Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:08 pm BST

PDB ID	:	5LSM
Title	:	Crystal structure of nitronate monooxygenase (SO_0471) from Shewanella oneidensis MR-1
Authors	:	Baker, G.E.; Race, P.R.
Deposited on	:	2016-09-04
Resolution	:	2.50 Å(reported)

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

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

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

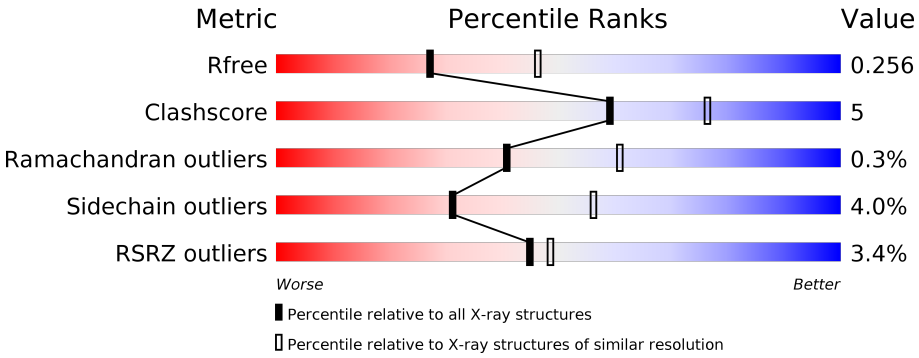
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	359	2% 82% 11% • 6%
1	B	359	3% 84% 8% 8%
1	C	359	2% 80% 13% • 6%
1	D	359	3% 83% 8% • 7%
1	E	359	4% 84% 10% • 6%
1	F	359	7% 80% 13% • 6%

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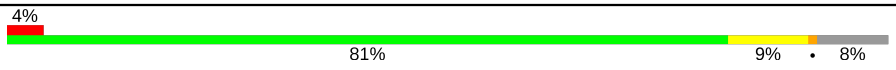
Mol	Chain	Length	Quality of chain
1	G	359	
1	H	359	

2 Entry composition (i)

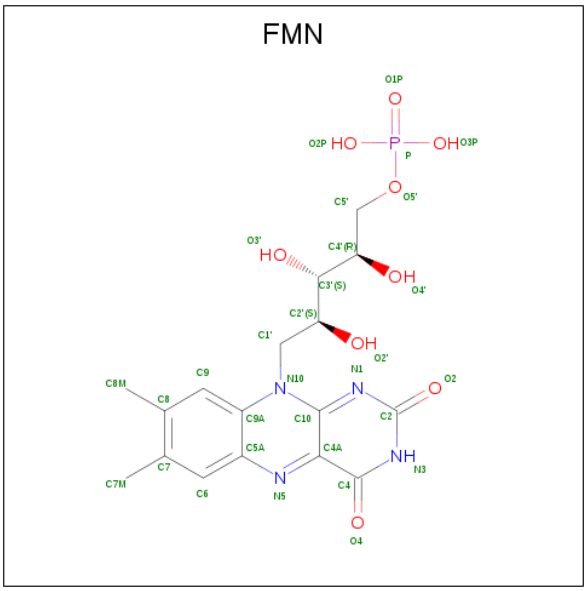
There are 4 unique types of molecules in this entry. The entry contains 19985 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FMN-dependent nitronate monooxygenase.

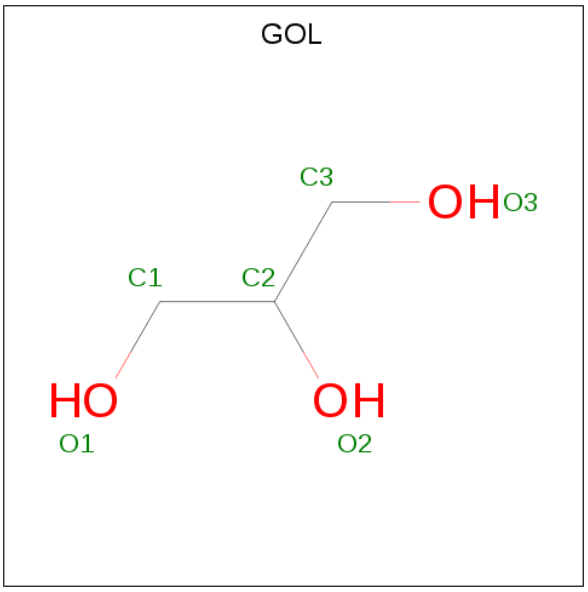
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2498	1592	426	466	14			
1	B	332	Total	C	N	O	S	0	0	0
			2413	1544	411	444	14			
1	C	338	Total	C	N	O	S	0	0	0
			2429	1551	414	451	13			
1	D	333	Total	C	N	O	S	0	0	0
			2380	1513	408	444	15			
1	E	339	Total	C	N	O	S	0	0	0
			2440	1555	419	452	14			
1	F	337	Total	C	N	O	S	0	0	0
			2418	1540	415	450	13			
1	G	331	Total	C	N	O	S	0	0	0
			2344	1497	398	435	14			
1	H	331	Total	C	N	O	S	0	0	0
			2367	1509	404	440	14			

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



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: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

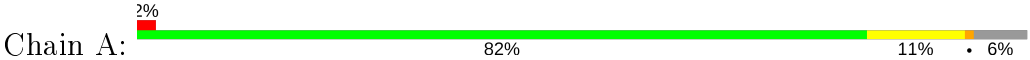
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	64	Total O 64 64	0	0
4	B	59	Total O 59 59	0	0
4	C	59	Total O 59 59	0	0
4	D	65	Total O 65 65	0	0
4	E	47	Total O 47 47	0	0
4	F	43	Total O 43 43	0	0
4	G	40	Total O 40 40	0	0
4	H	47	Total O 47 47	0	0

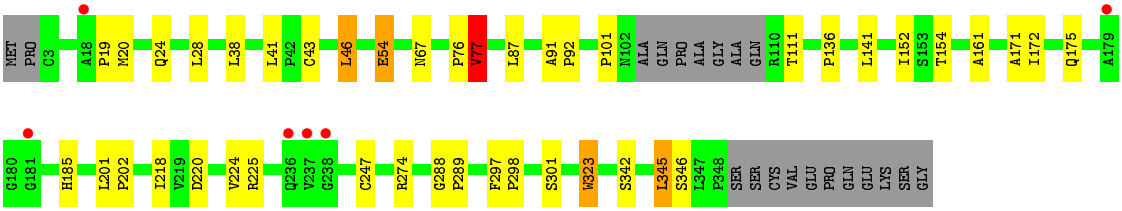
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: FMN-dependent nitronate monooxygenase

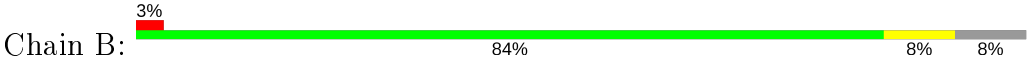
Chain A:

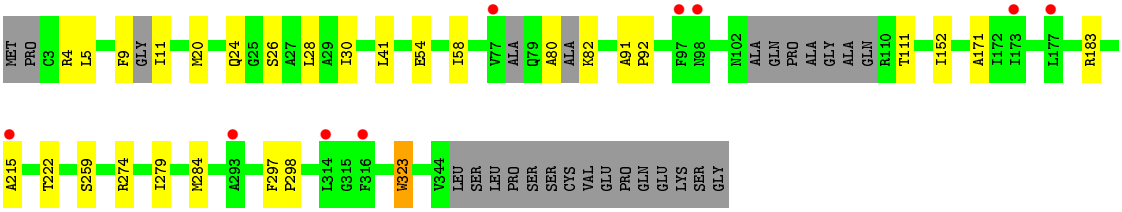




- Molecule 1: FMN-dependent nitronate monooxygenase

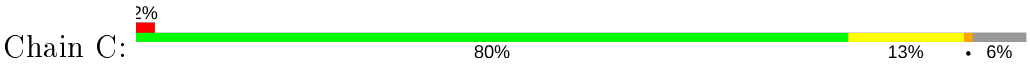
Chain B:

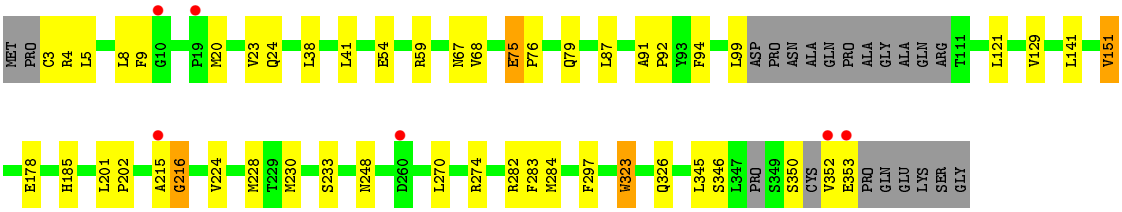




- Molecule 1: FMN-dependent nitronate monooxygenase

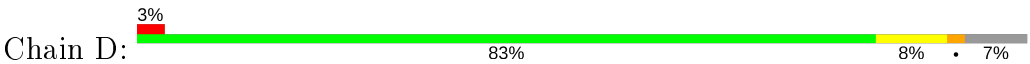
Chain C:

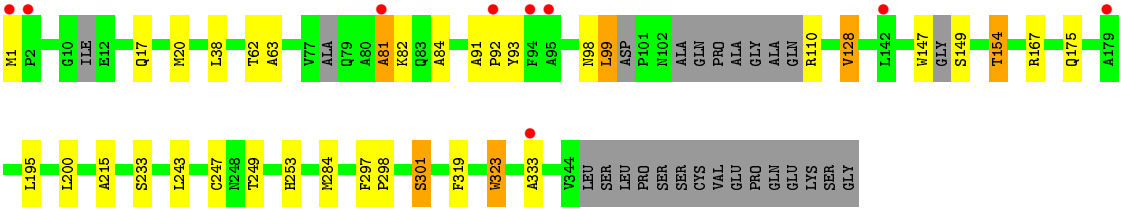




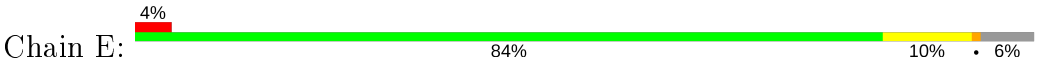
- Molecule 1: FMN-dependent nitronate monooxygenase

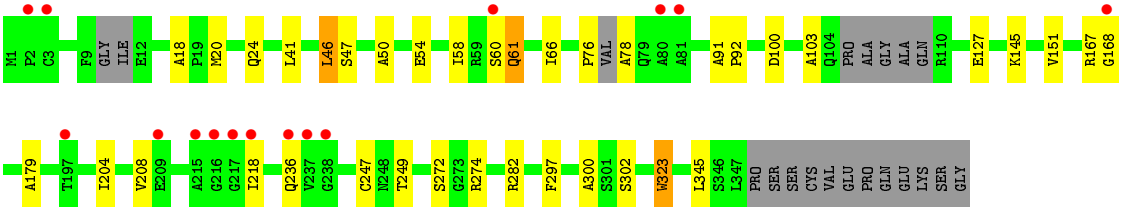
Chain D:



