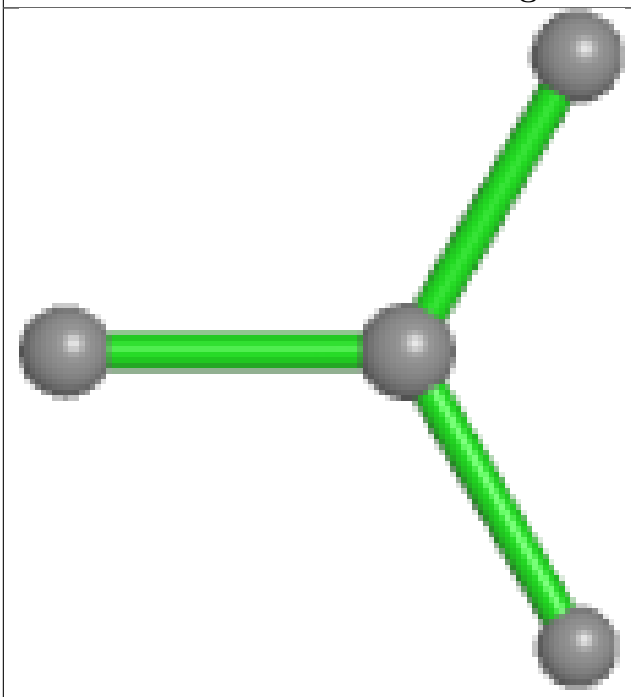


Torsions

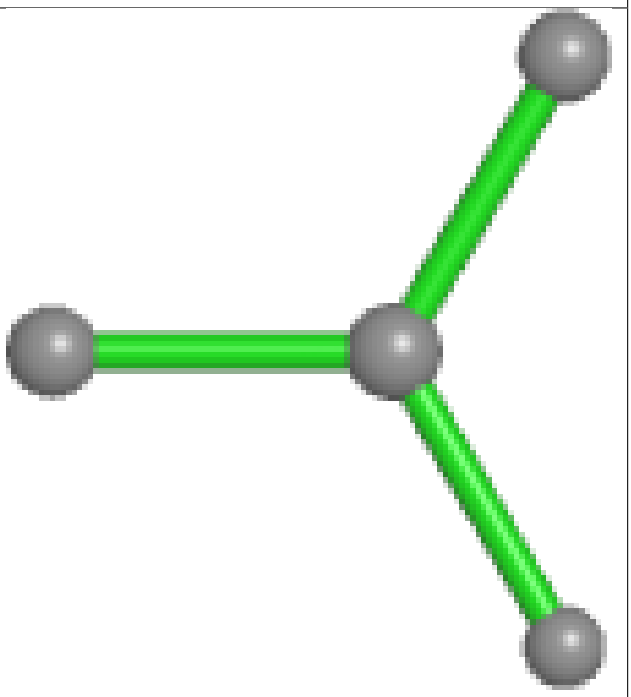


Rings

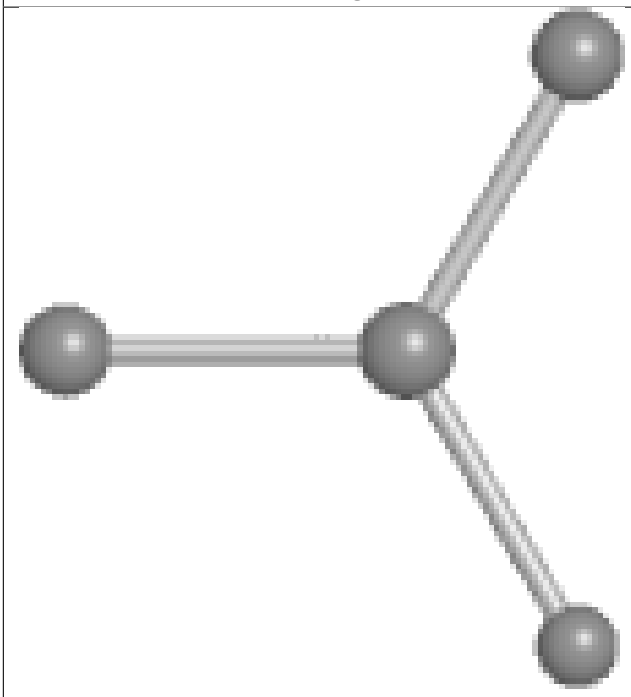
Ligand DMS H 304



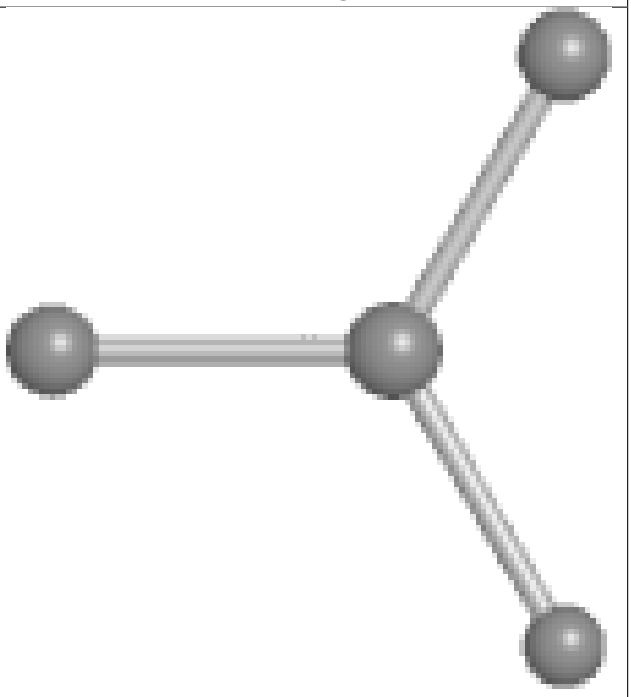
Bond lengths



Bond angles

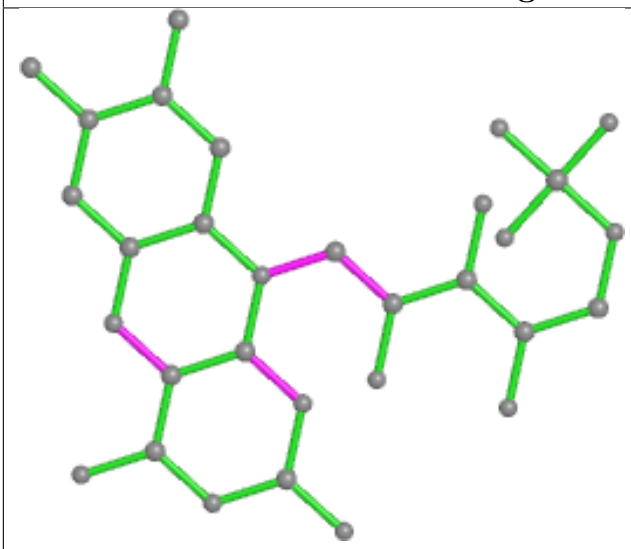


Torsions

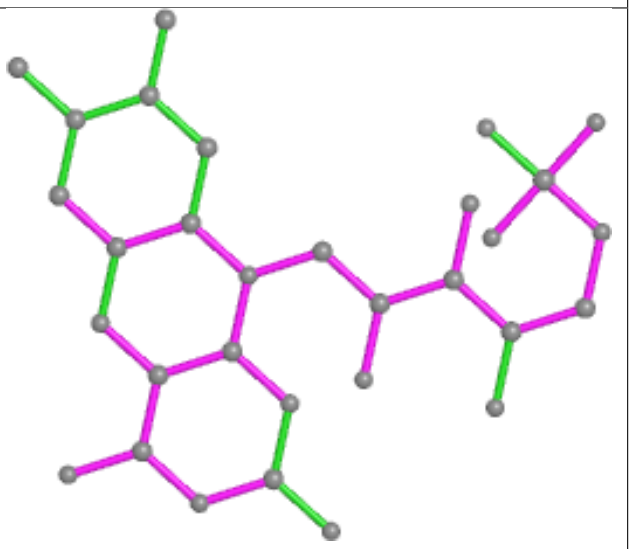


Rings

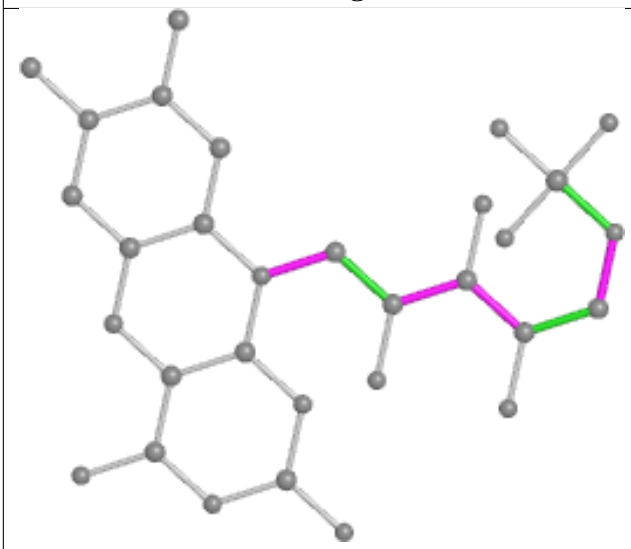
Ligand FMN H 301



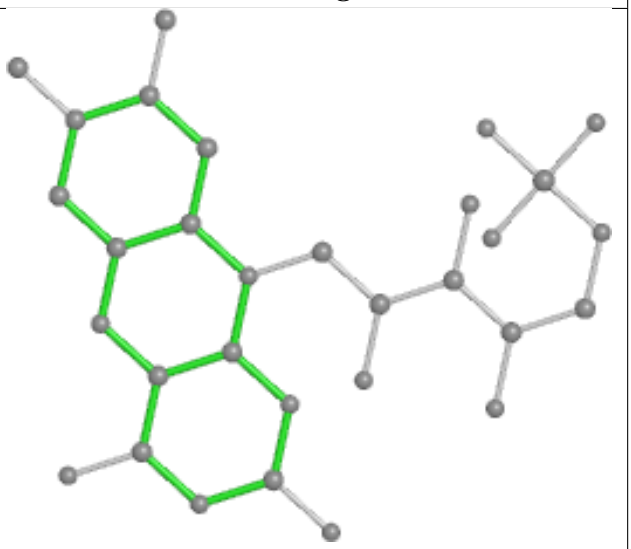
Bond lengths



Bond angles

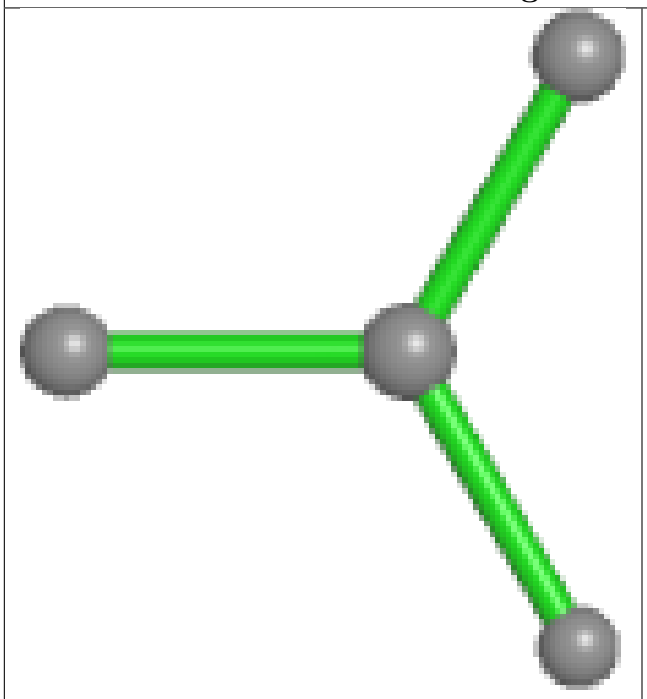


Torsions

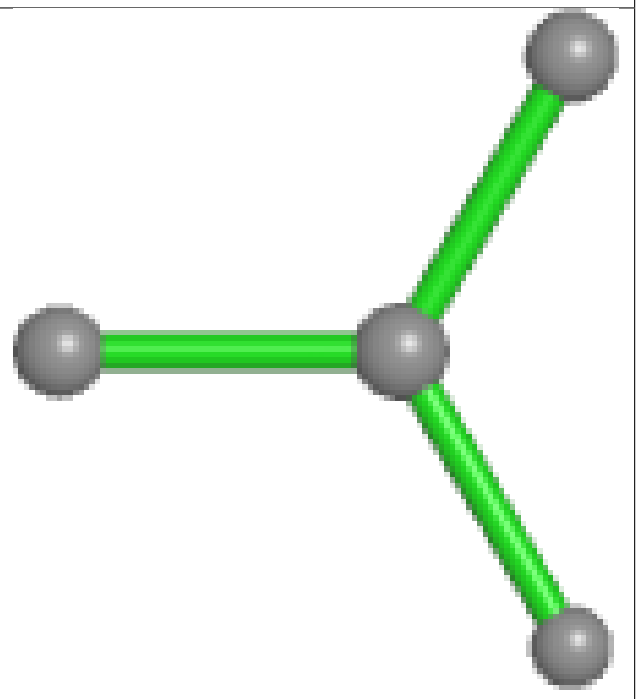


Rings

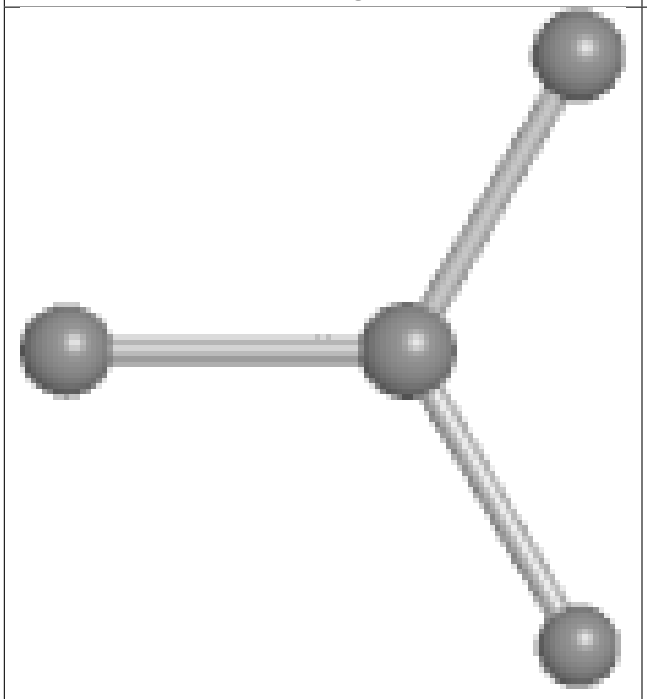
Ligand DMS D 304



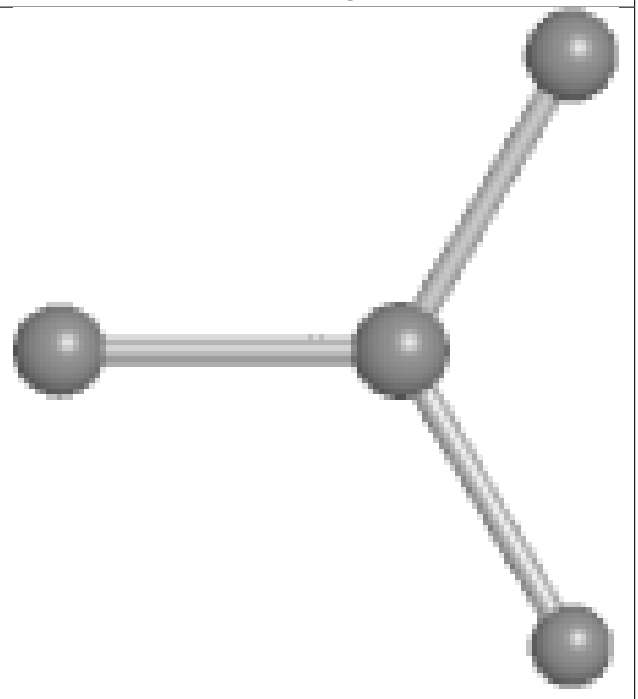
Bond lengths



Bond angles

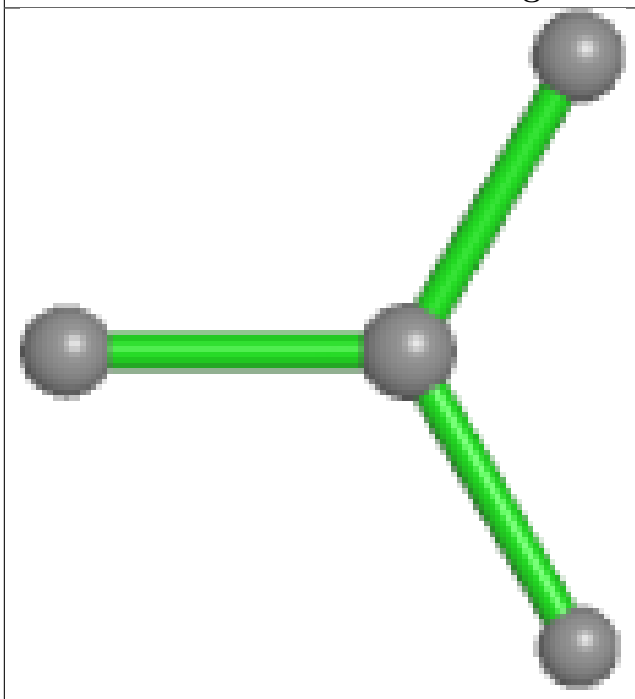


Torsions

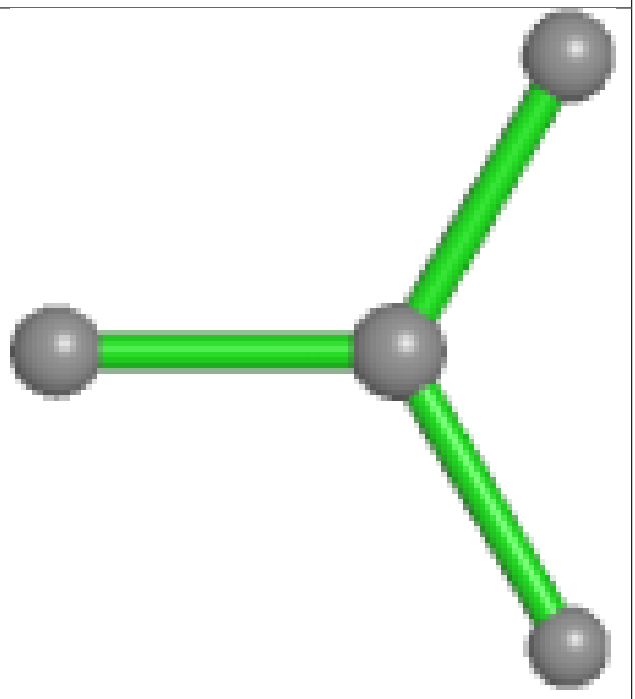


Rings

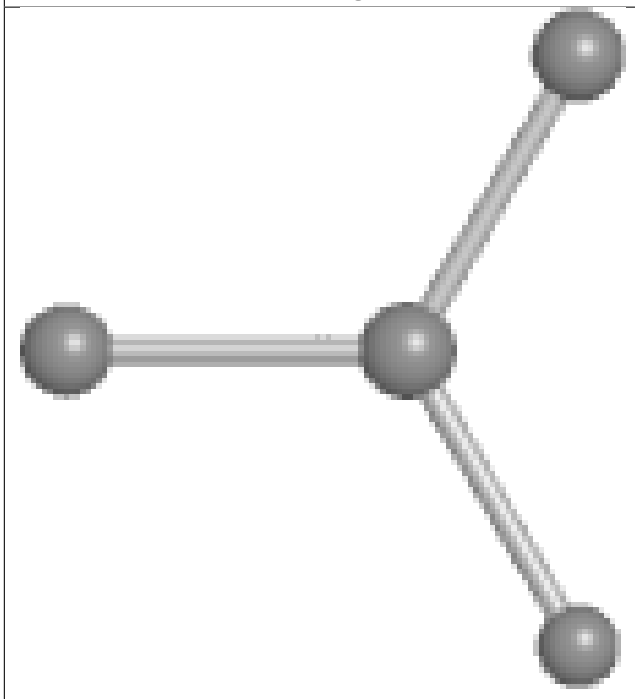
Ligand DMS E 303



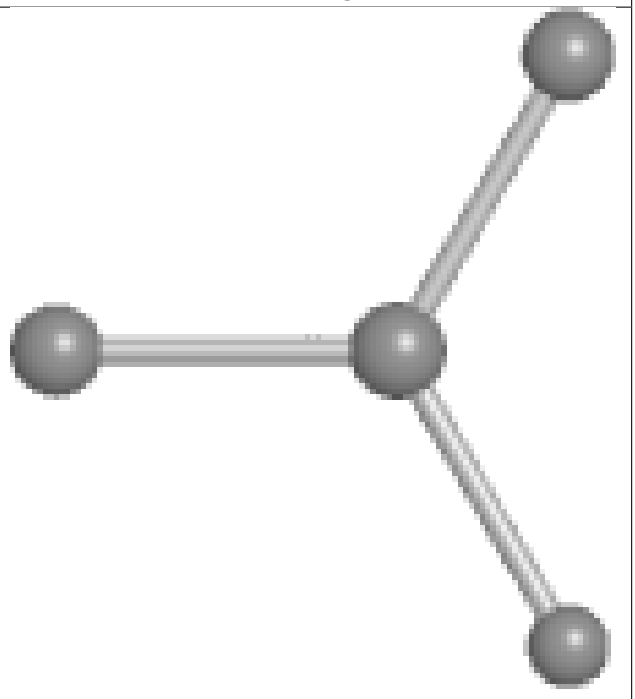
Bond lengths



Bond angles

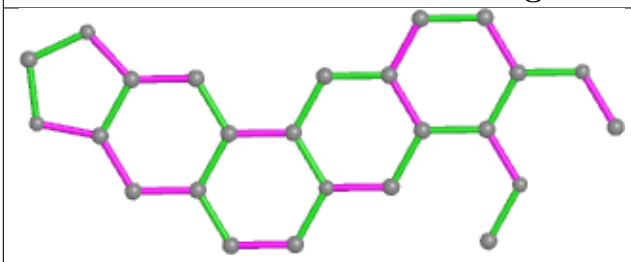


Torsions

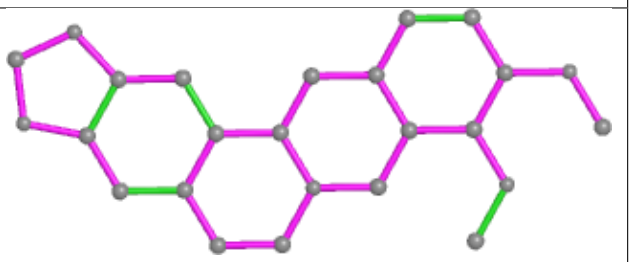


Rings

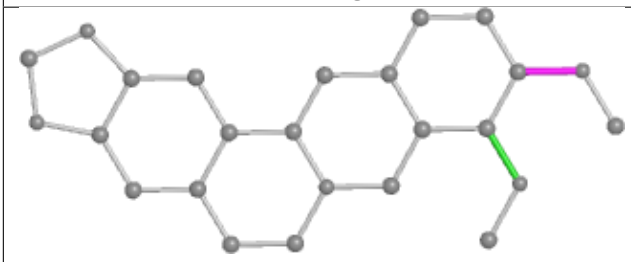
Ligand BER E 302



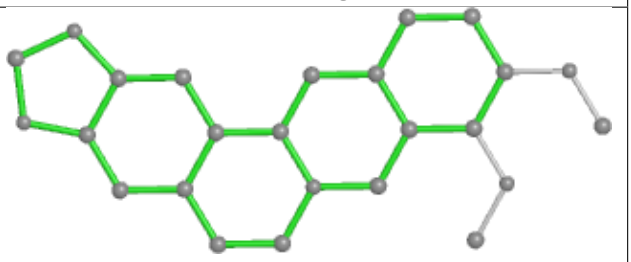
Bond lengths



Bond angles

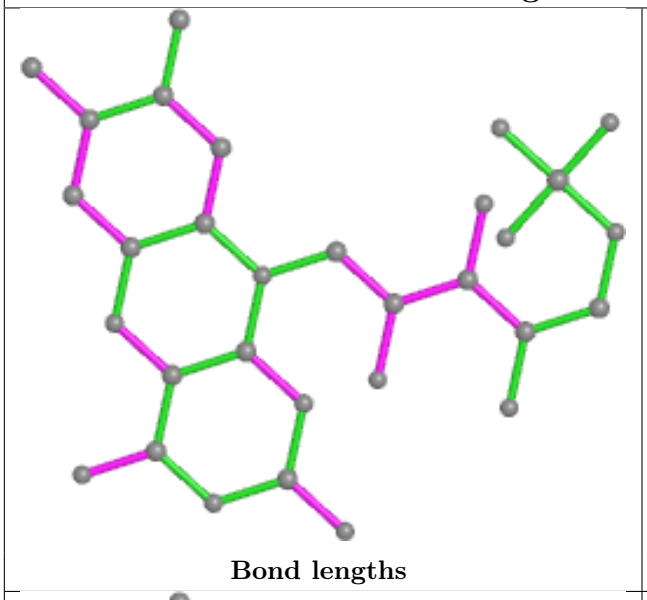


Torsions

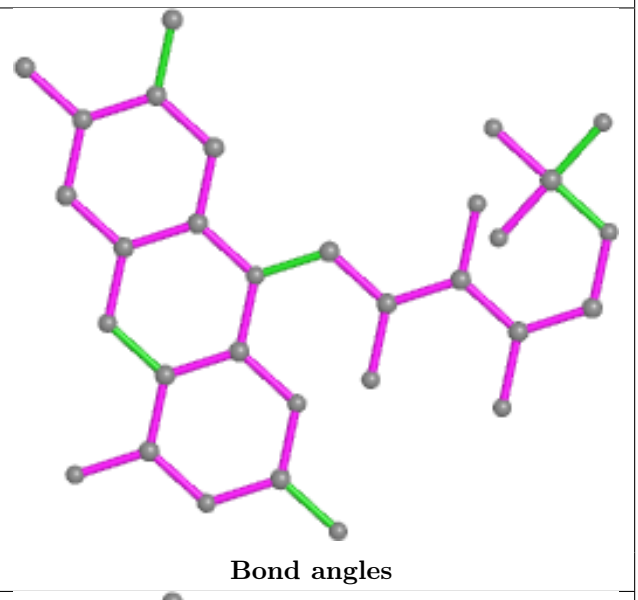


Rings

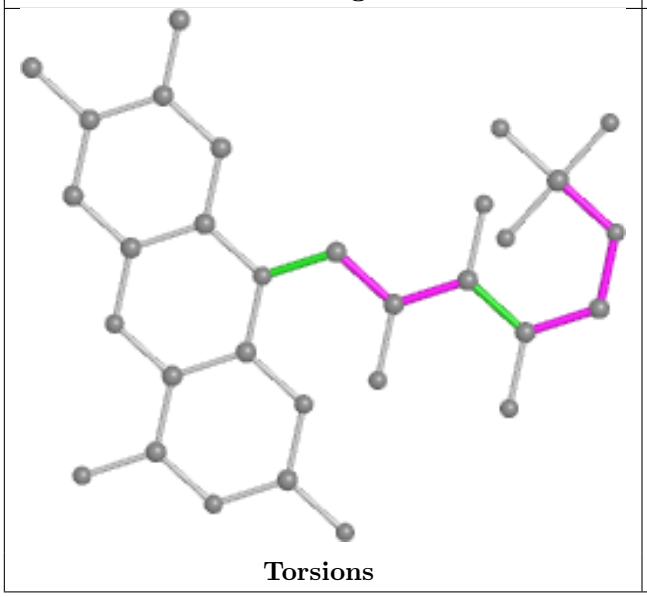
Ligand FMN F 301



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, 95^{th} 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	216/217 (99%)	0.27	5 (2%) 60 56	17, 27, 52, 58	0