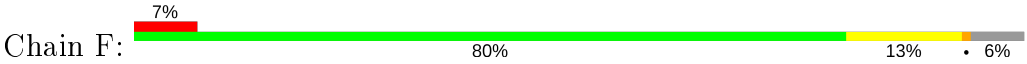


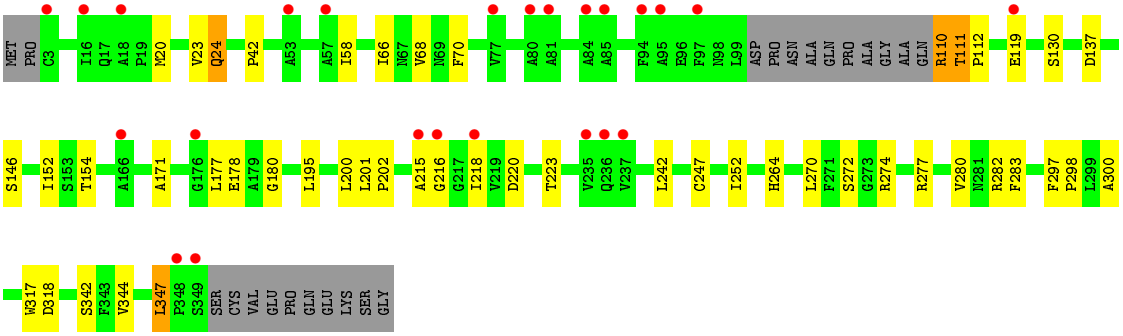
• Molecule 1: FMN-dependent nitronate monooxygenase



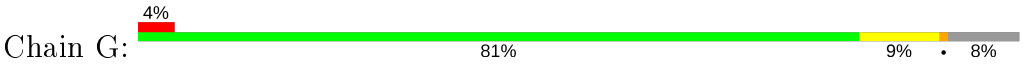


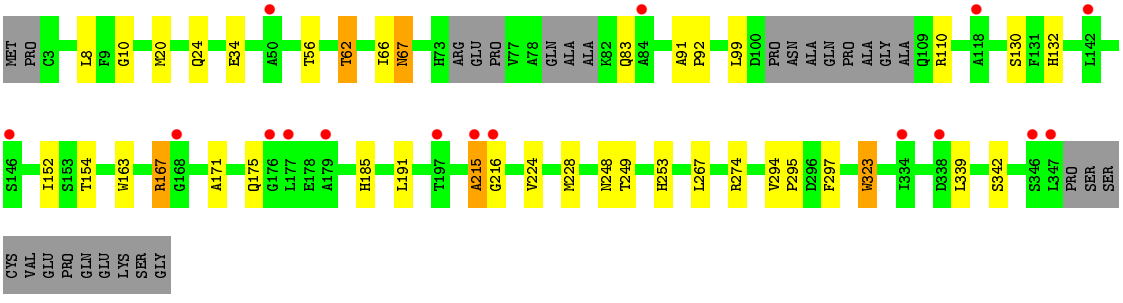
• Molecule 1: FMN-dependent nitronate monooxygenase



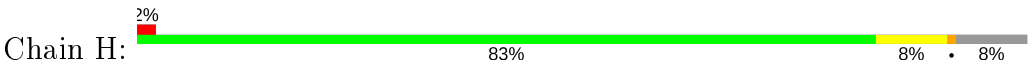


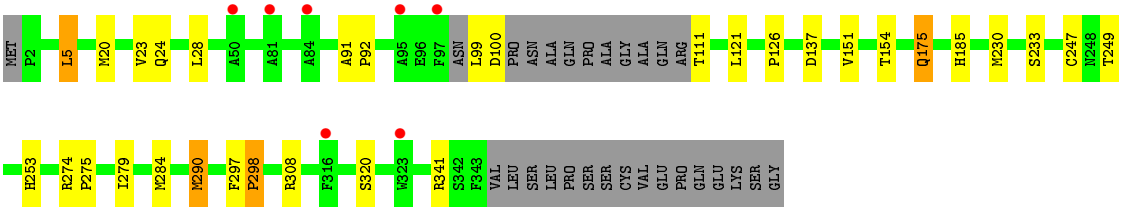
• Molecule 1: FMN-dependent nitronate monooxygenase





• Molecule 1: FMN-dependent nitronate monooxygenase




MET P2 L5 M20 V23 Q24 L28 A50 A81 A84 A91 P92 A95 E96 F97 ASN L99 D100 PRO ASN ALA GLN PRO ALA GLY ALA GLN ARG T111 L121 P126 D137 V151 T154 Q175 H185 M230 S233 C247 N248 T249
H253 R274 P275 I279 M284 M290 F297 P298 R308 F316 S320 W323 R341 S342 F343 VAL LEU SER LEU PRO SER SER CYS VAL GLU PRO GLN GLU LYS SER GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.00Å 99.91Å 108.56Å 95.31° 106.23° 91.62°	Depositor
Resolution (Å)	34.16 – 2.50 34.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (34.16-2.50) 94.8 (34.16-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.185 , 0.256 0.192 , 0.256	Depositor DCC
R_{free} test set	5038 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19985	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: FMN, GOL

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	0.48	0/2550	0.55	0/3474
1	B	0.43	0/2463	0.53	0/3357
1	C	0.43	0/2479	0.55	0/3382
1	D	0.44	0/2429	0.52	0/3313
1	E	0.42	0/2492	0.51	0/3403
1	F	0.44	1/2470 (0.0%)	0.62	4/3372 (0.1%)
1	G	0.41	0/2393	0.52	0/3272
1	H	0.45	0/2418	0.53	0/3298
All	All	0.44	1/19694 (0.0%)	0.54	4/26871 (0.0%)

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	B	0	1
1	C	0	3
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	111	THR	C-N	-7.95	1.19	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	110	ARG	O-C-N	-12.79	102.24	122.70
1	F	110	ARG	C-N-CA	10.01	146.72	121.70
1	F	110	ARG	CA-C-N	9.39	137.86	117.20
1	F	111	THR	O-C-N	6.60	133.63	121.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	215	ALA	Peptide
1	C	215	ALA	Peptide
1	C	216	GLY	Peptide
1	C	346	SER	Peptide
1	D	81	ALA	Peptide
1	E	46	LEU	Peptide
1	F	110	ARG	Peptide
1	F	215	ALA	Peptide
1	G	215	ALA	Peptide
1	G	216	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2498	0	2458	27	0
1	B	2413	0	2361	19	0
1	C	2429	0	2340	28	0
1	D	2380	0	2253	22	0
1	E	2440	0	2350	21	0
1	F	2418	0	2317	25	0
1	G	2344	0	2224	21	0
1	H	2367	0	2262	20	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	3	0
2	E	31	0	19	3	0
2	F	31	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	31	0	19	4	0
2	H	31	0	19	1	0
3	A	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
4	A	64	0	0	0	0
4	B	59	0	0	2	0
4	C	59	0	0	4	0
4	D	65	0	0	5	0
4	E	47	0	0	0	0
4	F	43	0	0	2	0
4	G	40	0	0	0	0
4	H	47	0	0	0	0
All	All	19985	0	18749	181	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 5.

All (181) 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:24:GLN:HG3	1:B:28:LEU:HD23	1.45	0.95
1:D:284:MET:HE1	4:D:519:HOH:O	1.69	0.90
1:F:152:ILE:HD11	1:F:171:ALA:HB3	1.55	0.89
1:A:24:GLN:HG3	1:A:28:LEU:HD23	1.58	0.85
1:G:8:LEU:O	1:G:10:GLY:N	2.14	0.80
1:C:284:MET:HE1	4:C:519:HOH:O	1.81	0.80
1:F:218:ILE:HA	1:F:223:THR:HG21	1.64	0.80
1:F:152:ILE:CD1	1:F:171:ALA:HB3	2.13	0.78
1:D:154:THR:HG22	4:D:517:HOH:O	1.88	0.73
1:G:20:MET:HA	2:G:401:FMN:N5	2.05	0.72
1:H:20:MET:HA	2:H:401:FMN:N5	2.05	0.71
1:F:218:ILE:HA	1:F:223:THR:CG2	2.21	0.70
1:D:215:ALA:O	4:D:501:HOH:O	2.10	0.69
1:D:154:THR:CG2	4:D:517:HOH:O	2.43	0.67
1:B:284:MET:HE1	4:B:505:HOH:O	1.94	0.67
1:E:60:SER:O	1:E:61:GLN:HG2	1.94	0.66
1:B:20:MET:HA	2:B:401:FMN:N5	2.11	0.66
1:H:274:ARG:HB2	1:H:297:PHE:HD1	1.60	0.66
1:B:41:LEU:HD11	1:B:54:GLU:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLN:HG3	1:A:28:LEU:CD2	2.28	0.63
1:E:20:MET:HA	2:E:401:FMN:N5	2.13	0.63
1:D:284:MET:CE	4:D:519:HOH:O	2.33	0.63
1:G:274:ARG:HG3	1:G:297:PHE:HB2	1.80	0.63
1:D:20:MET:HA	2:D:401:FMN:N5	2.13	0.63
1:B:9:PHE:O	1:B:11:ILE:N	2.32	0.62
1:C:20:MET:HA	2:C:401:FMN:N5	2.14	0.61
1:C:274:ARG:HG3	1:C:297:PHE:HB2	1.81	0.61
1:F:20:MET:HA	2:F:401:FMN:N5	2.14	0.61
1:B:30:ILE:HD11	1:B:58:ILE:HA	1.83	0.60
1:G:152:ILE:HG22	1:G:171:ALA:HB3	1.85	0.59
1:H:308:ARG:HD3	1:H:320:SER:HA	1.85	0.58
1:B:152:ILE:HG22	1:B:171:ALA:HB3	1.86	0.57
1:H:24:GLN:HG3	1:H:28:LEU:HD23	1.85	0.57
1:A:20:MET:HA	2:A:401:FMN:N5	2.19	0.57
1:B:323:TRP:HB2	2:B:401:FMN:HM72	1.87	0.57
1:D:323:TRP:HB2	2:D:401:FMN:HM72	1.86	0.56
1:F:272:SER:C	1:F:300:ALA:HB3	2.25	0.56
1:E:76:PRO:O	1:E:78:ALA:N	2.37	0.56
1:G:20:MET:HB3	2:G:401:FMN:C6	2.36	0.56
1:C:352:VAL:N	1:C:353:GLU:HA	2.20	0.56
1:A:76:PRO:O	1:A:77:VAL:HB	2.06	0.55
1:B:24:GLN:HG3	1:B:28:LEU:CD2	2.28	0.55
1:H:274:ARG:HG3	1:H:297:PHE:HB2	1.89	0.55
1:A:154:THR:HG23	1:A:175:GLN:HG2	1.90	0.54
1:H:154:THR:HG23	1:H:175:GLN:HG2	1.89	0.54
1:G:34:GLU:OE1	1:G:62:THR:HG23	2.08	0.53
1:C:216:GLY:HA2	4:C:511:HOH:O	2.08	0.53
1:E:20:MET:H	1:E:24:GLN:HE21	1.56	0.53
1:H:99:LEU:O	1:H:100:ASP:C	2.47	0.53
1:H:274:ARG:HB2	1:H:297:PHE:CD1	2.42	0.53
1:C:185:HIS:O	1:C:274:ARG:NH2	2.40	0.52
1:A:154:THR:CG2	1:A:175:GLN:HG2	2.40	0.52
1:E:274:ARG:HG3	1:E:297:PHE:HB2	1.91	0.52
1:D:62:THR:O	1:D:63:ALA:HB3	2.10	0.52
1:D:81:ALA:CB	1:D:84:ALA:HB3	2.40	0.51
1:C:284:MET:CE	4:C:519:HOH:O	2.46	0.51
1:G:249:THR:HG22	1:G:253:HIS:HB3	1.93	0.51
1:A:201:LEU:HB3	1:A:202:PRO:HD3	1.93	0.51
1:B:323:TRP:HB2	2:B:401:FMN:C7M	2.41	0.50
1:G:274:ARG:HG3	1:G:297:PHE:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:SER:CB	1:E:50:ALA:HB3	2.42	0.50
1:F:216:GLY:HA2	4:F:507:HOH:O	2.11	0.50
1:G:91:ALA:HB3	1:G:92:PRO:HD3	1.93	0.50
1:H:279:ILE:O	1:H:284:MET:HE3	2.12	0.50
1:C:41:LEU:HD11	1:C:54:GLU:HG2	1.94	0.50
1:C:178:GLU:HA	1:C:326:GLN:HG3	1.94	0.49
1:A:225:ARG:HD2	1:A:346:SER:HB3	1.94	0.49
1:G:185:HIS:O	1:G:274:ARG:NH2	2.37	0.49
1:G:152:ILE:CG2	1:G:171:ALA:HB3	2.41	0.49
1:E:272:SER:C	1:E:300:ALA:HB3	2.33	0.49
1:E:41:LEU:HD11	1:E:54:GLU:HG2	1.94	0.49
1:B:26:SER:O	1:B:30:ILE:HD12	2.13	0.49
1:C:91:ALA:HB3	1:C:92:PRO:HD3	1.95	0.49
1:F:344:VAL:HA	1:F:347:LEU:HD21	1.95	0.49
1:H:274:ARG:HD3	1:H:297:PHE:CD1	2.48	0.48
1:A:152:ILE:HG22	1:A:171:ALA:HB3	1.96	0.48
1:F:347:LEU:HD23	4:F:511:HOH:O	2.13	0.48
1:D:323:TRP:HB2	2:D:401:FMN:C7M	2.44	0.48
1:F:178:GLU:N	1:F:178:GLU:OE1	2.46	0.47
1:F:24:GLN:NE2	1:F:42:PRO:HD3	2.28	0.47
1:C:3:CYS:N	1:C:353:GLU:O	2.47	0.47
1:E:46:LEU:HA	1:E:47:SER:CB	2.44	0.47
1:C:5:LEU:O	1:C:8:LEU:O	2.33	0.47
1:H:249:THR:HG22	1:H:253:HIS:HB3	1.97	0.47
1:B:183:ARG:HD2	4:B:519:HOH:O	2.15	0.47
1:A:218:ILE:N	1:A:218:ILE:HD12	2.30	0.46
1:C:38:LEU:HD21	1:C:67:ASN:HB2	1.96	0.46
1:A:20:MET:HA	2:A:401:FMN:C5A	2.45	0.46
1:F:68:VAL:HG12	1:F:70:PHE:CE2	2.49	0.46
1:G:66:ILE:HG22	1:G:67:ASN:N	2.31	0.46
1:A:201:LEU:HB3	1:A:202:PRO:CD	2.45	0.46
1:E:145:LYS:NZ	1:E:168:GLY:O	2.33	0.46
1:E:58:ILE:HG21	1:E:66:ILE:HG21	1.98	0.46
1:C:5:LEU:HB2	1:C:233:SER:HB3	1.98	0.45
1:A:185:HIS:O	1:A:274:ARG:NH2	2.44	0.45
1:A:161:ALA:HB1	1:A:172:ILE:HD13	1.98	0.45
1:A:76:PRO:O	1:A:77:VAL:CB	2.65	0.45
1:B:274:ARG:HG3	1:B:297:PHE:HB2	1.98	0.45
1:F:220:ASP:OD1	1:F:223:THR:HB	2.16	0.45
1:G:323:TRP:HB2	2:G:401:FMN:HM72	1.99	0.45
1:H:154:THR:CG2	1:H:175:GLN:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:297:PHE:O	1:H:298:PRO:CB	2.65	0.45
1:F:282:ARG:HB3	1:F:318:ASP:HB3	1.98	0.45
1:C:350:SER:O	1:C:352:VAL:N	2.50	0.45
1:F:201:LEU:N	1:F:202:PRO:HD2	2.32	0.45
1:C:9:PHE:CD1	1:C:9:PHE:N	2.85	0.44
1:B:41:LEU:CD1	1:B:54:GLU:HG2	2.46	0.44
1:A:288:GLY:HA3	1:A:289:PRO:C	2.37	0.44
1:H:185:HIS:O	1:H:274:ARG:NH2	2.41	0.44
1:H:5:LEU:HD22	1:H:233:SER:HB2	1.99	0.44
1:C:201:LEU:HB3	1:C:202:PRO:CD	2.48	0.44
1:A:220:ASP:O	1:A:224:VAL:HG23	2.17	0.44
1:F:264:HIS:CE1	1:F:280:VAL:HG21	2.53	0.44
1:A:225:ARG:NH1	1:A:346:SER:O	2.50	0.44
1:H:24:GLN:HG3	1:H:28:LEU:CD2	2.48	0.44
1:C:216:GLY:CA	4:C:511:HOH:O	2.66	0.43
1:C:323:TRP:HB2	2:C:401:FMN:HM72	2.00	0.43
1:D:195:LEU:HB2	1:D:200:LEU:HB2	1.99	0.43
1:C:68:VAL:HG21	1:C:121:LEU:HD21	2.00	0.43
1:G:224:VAL:O	1:G:228:MET:HG2	2.18	0.43
1:A:19:PRO:O	2:A:401:FMN:C4A	2.66	0.43
1:D:249:THR:HG22	1:D:253:HIS:HB3	2.00	0.43
1:D:81:ALA:HB2	1:D:84:ALA:HB3	2.01	0.43
1:E:100:ASP:OD1	1:H:341:ARG:NH2	2.52	0.43
1:E:91:ALA:N	1:E:92:PRO:CD	2.82	0.43
1:G:154:THR:HG23	1:G:175:GLN:HB2	2.00	0.43
1:H:121:LEU:HD22	1:H:126:PRO:HG3	2.00	0.43
1:A:41:LEU:HD11	1:A:54:GLU:HG2	2.00	0.43
1:C:352:VAL:N	1:C:353:GLU:CA	2.81	0.42
1:H:91:ALA:N	1:H:92:PRO:HD2	2.34	0.42
1:C:224:VAL:O	1:C:228:MET:HG2	2.20	0.42
1:D:297:PHE:HA	1:D:298:PRO:HA	1.78	0.42
1:E:103:ALA:HB1	1:E:302:SER:HB2	2.00	0.42
1:C:129:VAL:O	1:C:151:VAL:HA	2.19	0.42
1:C:345:LEU:HD12	1:C:345:LEU:HA	1.94	0.42
1:D:93:TYR:CD1	1:D:319:PHE:HZ	2.38	0.42
1:A:323:TRP:HB2	2:A:401:FMN:HM72	2.02	0.42
1:D:110:ARG:NH2	1:D:301:SER:OG	2.52	0.42
1:E:323:TRP:HB2	2:E:401:FMN:HM72	2.01	0.42
1:A:297:PHE:HA	1:A:298:PRO:HA	1.91	0.42
1:B:91:ALA:N	1:B:92:PRO:CD	2.83	0.42
1:E:204:ILE:O	1:E:208:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLU:HG3	1:C:76:PRO:HD2	2.02	0.42
1:D:62:THR:OG1	1:D:63:ALA:N	2.52	0.42
1:D:81:ALA:HB1	1:D:84:ALA:HB3	2.01	0.42
1:E:18:ALA:HB2	1:E:236:GLN:HG2	2.01	0.42
1:A:342:SER:O	1:A:345:LEU:HD22	2.20	0.41
1:B:279:ILE:O	1:B:284:MET:HE3	2.20	0.41
1:F:111:THR:HA	1:F:112:PRO:HD3	1.65	0.41
1:F:270:LEU:HB3	1:F:283:PHE:CE2	2.55	0.41
1:F:58:ILE:HG21	1:F:66:ILE:HD13	2.02	0.41
1:G:339:LEU:O	1:G:342:SER:OG	2.22	0.41
1:E:274:ARG:HG3	1:E:297:PHE:CB	2.50	0.41
1:G:163:TRP:O	1:G:167:ARG:HG2	2.20	0.41
1:G:215:ALA:HB1	2:G:401:FMN:H5'2	2.01	0.41
1:E:179:ALA:HB1	2:E:401:FMN:H4'	2.02	0.41
1:F:297:PHE:HA	1:F:298:PRO:HA	1.85	0.41
1:H:275:PRO:HG3	1:H:290:MET:CE	2.50	0.41
1:A:136:PRO:HG2	1:A:141:LEU:HD13	2.03	0.41
1:B:297:PHE:HA	1:B:298:PRO:HA	1.82	0.41
1:B:222:THR:CG2	1:C:230:MET:HA	2.51	0.41
1:E:127:GLU:H	1:E:127:GLU:CD	2.24	0.41
1:E:218:ILE:N	1:E:218:ILE:HD12	2.35	0.41
1:G:294:VAL:HA	1:G:295:PRO:HD2	1.96	0.41
1:D:243:LEU:O	1:D:333:ALA:HA	2.20	0.41
1:G:191:LEU:HD13	1:G:267:LEU:HD23	2.03	0.41
1:B:80:ALA:O	1:B:82:LYS:N	2.54	0.41
1:F:130:SER:HA	1:F:152:ILE:O	2.21	0.41
1:F:180:GLY:HA2	1:F:277:ARG:HB3	2.03	0.41
1:A:91:ALA:HB3	1:A:92:PRO:HD3	2.03	0.41
1:A:43:CYS:HA	1:A:46:LEU:HD22	2.03	0.40
1:A:38:LEU:HD21	1:A:67:ASN:HB2	2.03	0.40
1:F:195:LEU:HB2	1:F:200:LEU:HB2	2.03	0.40
1:G:130:SER:HA	1:G:152:ILE:O	2.21	0.40
1:C:94:PHE:HD1	1:C:99:LEU:HD11	1.87	0.40
1:D:91:ALA:N	1:D:92:PRO:CD	2.85	0.40
1:D:99:LEU:HA	1:D:99:LEU:HD12	1.91	0.40
1:F:23:VAL:HG11	1:F:242:LEU:CD2	2.51	0.40
1:F:252:ILE:HG12	1:F:317:TRP:HB3	2.02	0.40
1:C:270:LEU:HB3	1:C:283:PHE:CE2	2.56	0.40
1:D:38:LEU:HD21	1:D:128:VAL:HG11	2.03	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	335/359 (93%)	317 (95%)	15 (4%)	3 (1%)	17	31
1	B	322/359 (90%)	314 (98%)	8 (2%)	0	100	100
1	C	330/359 (92%)	309 (94%)	21 (6%)	0	100	100
1	D	321/359 (89%)	302 (94%)	18 (6%)	1 (0%)	41	61
1	E	331/359 (92%)	312 (94%)	18 (5%)	1 (0%)	41	61
1	F	333/359 (93%)	314 (94%)	18 (5%)	1 (0%)	41	61
1	G	323/359 (90%)	304 (94%)	18 (6%)	1 (0%)	41	61
1	H	325/359 (90%)	306 (94%)	17 (5%)	2 (1%)	25	43
All	All	2620/2872 (91%)	2478 (95%)	133 (5%)	9 (0%)	41	61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	THR
1	H	298	PRO
1	A	77	VAL
1	D	82	LYS
1	E	61	GLN
1	F	137	ASP
1	A	101	PRO
1	G	110	ARG
1	H	137	ASP