1	B	216/217 (99%)	0.06	6 (2%) 53 48	18, 28, 50, 53	0
1	C	216/217 (99%)	0.23	7 (3%) 47 42	19, 33, 45, 57	0
1	D	216/217 (99%)	0.24	9 (4%) 36 30	17, 31, 47, 55	0
1	E	217/217 (100%)	0.02	3 (1%) 75 72	19, 28, 48, 55	0
1	F	216/217 (99%)	0.37	12 (5%) 24 19	19, 27, 51, 59	0
1	G	217/217 (100%)	0.12	2 (0%) 84 82	20, 32, 46, 57	0
1	H	216/217 (99%)	0.14	8 (3%) 41 36	19, 32, 47, 54	0
All	All	1730/1736 (99%)	0.18	52 (3%) 50 44	17, 30, 49, 59	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	PHE	7.1
1	C	65	ALA	5.9
1	F	123	PHE	5.8
1	H	202	THR	3.4
1	G	65	ALA	3.4
1	G	1	MET	3.4
1	D	66	GLY	3.4
1	C	66	GLY	3.3
1	C	179	LYS	3.3
1	D	65	ALA	3.1
1	D	70	PHE	3.1
1	F	124	PHE	3.0
1	H	197	GLU	3.0
1	C	170	ALA	3.0
1	E	65	ALA	2.9
1	F	119	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	69	VAL	2.7
1	F	112	GLU	2.7
1	F	131	ASP	2.7
1	F	217	VAL	2.6
1	B	92	ASP	2.6
1	F	67	ASN	2.6
1	H	133	HIS	2.6
1	H	131	ASP	2.6
1	B	109	ALA	2.5
1	F	132	LEU	2.5
1	A	109	ALA	2.5
1	H	67	ASN	2.5
1	A	112	GLU	2.5
1	C	180	GLU	2.4
1	F	65	ALA	2.4
1	B	129	ARG	2.4
1	C	123	PHE	2.4
1	A	120	GLY	2.4
1	F	180	GLU	2.4
1	D	129	ARG	2.3
1	D	170	ALA	2.3
1	B	67	ASN	2.3
1	A	111	PRO	2.3
1	B	65	ALA	2.3
1	C	18	ALA	2.2
1	F	120	GLY	2.2
1	F	108	PHE	2.2
1	H	65	ALA	2.2
1	B	131	ASP	2.1
1	D	179	LYS	2.1
1	E	92	ASP	2.1
1	D	168	ASP	2.0
1	D	69	VAL	2.0
1	D	171	ILE	2.0
1	H	132	LEU	2.0
1	E	1	MET	2.0

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)