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/274 (91%)	241 (97%)	8 (3%)	39	65
1	B	237/274 (86%)	232 (98%)	5 (2%)	53	78
1	C	232/274 (85%)	220 (95%)	12 (5%)	23	44
1	D	224/274 (82%)	210 (94%)	14 (6%)	18	34
1	E	234/274 (85%)	227 (97%)	7 (3%)	41	68
1	F	229/274 (84%)	220 (96%)	9 (4%)	32	57
1	G	220/274 (80%)	210 (96%)	10 (4%)	27	51
1	H	223/274 (81%)	215 (96%)	8 (4%)	35	61
All	All	1848/2192 (84%)	1775 (96%)	73 (4%)	31	56

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	54	GLU
1	A	77	VAL
1	A	87	LEU
1	A	247	CYS
1	A	301	SER
1	A	323	TRP
1	A	345	LEU
1	B	4	ARG
1	B	5	LEU
1	B	111	THR
1	B	259	SER
1	B	323	TRP
1	C	4	ARG
1	C	23	VAL
1	C	24	GLN
1	C	59	ARG
1	C	75	GLU
1	C	79	GLN
1	C	87	LEU
1	C	141	LEU
1	C	151	VAL
1	C	248	ASN
1	C	282	ARG
1	C	323	TRP

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Mol	Chain	Res	Type
1	D	1	MET
1	D	17	GLN
1	D	98	ASN
1	D	99	LEU
1	D	128	VAL
1	D	147	TRP
1	D	149	SER
1	D	154	THR
1	D	167	ARG
1	D	175	GLN
1	D	233	SER
1	D	247	CYS
1	D	301	SER
1	D	323	TRP
1	E	151	VAL
1	E	167	ARG
1	E	247	CYS
1	E	249	THR
1	E	282	ARG
1	E	323	TRP
1	E	345	LEU
1	F	24	GLN
1	F	119	GLU
1	F	146	SER
1	F	154	THR
1	F	177	LEU
1	F	247	CYS
1	F	274	ARG
1	F	342	SER
1	F	347	LEU
1	G	24	GLN
1	G	56	THR
1	G	62	THR
1	G	67	ASN
1	G	83	GLN
1	G	99	LEU
1	G	132	HIS
1	G	167	ARG
1	G	248	ASN
1	G	323	TRP
1	H	5	LEU
1	H	23	VAL

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Mol	Chain	Res	Type
1	H	111	THR
1	H	151	VAL
1	H	175	GLN
1	H	230	MET
1	H	247	CYS
1	H	290	MET

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

Mol	Chain	Res	Type
1	E	24	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 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	E	402	-	5,5,5	0.37	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FMN	H	401	-	31,33,33	2.47	6 (19%)	40,50,50	2.23	7 (17%)
3	GOL	F	402	-	5,5,5	0.37	0	5,5,5	0.17	0
2	FMN	D	401	-	31,33,33	2.30	5 (16%)	40,50,50	2.12	7 (17%)
2	FMN	F	401	-	31,33,33	2.31	6 (19%)	40,50,50	2.12	10 (25%)
2	FMN	B	401	-	31,33,33	2.31	6 (19%)	40,50,50	2.13	6 (15%)
3	GOL	G	402	-	5,5,5	0.48	0	5,5,5	0.37	0
2	FMN	E	401	-	31,33,33	2.56	6 (19%)	40,50,50	2.20	9 (22%)
2	FMN	G	401	-	31,33,33	2.43	6 (19%)	40,50,50	2.22	8 (20%)
2	FMN	A	401	-	31,33,33	2.16	5 (16%)	40,50,50	2.14	8 (20%)
2	FMN	C	401	-	31,33,33	2.27	6 (19%)	40,50,50	2.25	8 (20%)
3	GOL	A	402	-	5,5,5	0.59	0	5,5,5	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	402	-	-	2/4/4/4	-
2	FMN	H	401	-	-	6/18/18/18	0/3/3/3
3	GOL	F	402	-	-	2/4/4/4	-
2	FMN	D	401	-	-	6/18/18/18	0/3/3/3
2	FMN	F	401	-	-	6/18/18/18	0/3/3/3
2	FMN	B	401	-	-	10/18/18/18	0/3/3/3
3	GOL	G	402	-	-	2/4/4/4	-
2	FMN	E	401	-	-	6/18/18/18	0/3/3/3
2	FMN	G	401	-	-	7/18/18/18	0/3/3/3
2	FMN	A	401	-	-	4/18/18/18	0/3/3/3
2	FMN	C	401	-	-	5/18/18/18	0/3/3/3
3	GOL	A	402	-	-	4/4/4/4	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	FMN	C4A-C10	11.04	1.49	1.38
2	H	401	FMN	C4A-C10	10.23	1.49	1.38
2	G	401	FMN	C4A-C10	10.08	1.48	1.38
2	D	401	FMN	C4A-C10	9.71	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FMN	C4A-C10	9.67	1.48	1.38
2	F	401	FMN	C4A-C10	9.61	1.48	1.38
2	B	401	FMN	C4A-C10	9.46	1.48	1.38
2	A	401	FMN	C4A-C10	8.74	1.47	1.38
2	E	401	FMN	C4-C4A	4.81	1.49	1.41
2	D	401	FMN	C4-C4A	4.64	1.49	1.41
2	G	401	FMN	C4-C4A	4.57	1.49	1.41
2	H	401	FMN	C4-C4A	4.43	1.49	1.41
2	F	401	FMN	C4-C4A	4.42	1.49	1.41
2	B	401	FMN	C4-C4A	4.37	1.48	1.41
2	H	401	FMN	C9A-N10	4.18	1.44	1.38
2	A	401	FMN	C4-C4A	3.87	1.48	1.41
2	G	401	FMN	C8-C7	3.82	1.50	1.40
2	C	401	FMN	C4-C4A	3.80	1.47	1.41
2	G	401	FMN	C9A-C5A	3.78	1.50	1.42
2	A	401	FMN	C9A-N10	3.70	1.43	1.38
2	A	401	FMN	C9A-C5A	3.62	1.49	1.42
2	E	401	FMN	C9A-C5A	3.60	1.49	1.42
2	C	401	FMN	C9A-C5A	3.59	1.49	1.42
2	A	401	FMN	C8-C7	3.49	1.49	1.40
2	B	401	FMN	C9A-C5A	3.43	1.49	1.42
2	H	401	FMN	C9A-C5A	3.38	1.49	1.42
2	B	401	FMN	C8-C7	3.38	1.49	1.40
2	B	401	FMN	C9A-N10	3.37	1.43	1.38
2	H	401	FMN	C8-C7	3.37	1.49	1.40
2	D	401	FMN	C9A-C5A	3.36	1.49	1.42
2	G	401	FMN	C9A-N10	3.34	1.43	1.38
2	F	401	FMN	C9A-C5A	3.31	1.49	1.42
2	D	401	FMN	C8-C7	3.28	1.49	1.40
2	F	401	FMN	C9A-N10	3.26	1.42	1.38
2	F	401	FMN	C8-C7	3.19	1.48	1.40
2	E	401	FMN	C8-C7	3.19	1.48	1.40
2	E	401	FMN	C10-N1	3.18	1.37	1.33
2	E	401	FMN	C9A-N10	3.11	1.42	1.38
2	C	401	FMN	C8-C7	3.09	1.48	1.40
2	C	401	FMN	C9A-N10	3.03	1.42	1.38
2	H	401	FMN	C10-N1	2.91	1.37	1.33
2	C	401	FMN	C10-N1	2.74	1.36	1.33
2	D	401	FMN	C9A-N10	2.69	1.42	1.38
2	G	401	FMN	C10-N1	2.38	1.36	1.33
2	B	401	FMN	C10-N1	2.27	1.36	1.33
2	F	401	FMN	C10-N1	2.20	1.36	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	401	FMN	C4-N3-C2	8.85	122.61	115.14
2	C	401	FMN	C4-N3-C2	8.32	122.17	115.14
2	D	401	FMN	C4-N3-C2	8.23	122.09	115.14
2	E	401	FMN	C4-N3-C2	8.10	121.98	115.14
2	G	401	FMN	C4-N3-C2	8.08	121.97	115.14
2	B	401	FMN	C4-N3-C2	8.07	121.96	115.14
2	A	401	FMN	C4-N3-C2	7.80	121.73	115.14
2	F	401	FMN	C4-N3-C2	7.55	121.52	115.14
2	G	401	FMN	C1'-N10-C9A	6.42	123.35	118.29
2	C	401	FMN	C1'-N10-C9A	6.06	123.06	118.29
2	A	401	FMN	C1'-N10-C9A	5.58	122.68	118.29
2	H	401	FMN	C1'-N10-C9A	5.50	122.62	118.29
2	H	401	FMN	C4A-N5-C5A	5.31	122.08	116.77
2	B	401	FMN	C1'-N10-C9A	5.25	122.43	118.29
2	F	401	FMN	C1'-N10-C9A	5.04	122.26	118.29
2	E	401	FMN	C1'-N10-C9A	4.90	122.15	118.29
2	C	401	FMN	C4A-N5-C5A	4.88	121.65	116.77
2	B	401	FMN	C4A-N5-C5A	4.86	121.63	116.77
2	E	401	FMN	C4-C4A-C10	-4.77	116.80	119.95
2	F	401	FMN	C4A-N5-C5A	4.74	121.51	116.77
2	D	401	FMN	C4A-N5-C5A	4.70	121.47	116.77
2	A	401	FMN	C4A-N5-C5A	4.68	121.44	116.77
2	G	401	FMN	C4A-N5-C5A	4.54	121.31	116.77
2	E	401	FMN	C4A-N5-C5A	4.48	121.25	116.77
2	G	401	FMN	C4-C4A-C10	-4.40	117.04	119.95
2	D	401	FMN	C1'-N10-C9A	4.38	121.74	118.29
2	D	401	FMN	C4A-C4-N3	-4.09	117.84	123.43
2	B	401	FMN	C4-C4A-C10	-4.02	117.29	119.95
2	D	401	FMN	C4-C4A-C10	-3.89	117.38	119.95
2	H	401	FMN	C4-C4A-C10	-3.82	117.42	119.95
2	G	401	FMN	C4A-C4-N3	-3.72	118.34	123.43
2	B	401	FMN	C4A-C4-N3	-3.72	118.35	123.43
2	C	401	FMN	C4A-C4-N3	-3.68	118.40	123.43
2	H	401	FMN	C4A-C4-N3	-3.67	118.41	123.43
2	F	401	FMN	C4A-C4-N3	-3.62	118.48	123.43
2	A	401	FMN	C4A-C4-N3	-3.55	118.58	123.43
2	C	401	FMN	C4-C4A-C10	-3.45	117.67	119.95
2	A	401	FMN	C4-C4A-C10	-3.36	117.72	119.95
2	E	401	FMN	C4A-C4-N3	-3.35	118.85	123.43
2	F	401	FMN	C4-C4A-C10	-3.19	117.84	119.95
2	D	401	FMN	C4-C4A-N5	2.96	121.98	118.60
2	B	401	FMN	C4-C4A-N5	2.92	121.93	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	401	FMN	C4-C4A-N5	2.83	121.83	118.60
2	E	401	FMN	C4-C4A-N5	2.81	121.81	118.60
2	F	401	FMN	C9A-N10-C10	-2.75	118.31	121.91
2	A	401	FMN	C9A-N10-C10	-2.75	118.31	121.91
2	H	401	FMN	C4-C4A-N5	2.67	121.65	118.60
2	C	401	FMN	C9A-N10-C10	-2.61	118.49	121.91
2	F	401	FMN	O3P-P-O2P	2.56	117.43	107.64
2	G	401	FMN	C9A-N10-C10	-2.52	118.60	121.91
2	D	401	FMN	C9A-N10-C10	-2.50	118.64	121.91
2	E	401	FMN	C9A-N10-C10	-2.46	118.69	121.91
2	E	401	FMN	C5A-C9A-N10	2.42	119.47	117.72
2	F	401	FMN	O2P-P-O5'	-2.40	100.33	106.73
2	G	401	FMN	P-O5'-C5'	2.37	124.81	118.30
2	H	401	FMN	C9A-N10-C10	-2.21	119.01	121.91
2	F	401	FMN	C4-C4A-N5	2.20	121.11	118.60
2	C	401	FMN	O3P-P-O2P	2.17	115.92	107.64
2	A	401	FMN	C5'-C4'-C3'	-2.13	108.08	112.20
2	E	401	FMN	O3P-P-O2P	2.12	115.74	107.64
2	F	401	FMN	P-O5'-C5'	2.04	123.90	118.30
2	C	401	FMN	C5A-C9A-N10	2.02	119.18	117.72
2	A	401	FMN	P-O5'-C5'	2.02	123.87	118.30

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	402	GOL	C1-C2-C3-O3
3	E	402	GOL	O2-C2-C3-O3
2	H	401	FMN	O3'-C3'-C4'-C5'
3	F	402	GOL	C1-C2-C3-O3
2	D	401	FMN	C5'-O5'-P-O2P
2	B	401	FMN	C1'-C2'-C3'-C4'
2	B	401	FMN	O3'-C3'-C4'-C5'
3	G	402	GOL	C1-C2-C3-O3
2	E	401	FMN	C5'-O5'-P-O2P
2	G	401	FMN	C2'-C3'-C4'-C5'
2	G	401	FMN	O3'-C3'-C4'-O4'
2	G	401	FMN	O3'-C3'-C4'-C5'
2	G	401	FMN	C5'-O5'-P-O2P
2	G	401	FMN	C5'-O5'-P-O3P
2	A	401	FMN	C5'-O5'-P-O2P
2	C	401	FMN	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
3	A	402	GOL	O1-C1-C2-C3
3	A	402	GOL	C1-C2-C3-O3
2	H	401	FMN	O3'-C3'-C4'-O4'
2	F	401	FMN	O3'-C3'-C4'-O4'
2	B	401	FMN	O3'-C3'-C4'-O4'
2	H	401	FMN	C2'-C3'-C4'-O4'
2	F	401	FMN	C2'-C3'-C4'-O4'
2	B	401	FMN	C2'-C3'-C4'-O4'
2	G	401	FMN	C2'-C3'-C4'-O4'
2	F	401	FMN	O3'-C3'-C4'-C5'
2	H	401	FMN	C2'-C3'-C4'-C5'
2	F	401	FMN	C2'-C3'-C4'-C5'
3	F	402	GOL	O2-C2-C3-O3
3	G	402	GOL	O2-C2-C3-O3
3	A	402	GOL	O1-C1-C2-O2
2	D	401	FMN	O3'-C3'-C4'-C5'
2	B	401	FMN	C2'-C3'-C4'-C5'
2	E	401	FMN	C2'-C3'-C4'-C5'
2	D	401	FMN	C2'-C3'-C4'-O4'
3	A	402	GOL	O2-C2-C3-O3
2	D	401	FMN	O3'-C3'-C4'-O4'
2	E	401	FMN	O3'-C3'-C4'-C5'
2	E	401	FMN	C2'-C3'-C4'-O4'
2	B	401	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C4'-C5'-O5'-P
2	D	401	FMN	C2'-C3'-C4'-C5'
2	C	401	FMN	C4'-C5'-O5'-P
2	F	401	FMN	C5'-O5'-P-O2P
2	B	401	FMN	O2'-C2'-C3'-C4'
2	H	401	FMN	C4'-C5'-O5'-P
2	D	401	FMN	C4'-C5'-O5'-P
2	F	401	FMN	C4'-C5'-O5'-P
2	E	401	FMN	C4'-C5'-O5'-P
2	G	401	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C2'-C3'-C4'-O4'
2	C	401	FMN	C2'-C3'-C4'-O4'
2	E	401	FMN	O3'-C3'-C4'-O4'
2	B	401	FMN	O2'-C2'-C3'-O3'
2	H	401	FMN	C5'-O5'-P-O2P
2	B	401	FMN	C5'-O5'-P-O2P
2	A	401	FMN	O3'-C3'-C4'-O4'
2	C	401	FMN	O3'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
2	B	401	FMN	C1'-C2'-C3'-O3'
2	C	401	FMN	O3'-C3'-C4'-C5'

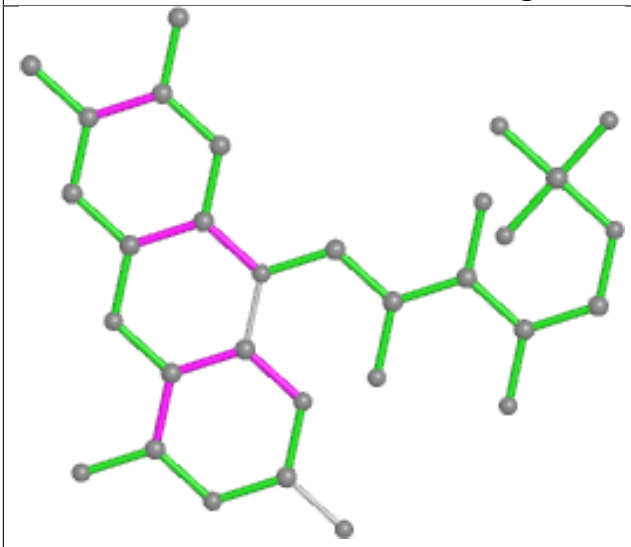
There are no ring outliers.

8 monomers are involved in 21 short contacts:

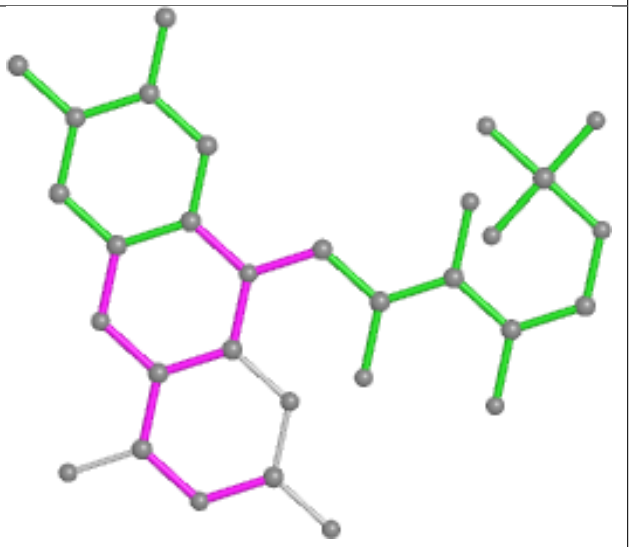
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	401	FMN	1	0
2	D	401	FMN	3	0
2	F	401	FMN	1	0
2	B	401	FMN	3	0
2	E	401	FMN	3	0
2	G	401	FMN	4	0
2	A	401	FMN	4	0
2	C	401	FMN	2	0

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.