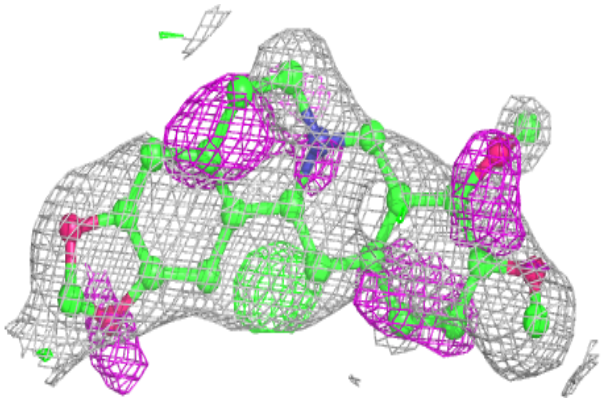
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

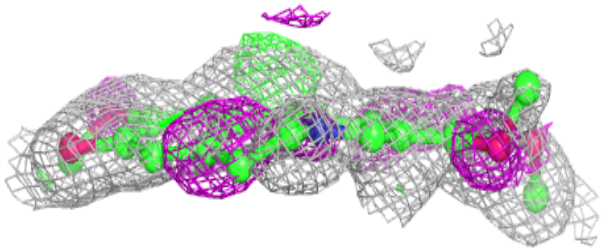
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BER	H	302	25/25	0.67	0.36	33,37,43,52	0
5	BER	D	302	25/25	0.70	0.33	30,39,44,46	0
5	BER	G	302	25/25	0.70	0.39	29,43,47,48	0
5	BER	C	302	25/25	0.70	0.29	31,38,44,48	0
3	GOL	D	303	6/6	0.76	0.20	37,39,43,46	0
5	BER	E	302	25/25	0.77	0.27	39,46,49,50	0
4	DMS	B	302	4/4	0.80	0.14	34,52,53,58	0
4	DMS	D	304	4/4	0.81	0.19	38,39,42,55	0
3	GOL	A	302	6/6	0.85	0.20	29,32,33,35	0
4	DMS	E	303	4/4	0.86	0.14	18,30,40,41	0
4	DMS	C	303	4/4	0.89	0.16	39,41,46,55	0
2	FMN	H	301	31/31	0.90	0.14	26,30,38,40	0
2	FMN	D	301	31/31	0.90	0.13	25,29,36,42	0
2	FMN	F	301	31/31	0.90	0.16	18,24,32,34	0
2	FMN	C	301	31/31	0.92	0.14	25,29,38,46	0
2	FMN	E	301	31/31	0.92	0.12	20,25,30,35	0
3	GOL	H	303	6/6	0.92	0.13	34,38,46,47	0
2	FMN	A	301	31/31	0.93	0.13	18,21,26,29	0
2	FMN	B	301	31/31	0.93	0.11	19,23,31,37	0
4	DMS	G	303	4/4	0.93	0.20	38,46,47,56	0
2	FMN	G	301	31/31	0.93	0.11	24,29,37,39	0
4	DMS	H	304	4/4	0.94	0.21	37,43,43,55	0

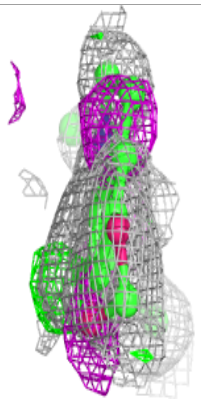
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BER H 302:

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

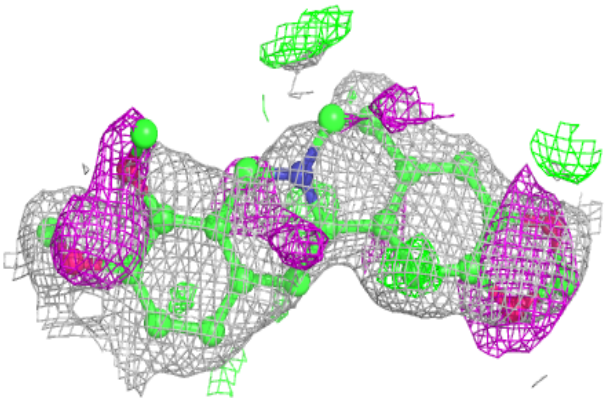


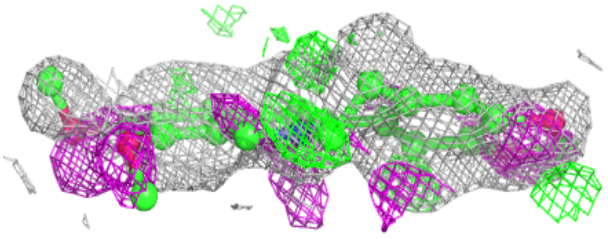


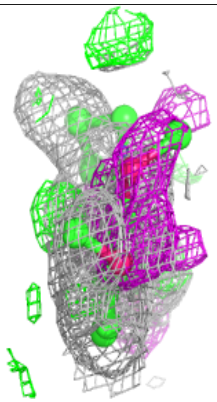


Electron density around BER D 302:

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

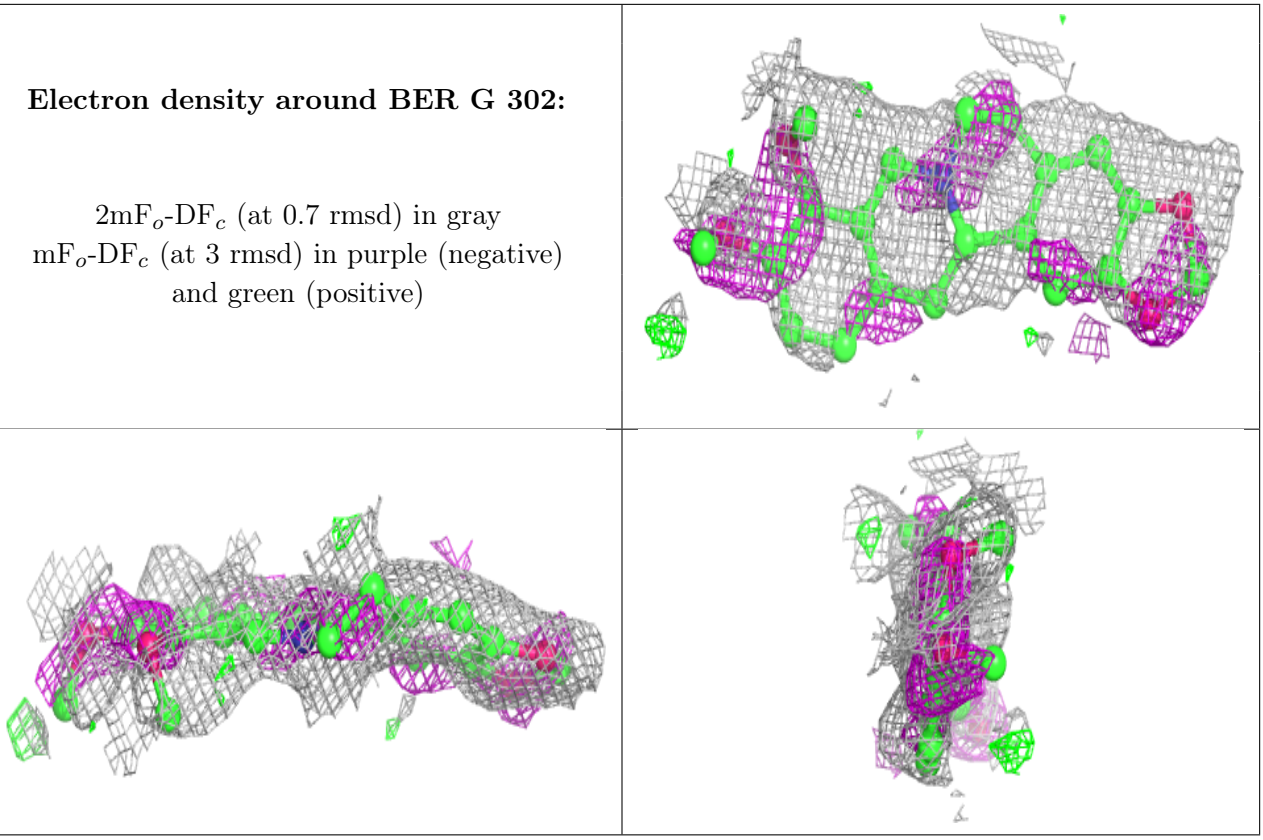






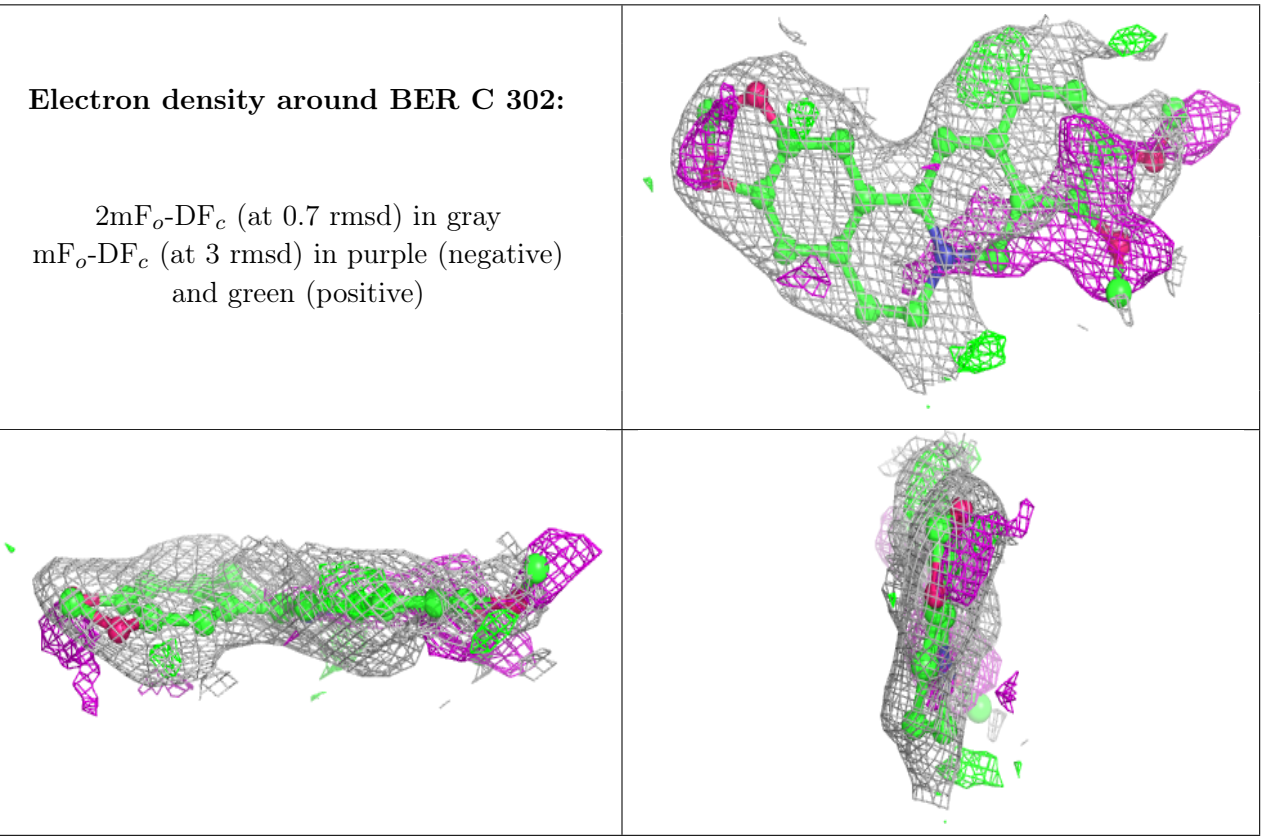
Electron density around BER G 302:

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



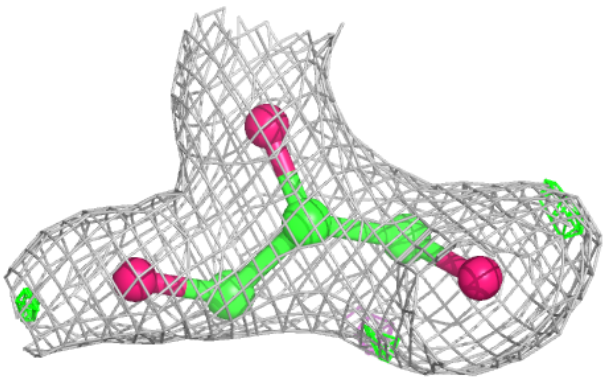
Electron density around BER C 302:

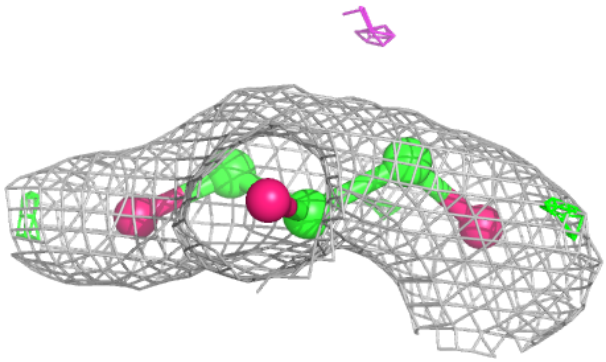
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

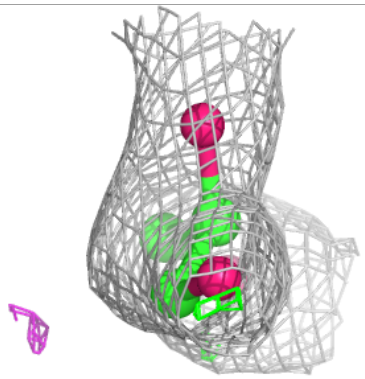


Electron density around GOL D 303:

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

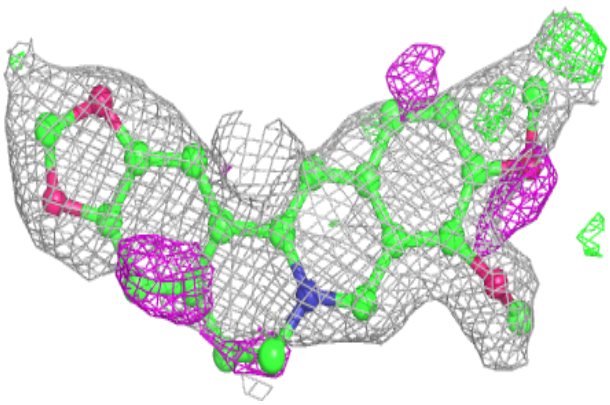


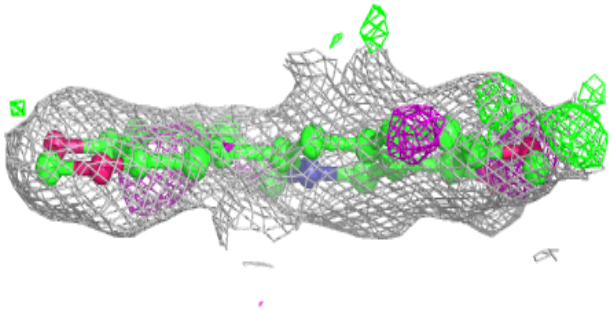


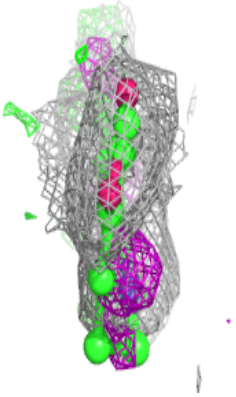


Electron density around BER E 302:

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

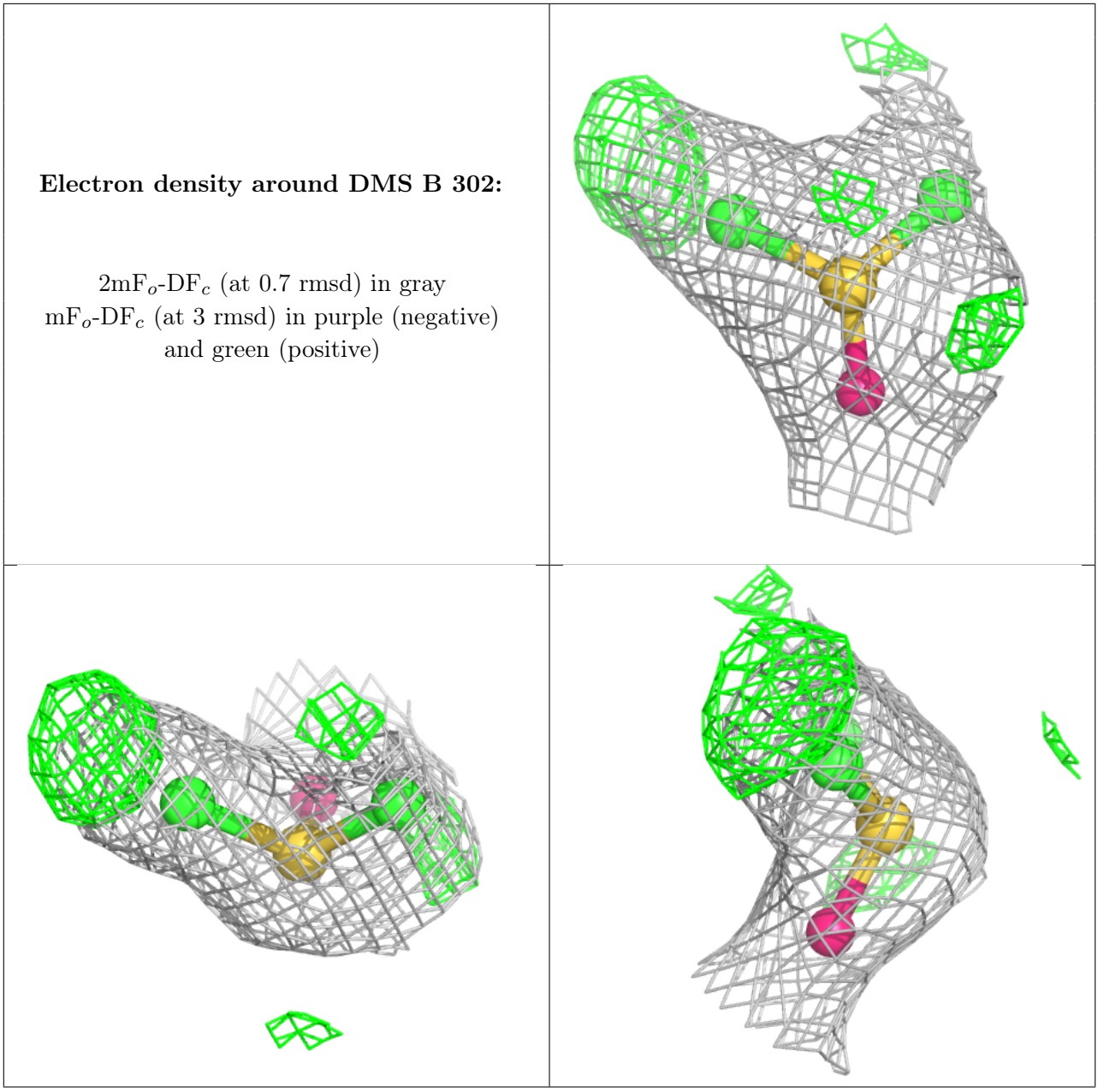






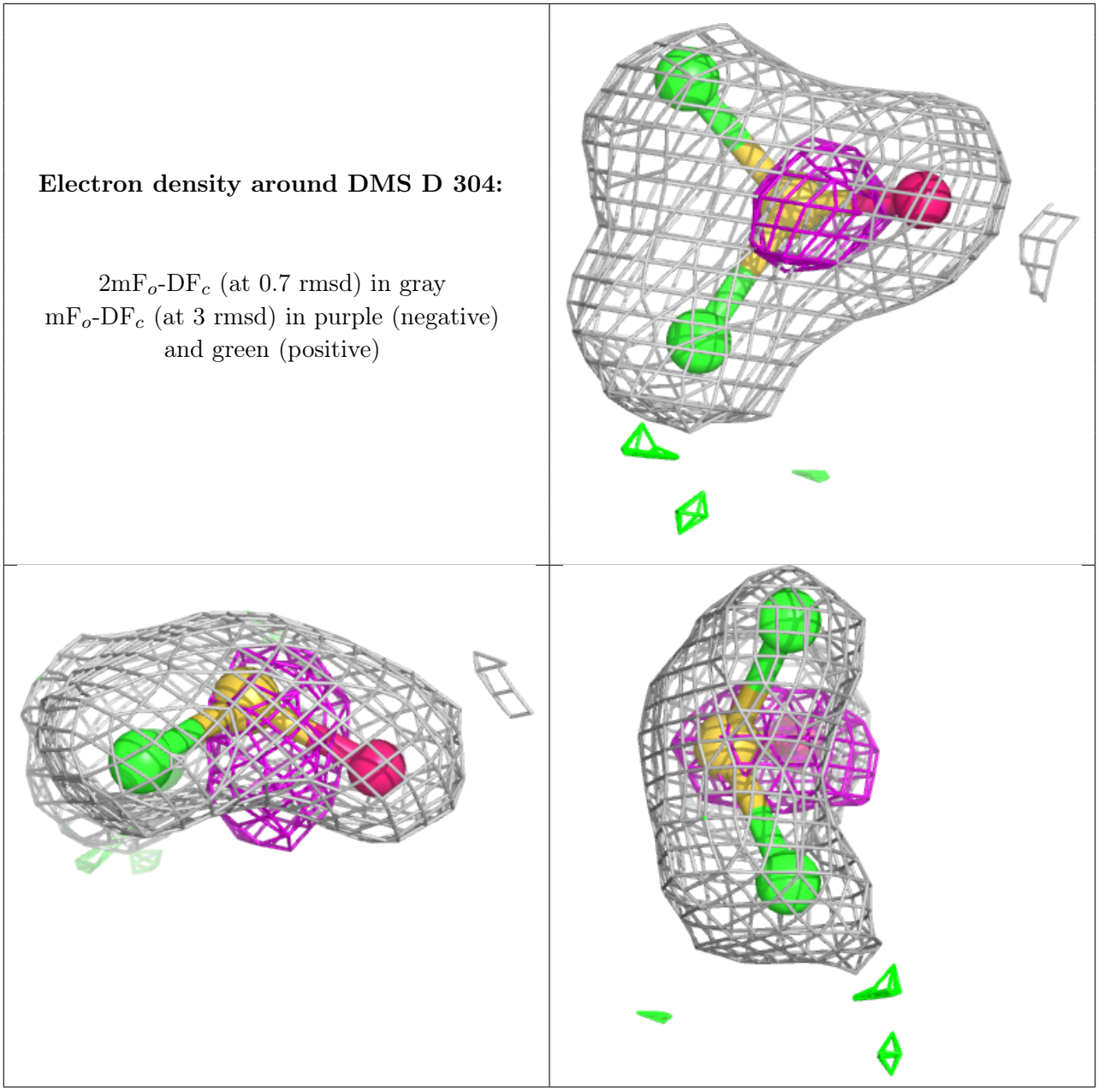
Electron density around DMS B 302:

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



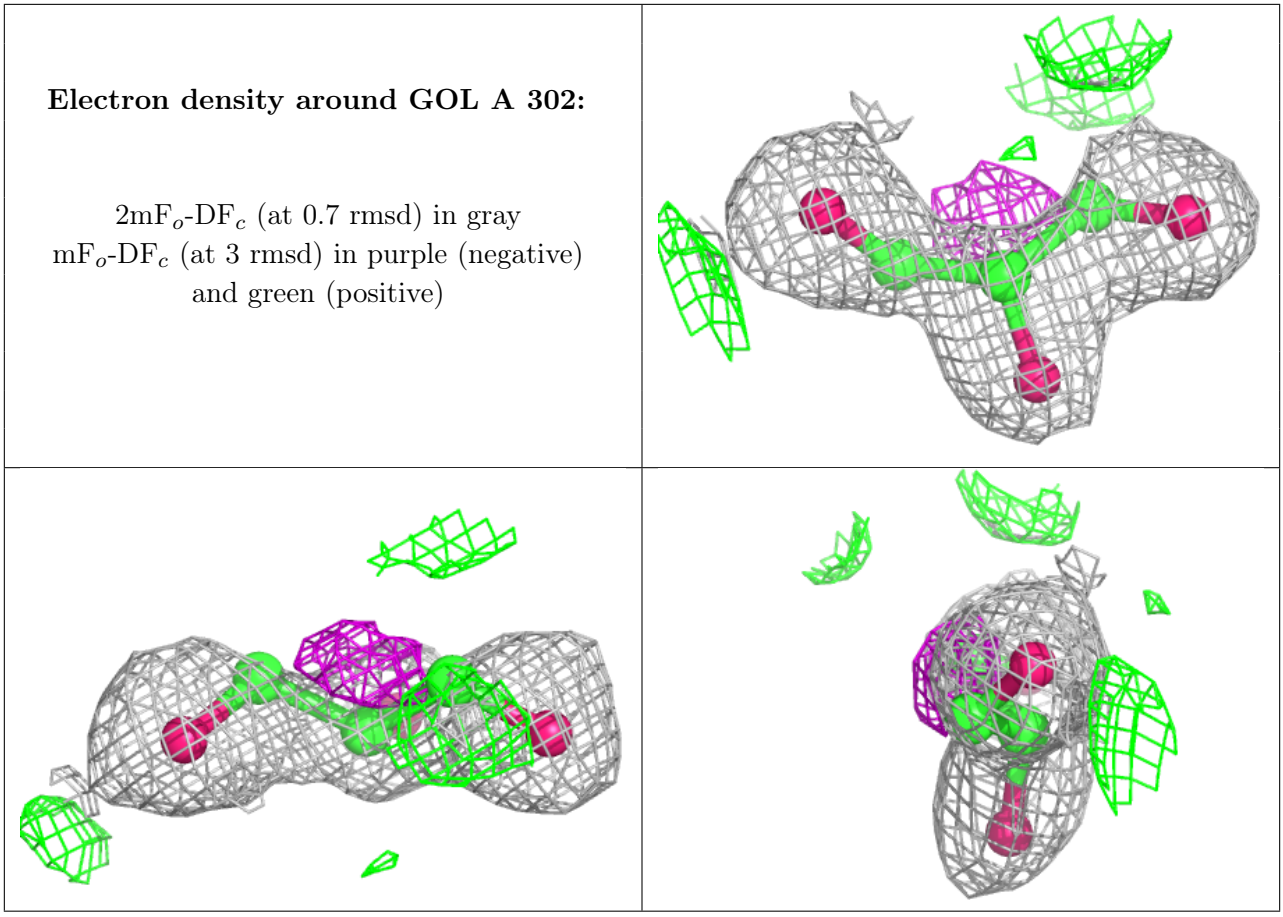
Electron density around DMS D 304:

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



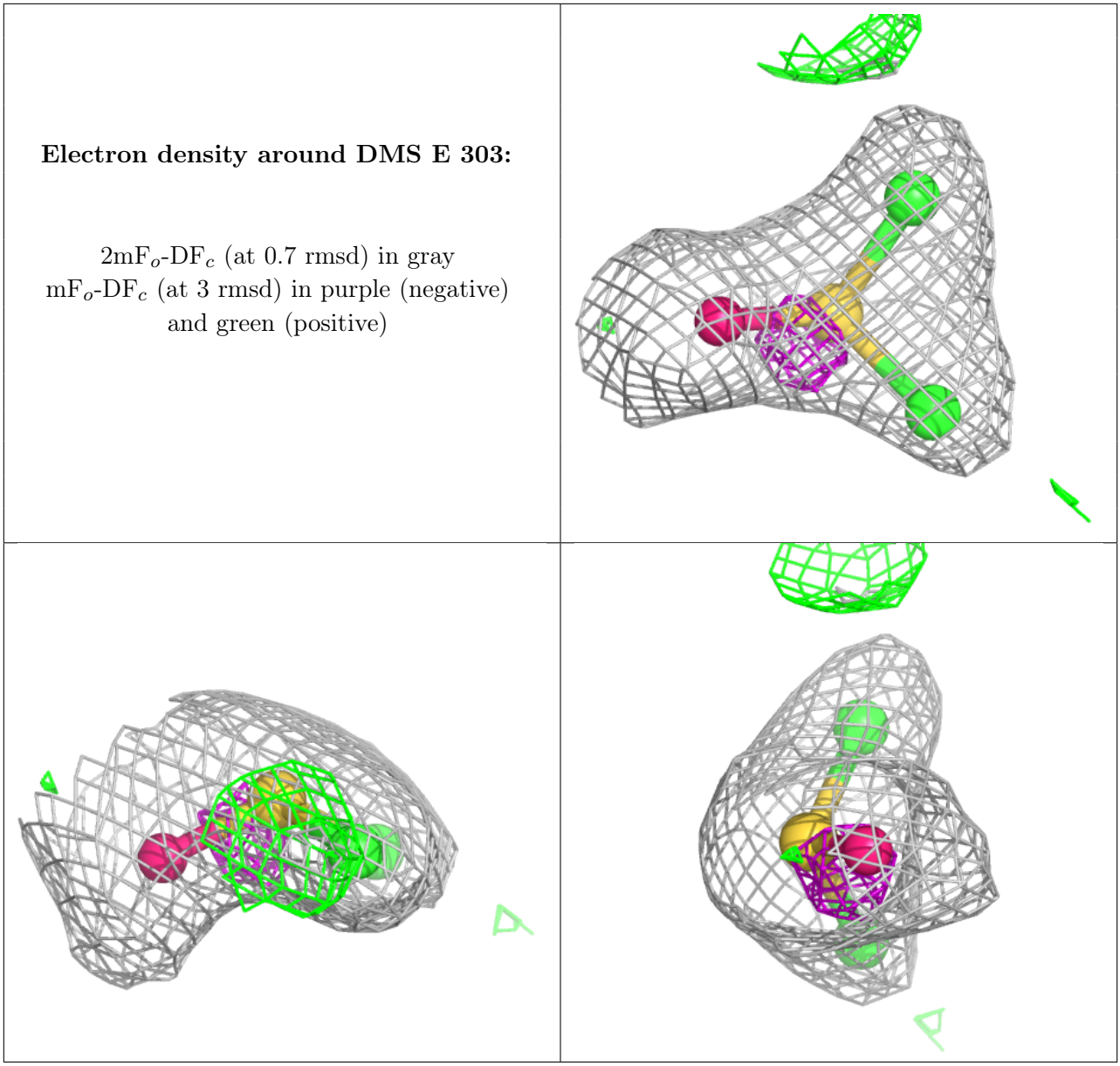
Electron density around GOL A 302:

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



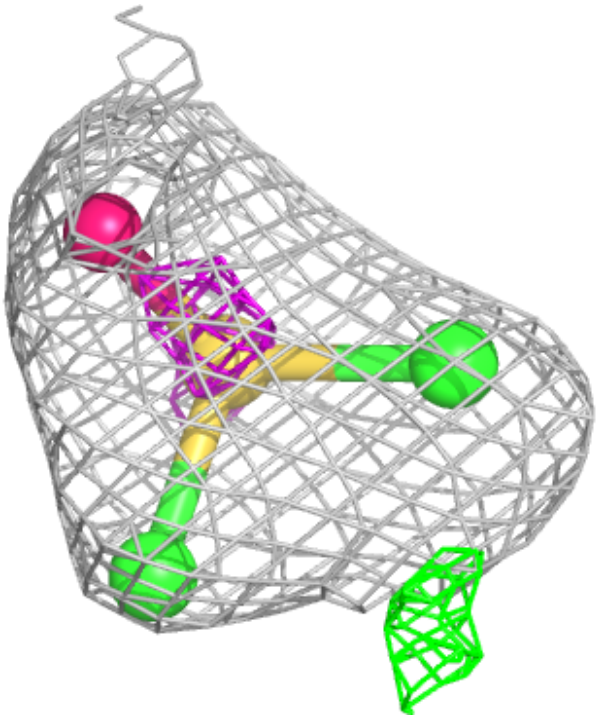
Electron density around DMS E 303:

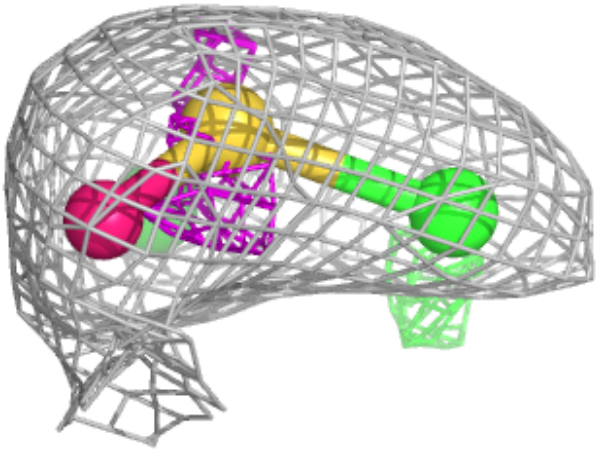
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

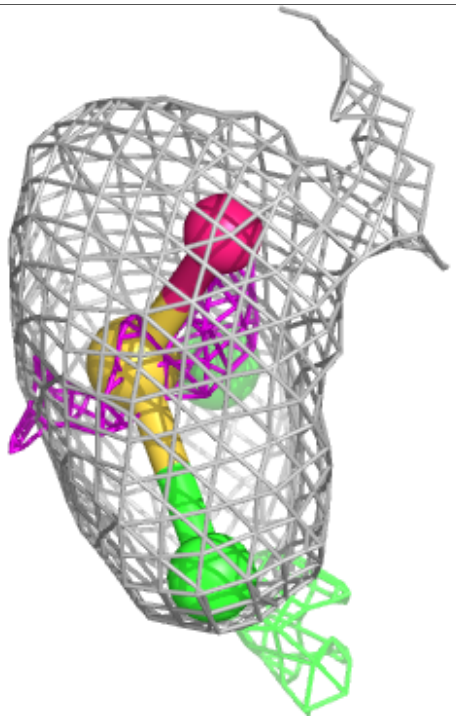


Electron density around DMS C 303:

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

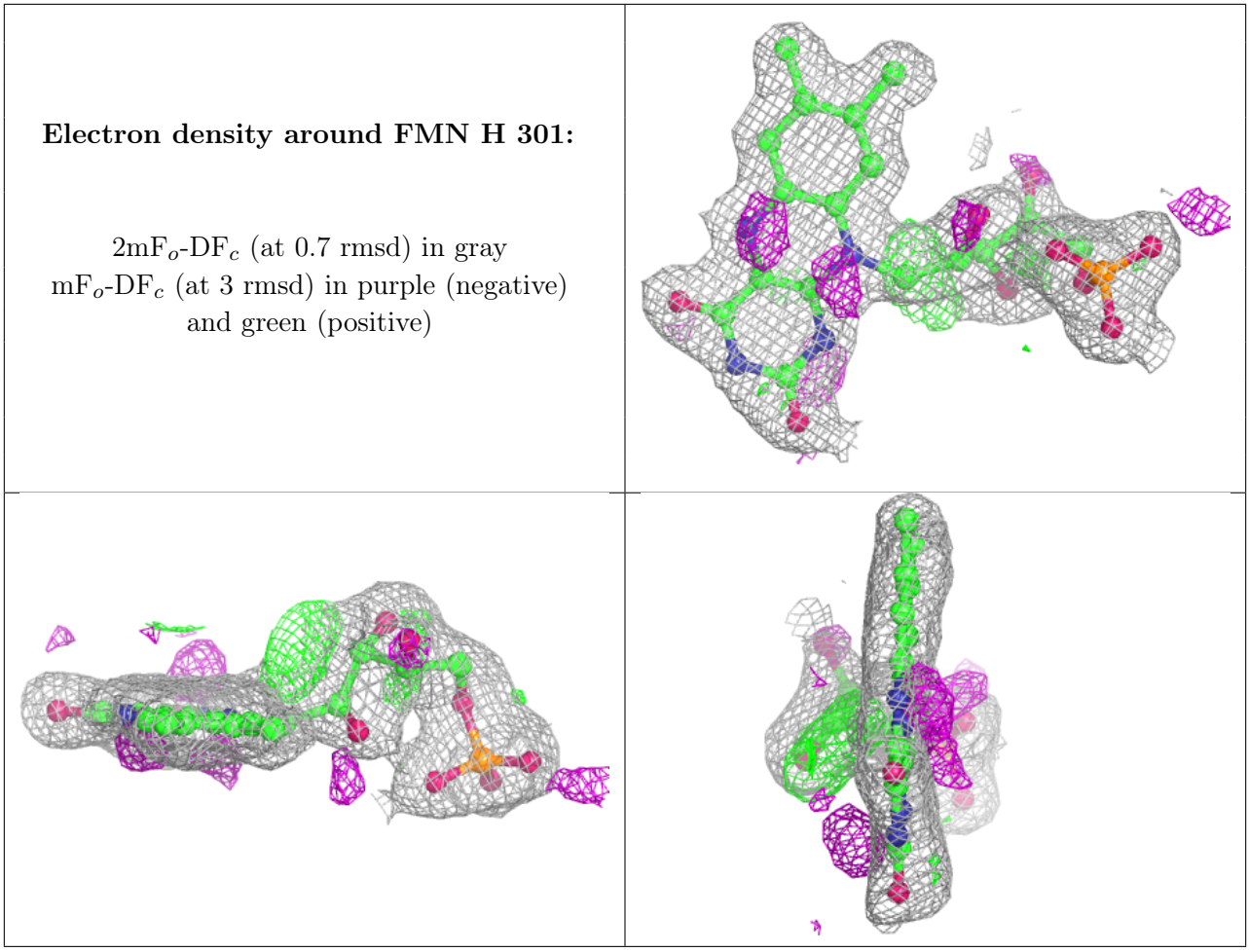






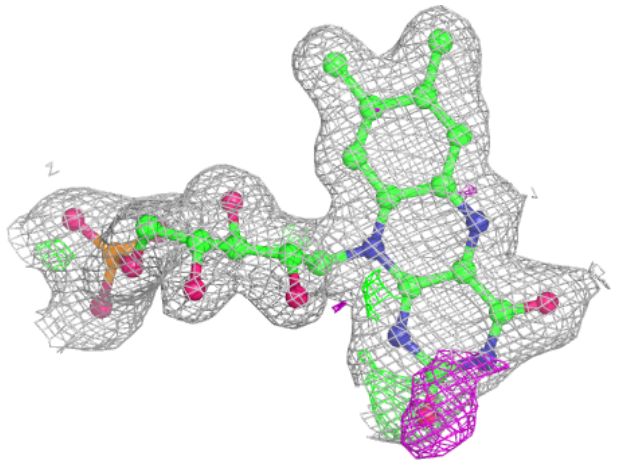
Electron density around FMN H 301:

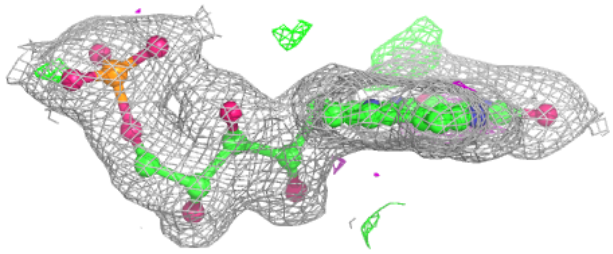
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

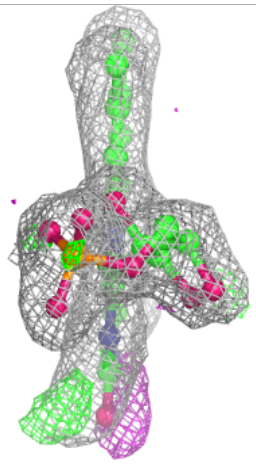


Electron density around FMN D 301:

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

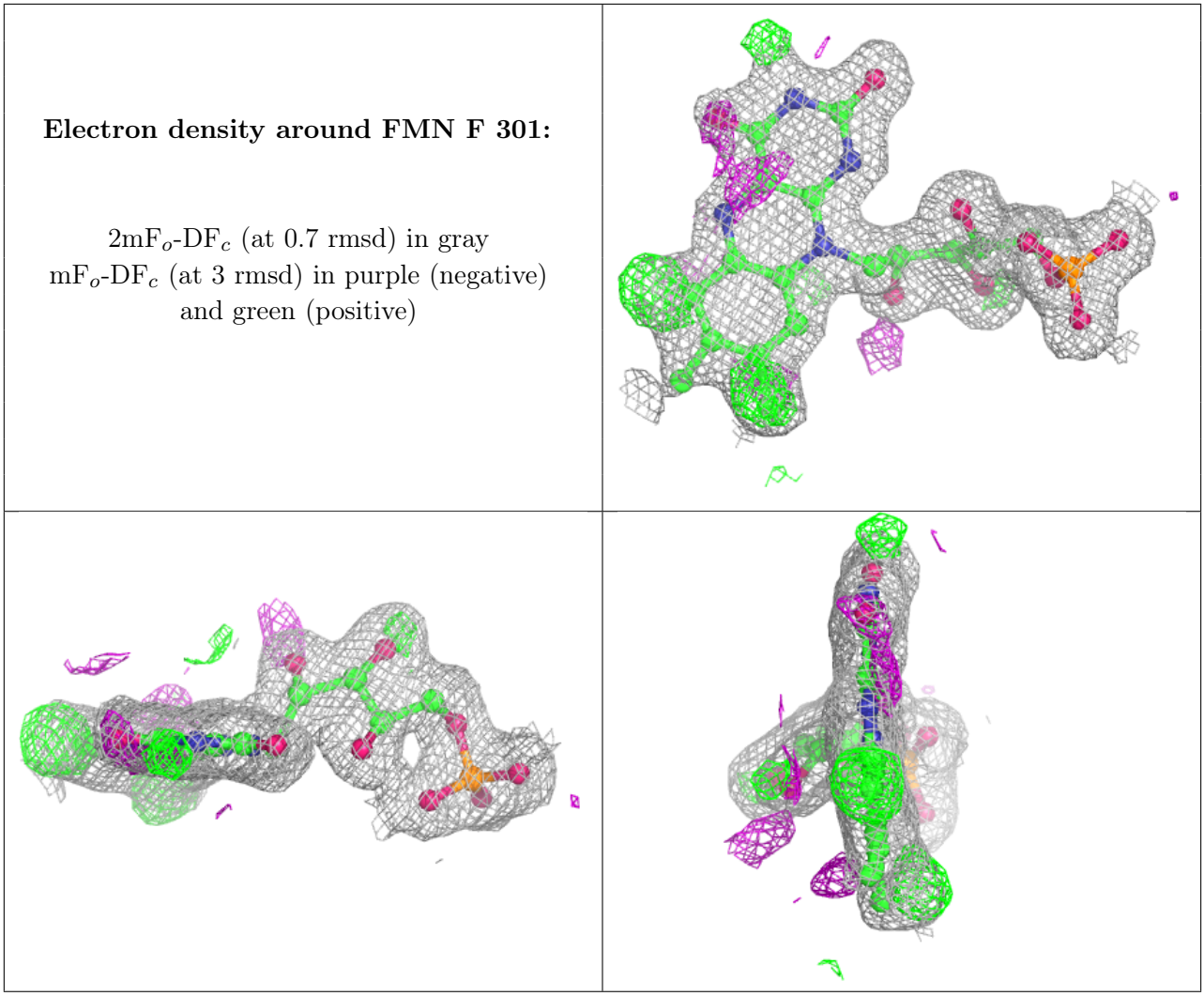






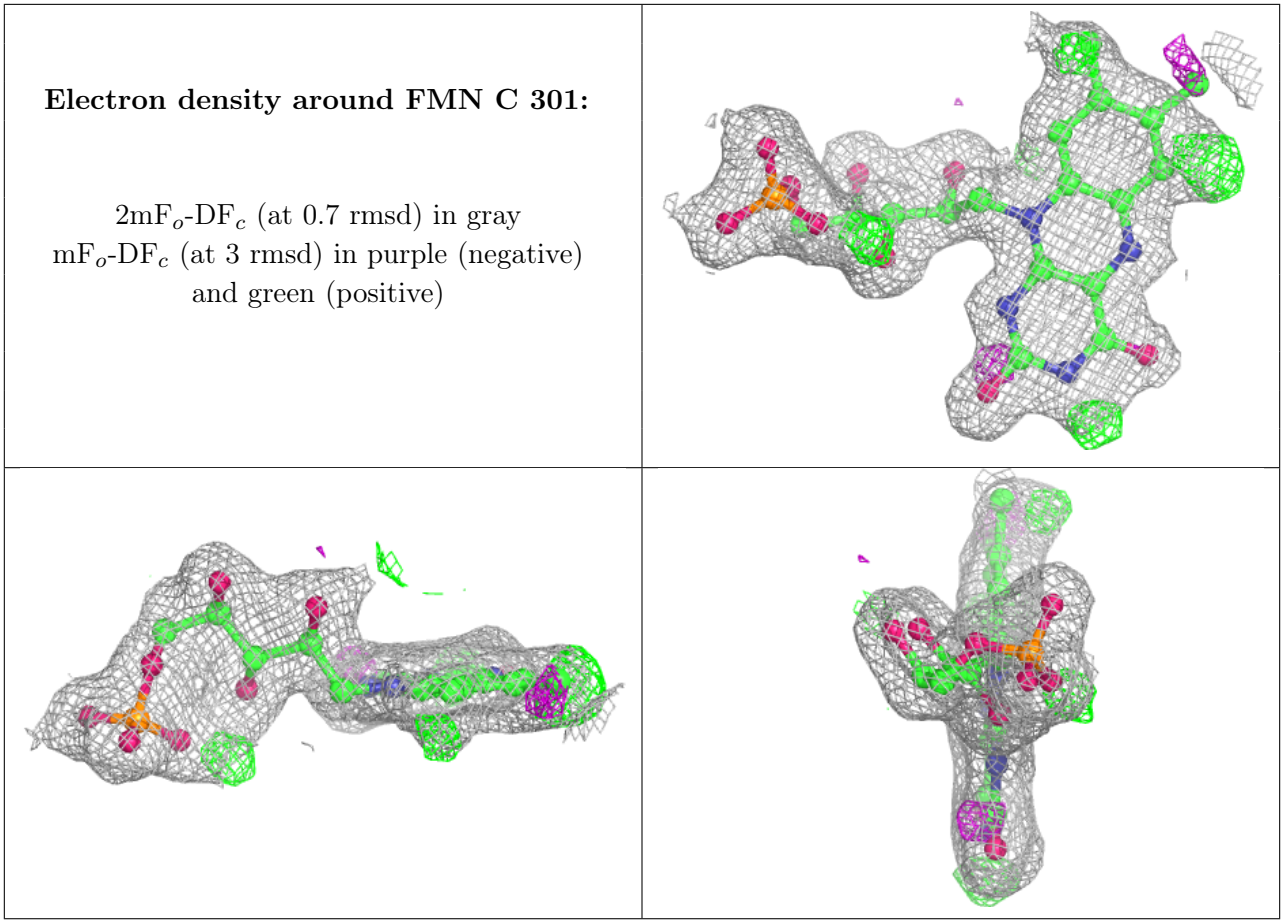
Electron density around FMN F 301:

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



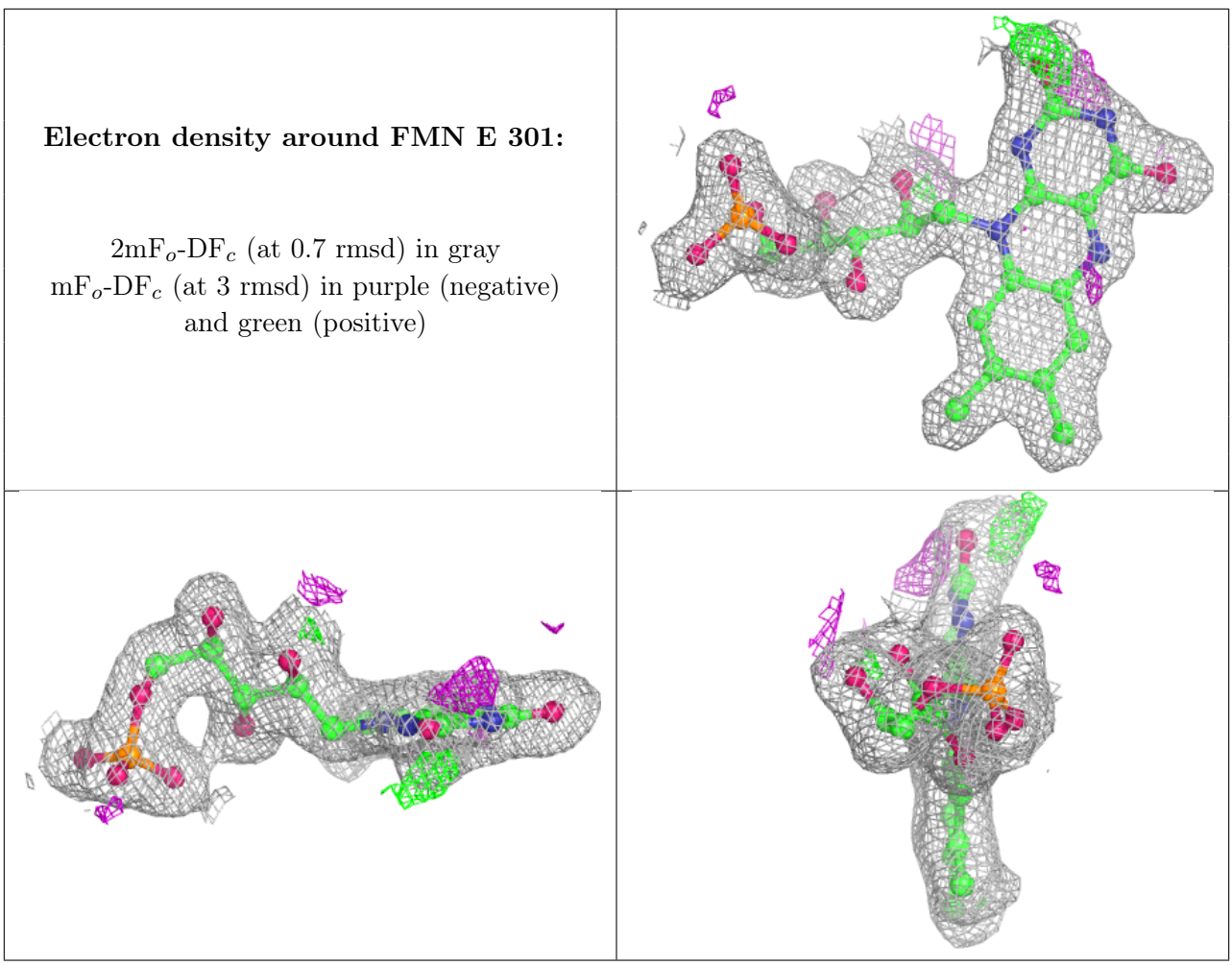
Electron density around FMN C 301:

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



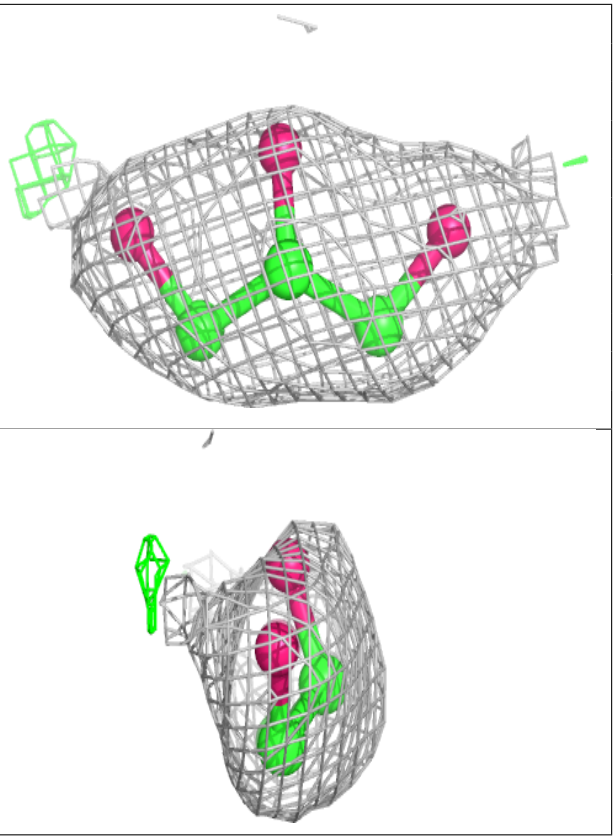
Electron density around FMN E 301:

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



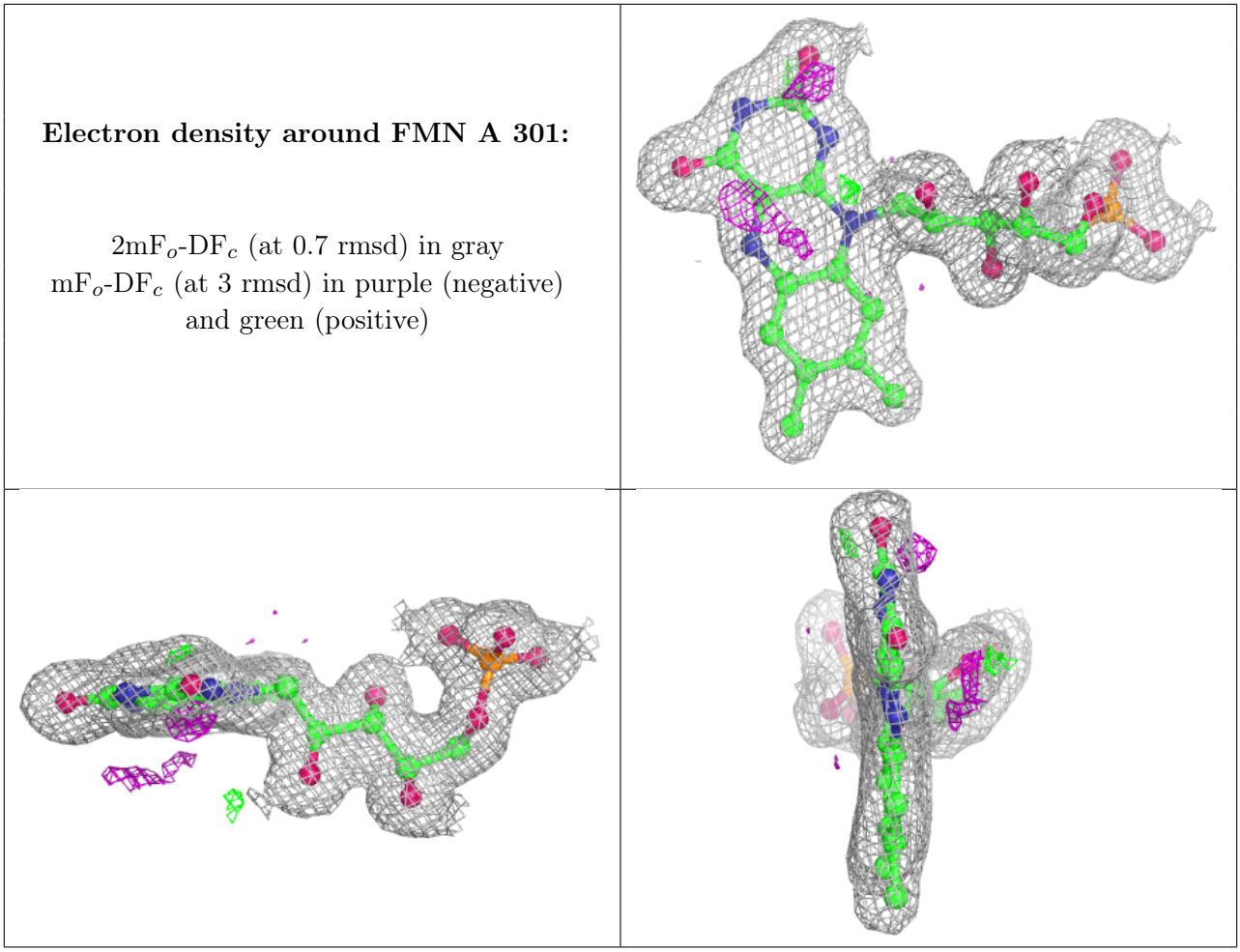
Electron density around GOL H 303:

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



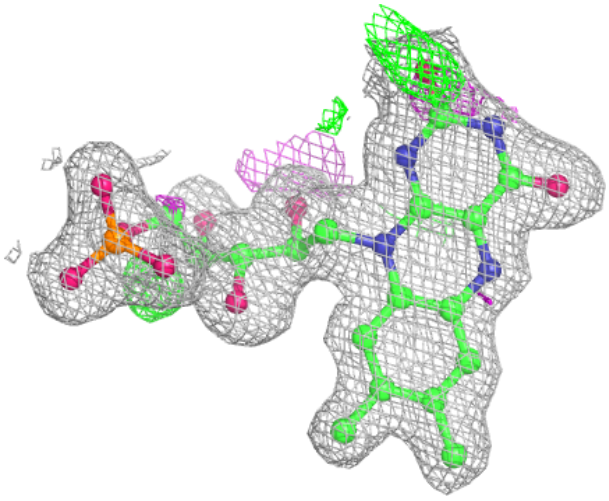
Electron density around FMN A 301:

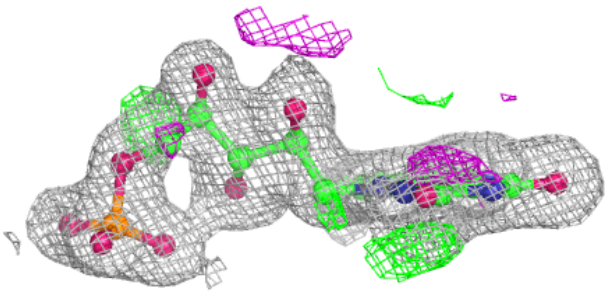
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

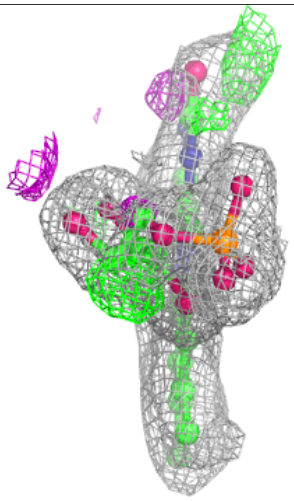


Electron density around FMN B 301:

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

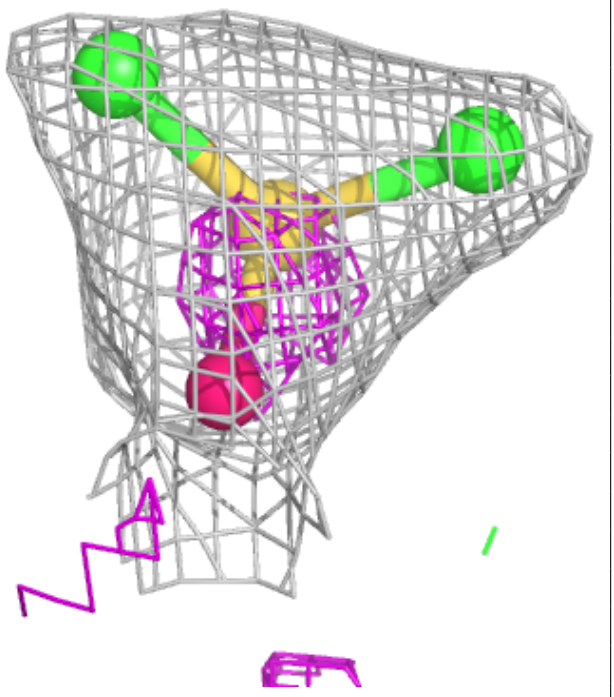


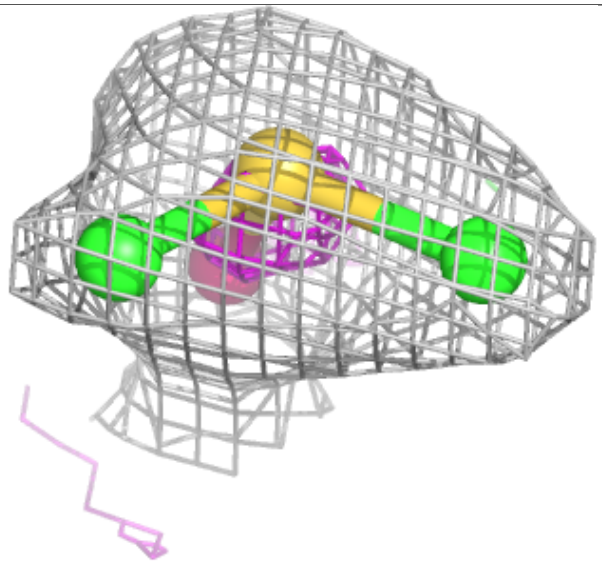


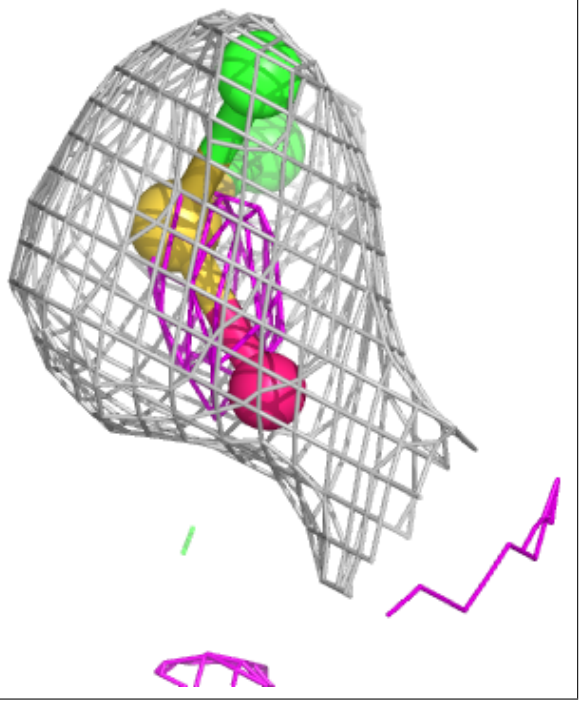


Electron density around DMS G 303:

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

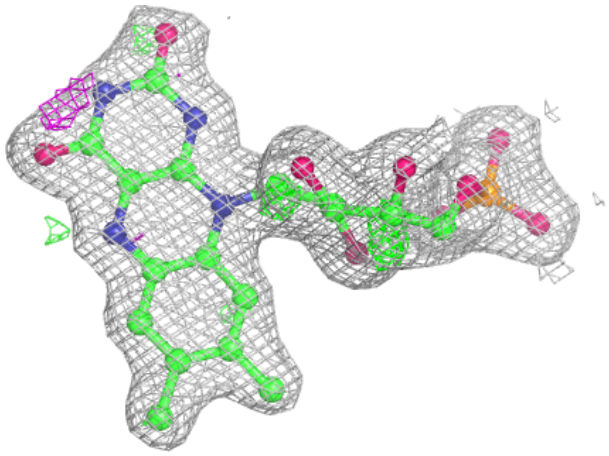


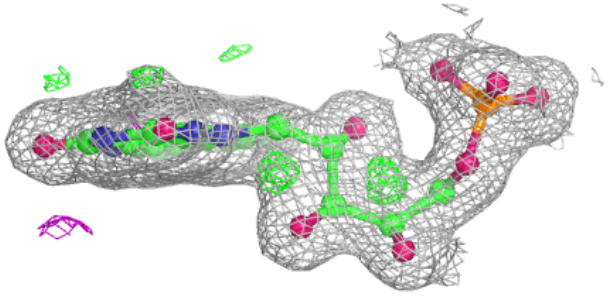


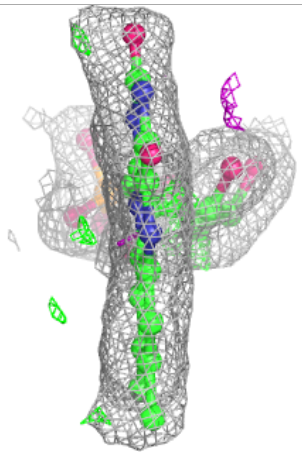


Electron density around FMN G 301:

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

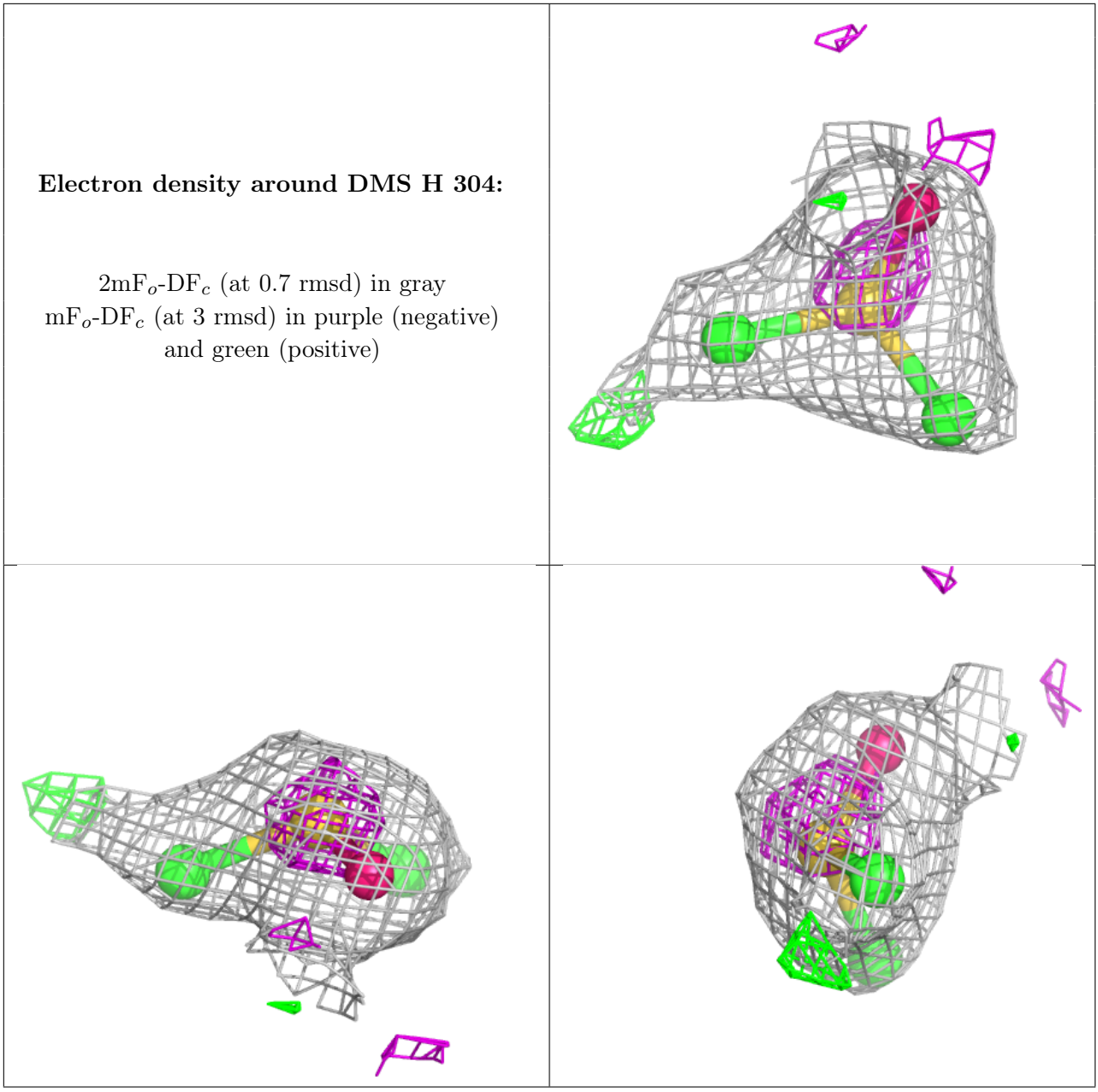






Electron density around DMS H 304:

$2mF_o$-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.