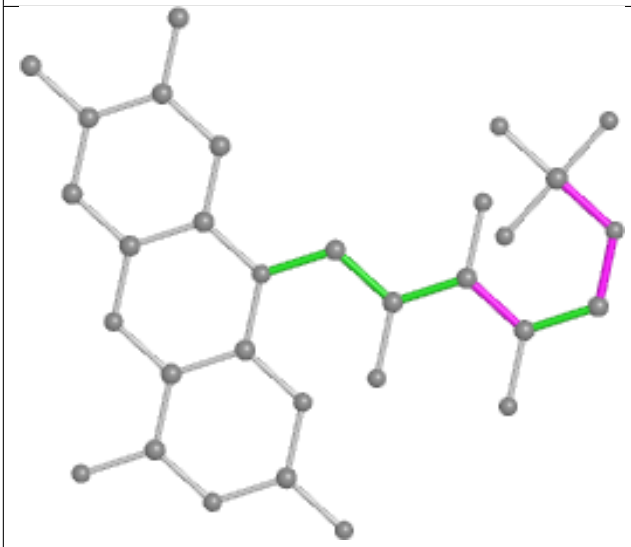
Ligand FMN H 401



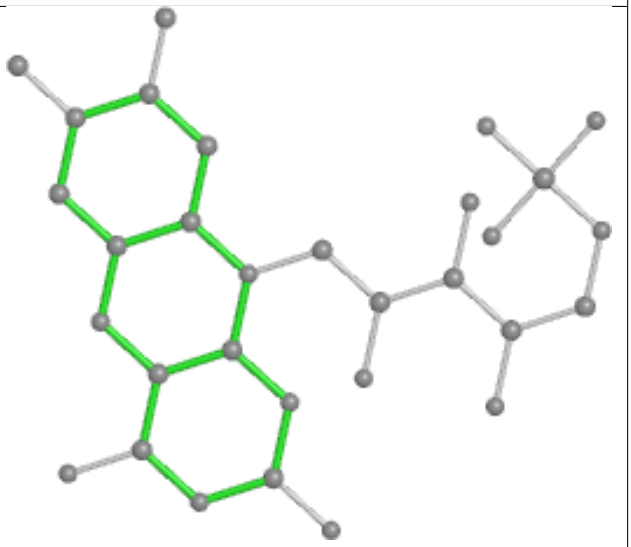
Bond lengths



Bond angles

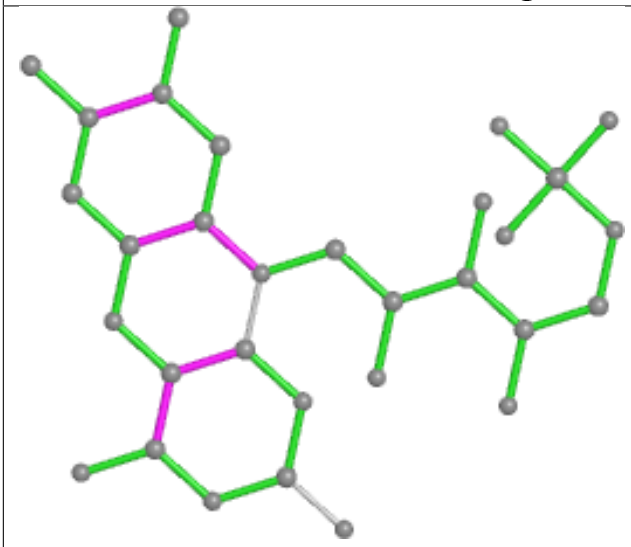


Torsions

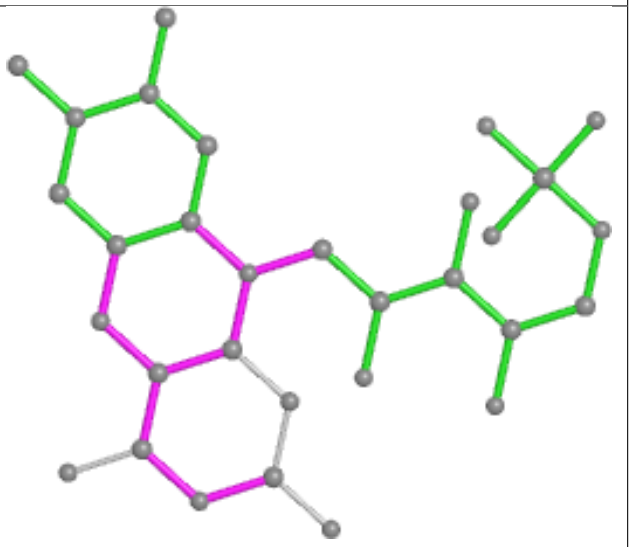


Rings

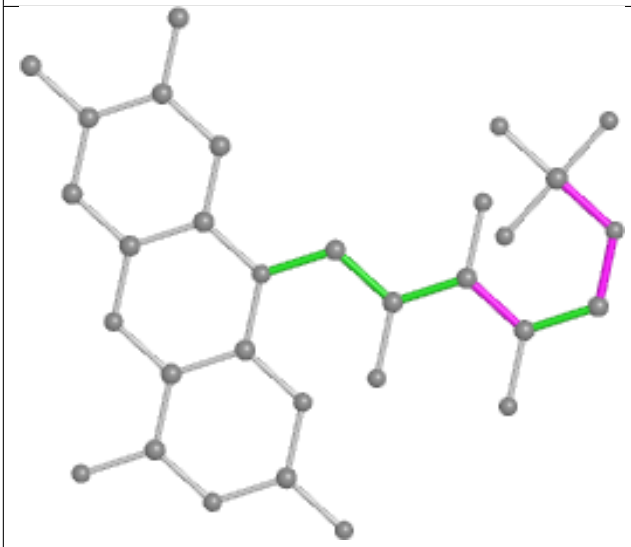
Ligand FMN D 401



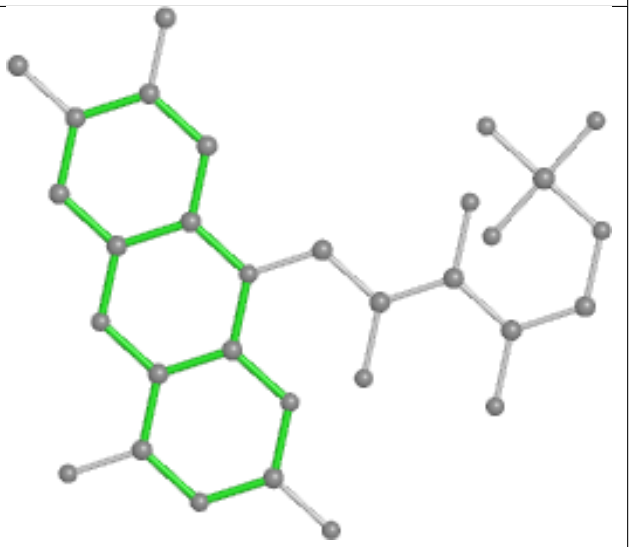
Bond lengths



Bond angles

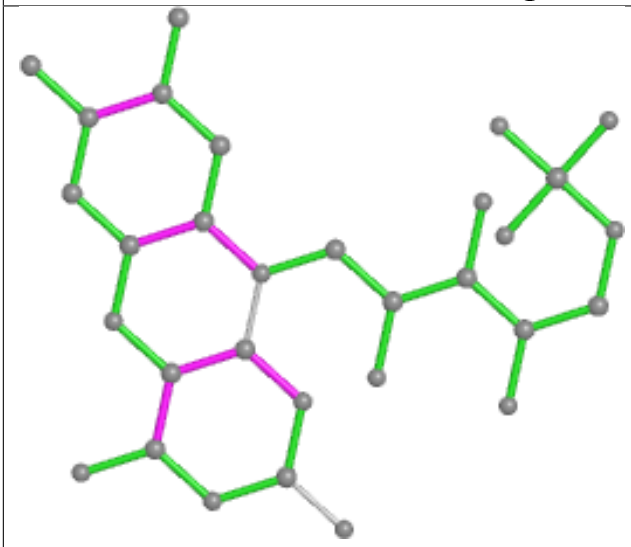


Torsions

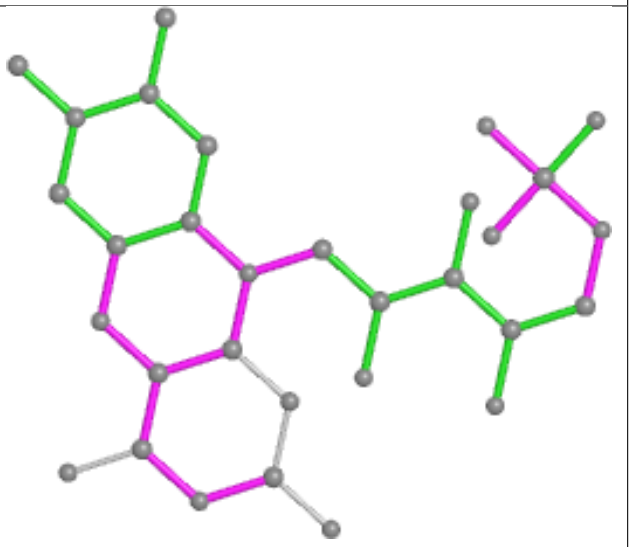


Rings

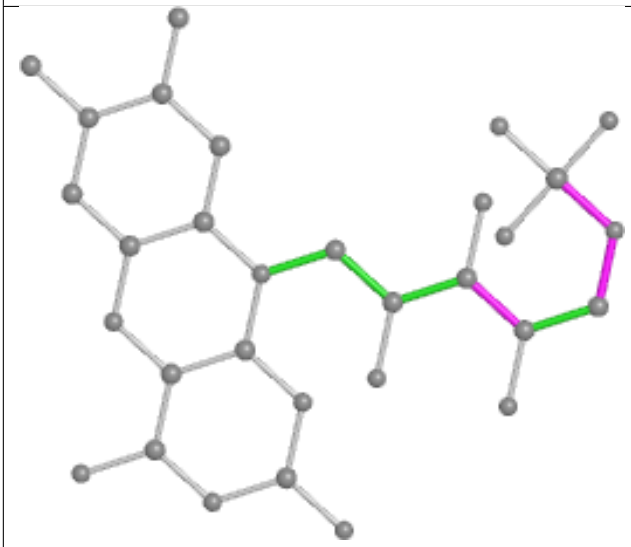
Ligand FMN F 401



Bond lengths



Bond angles



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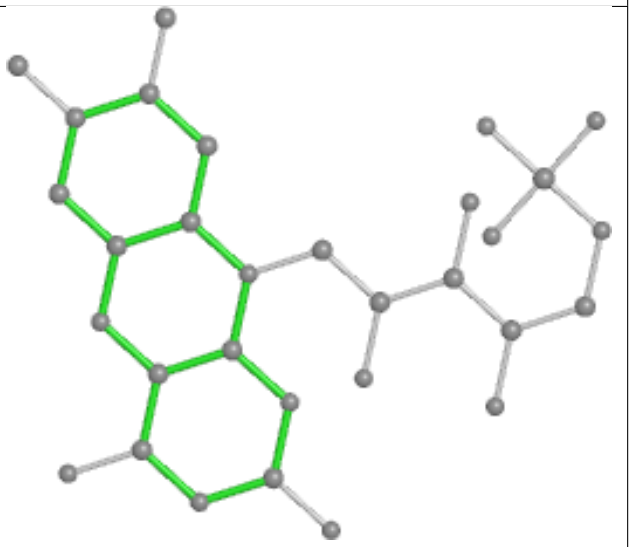
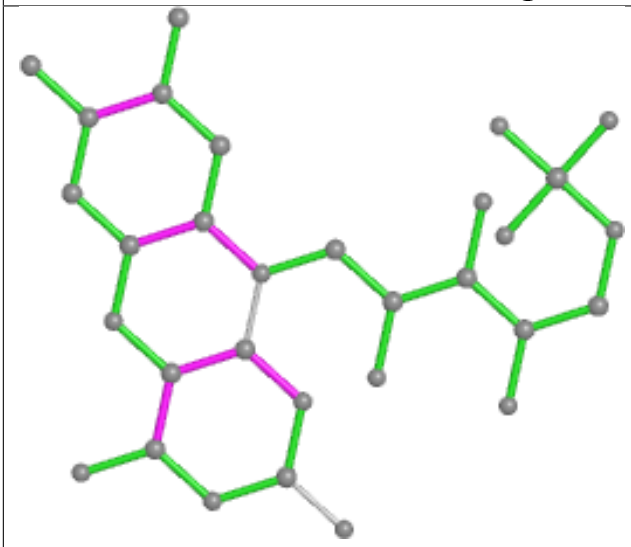
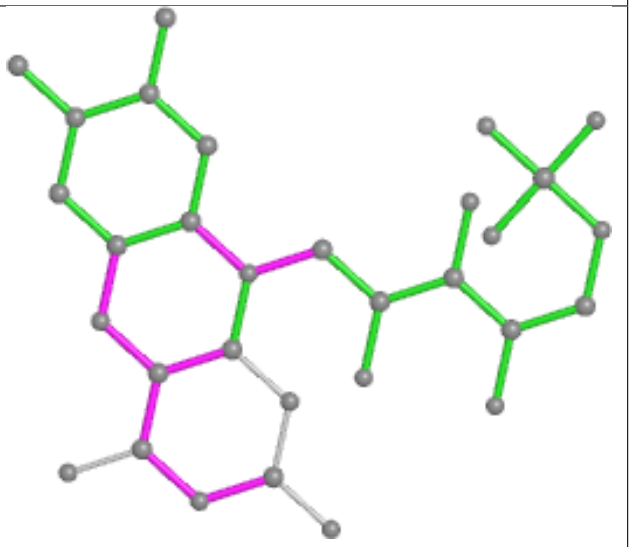


Rings

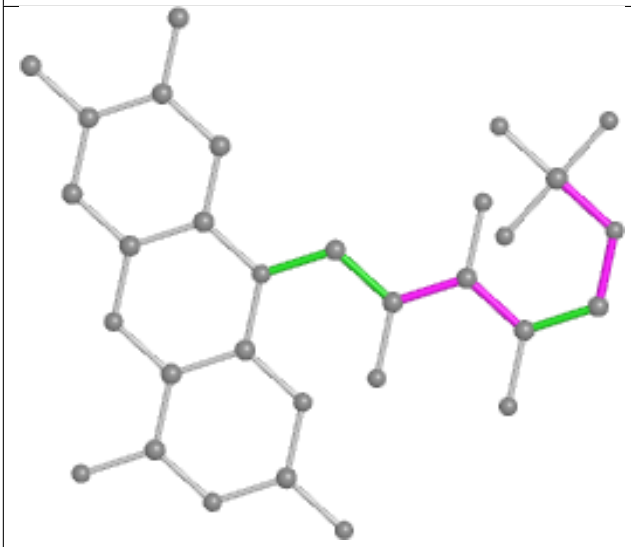
Ligand FMN B 401



Bond lengths



Bond angles



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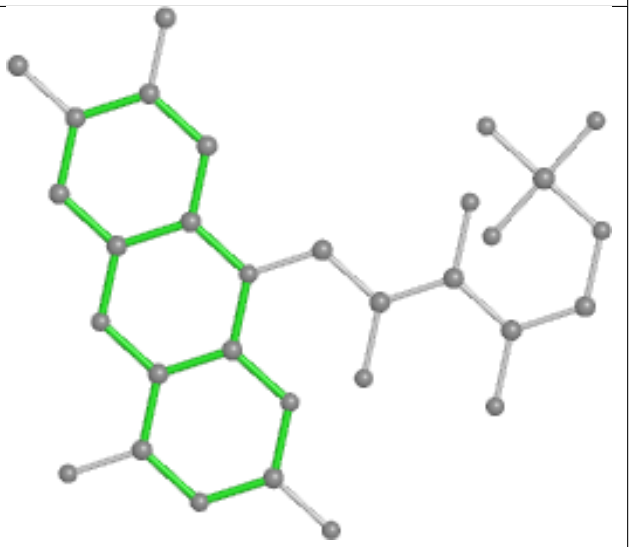
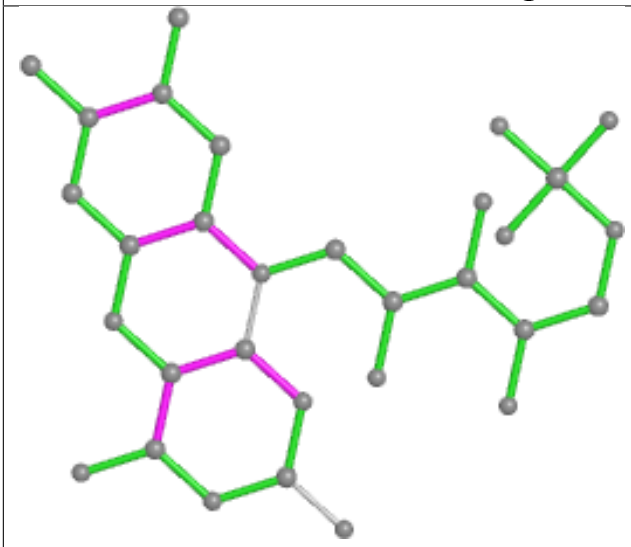
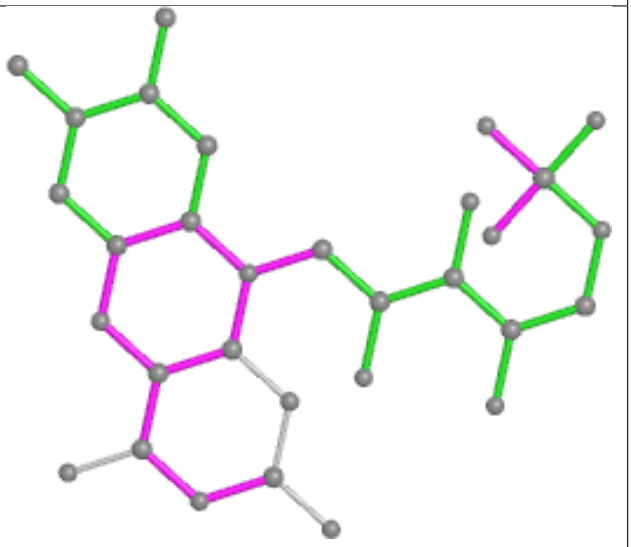


Rings

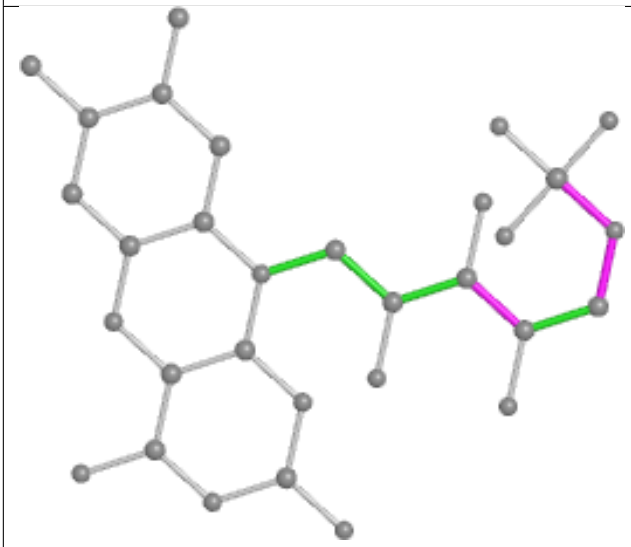
Ligand FMN E 401



Bond lengths



Bond angles



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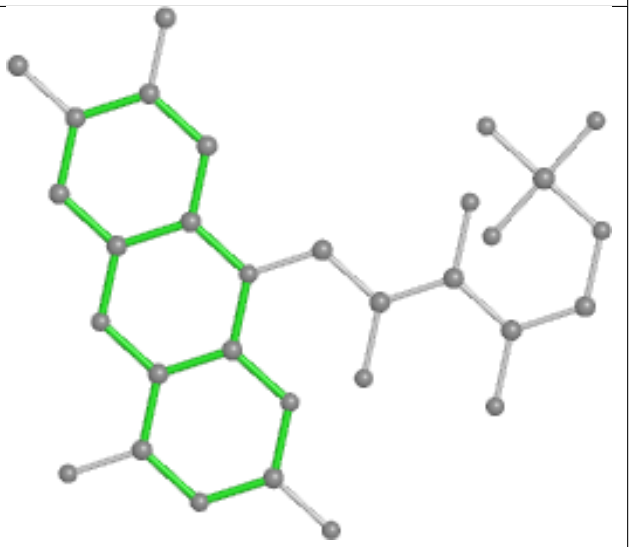
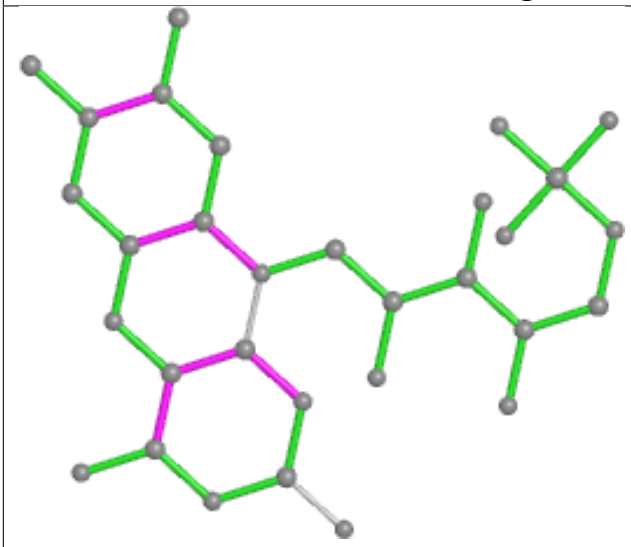
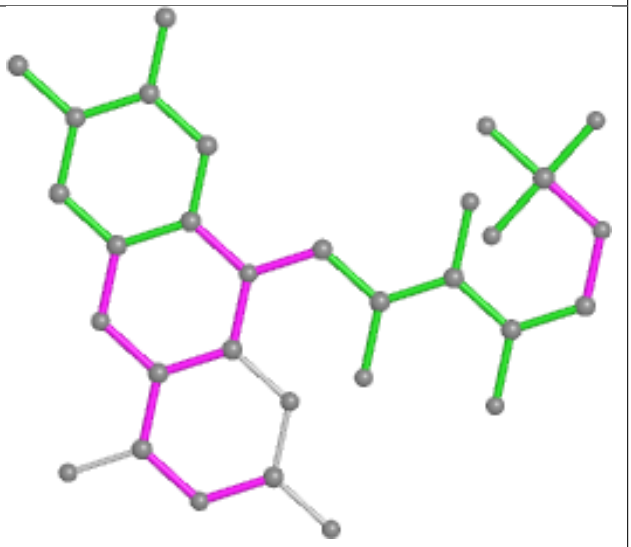


Rings

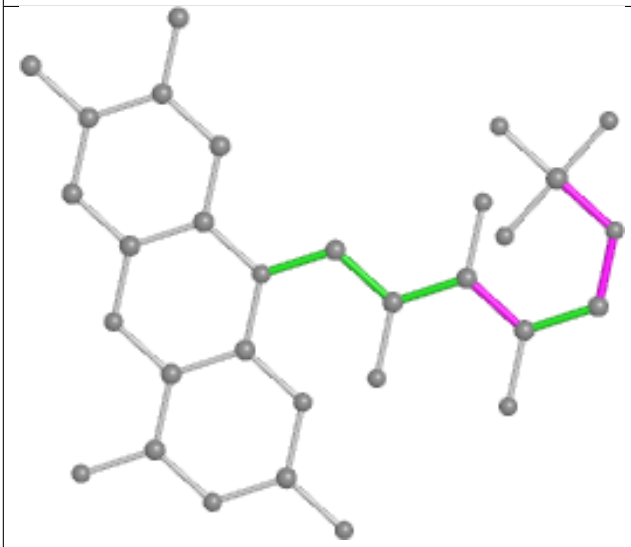
Ligand FMN G 401



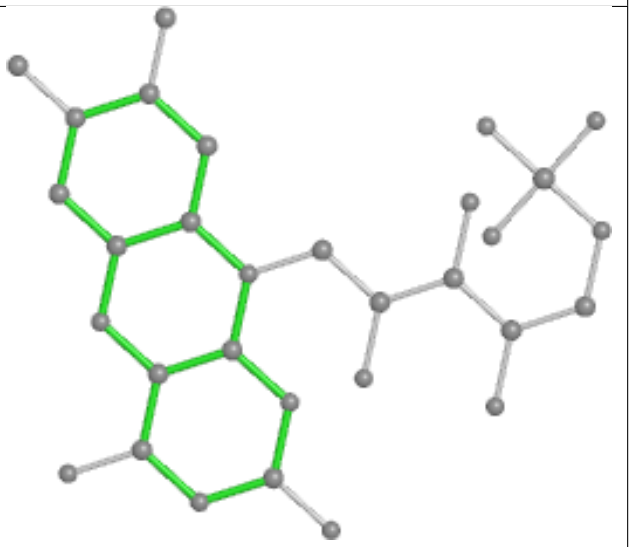
Bond lengths



Bond angles

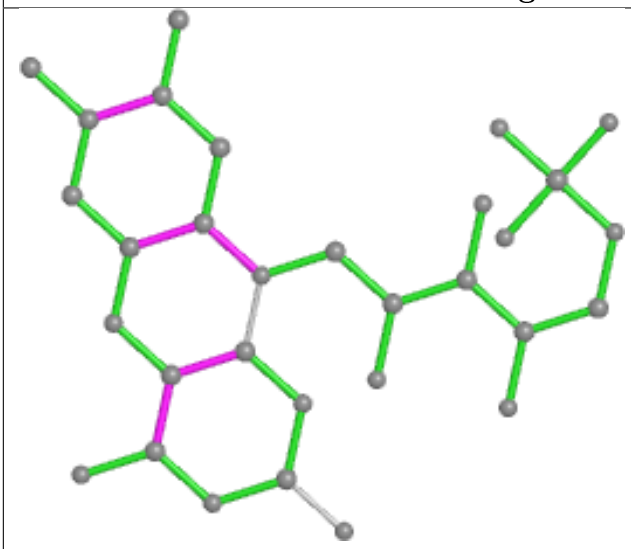


Torsions

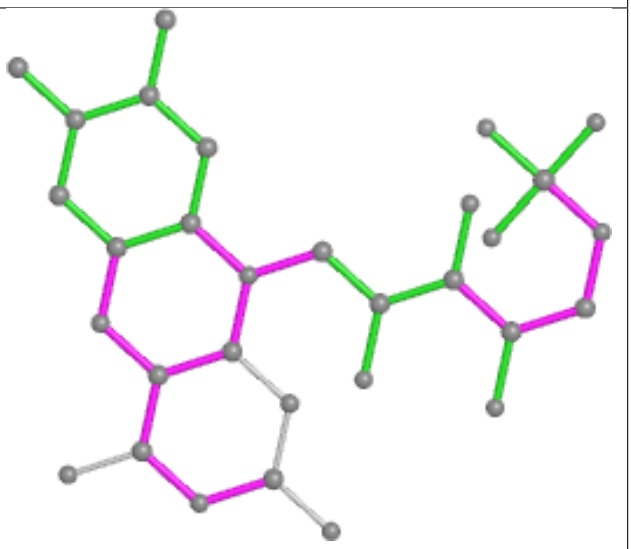


Rings

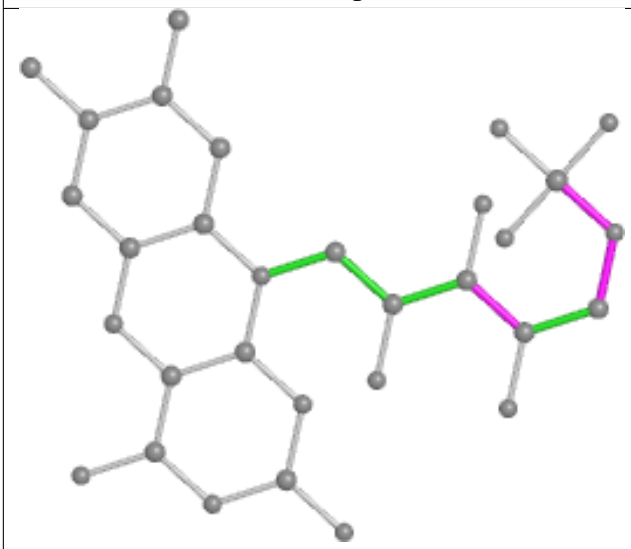
Ligand FMN A 401



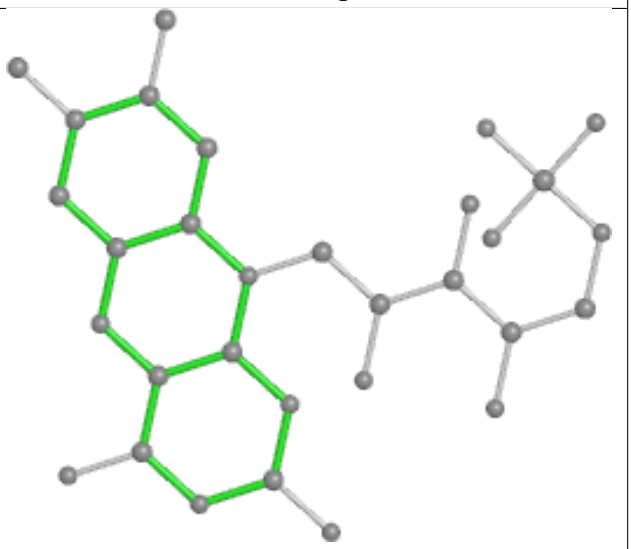
Bond lengths



Bond angles

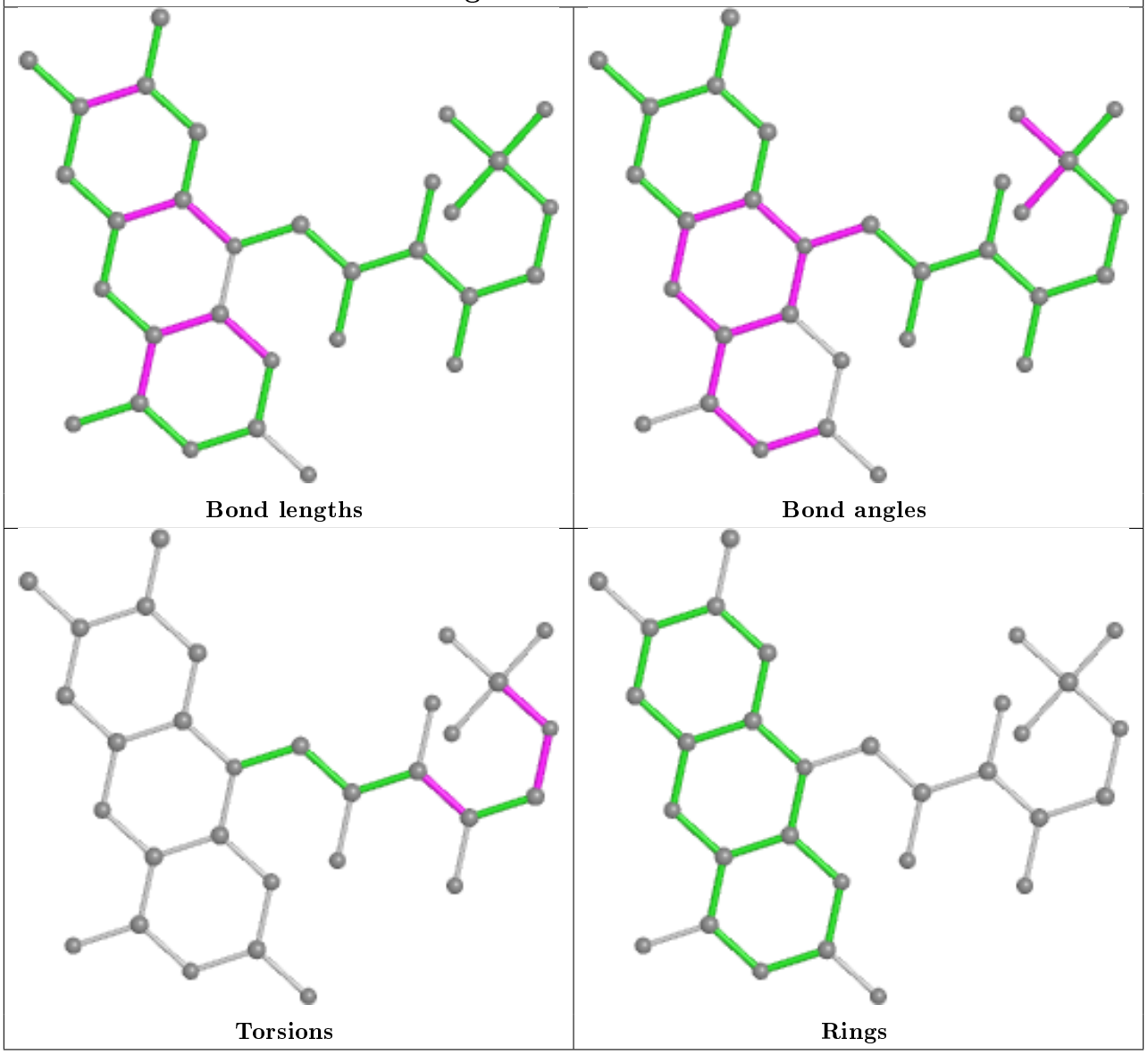


Torsions



Rings

Ligand FMN C 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	111:THR	C	112:PRO	N	1.19

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	339/359 (94%)	-0.12	6 (1%)	68	71	21, 35, 58, 88	0
1	B	332/359 (92%)	0.03	9 (2%)	54	58	26, 42, 62, 78	0
1	C	338/359 (94%)	-0.06	6 (1%)	68	71	25, 40, 63, 90	0
1	D	333/359 (92%)	0.06	9 (2%)	54	58	26, 43, 65, 105	0
1	E	339/359 (94%)	0.14	15 (4%)	34	37	27, 43, 69, 104	0
1	F	337/359 (93%)	0.21	24 (7%)	16	16	28, 46, 67, 95	0
1	G	331/359 (92%)	0.34	16 (4%)	30	32	28, 50, 78, 91	0
1	H	331/359 (92%)	0.02	7 (2%)	63	66	24, 39, 62, 83	0
All	All	2680/2872 (93%)	0.08	92 (3%)	45	48	21, 42, 68, 105	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	77	VAL	4.2
1	F	3	CYS	4.1
1	E	3	CYS	4.1
1	D	2	PRO	3.8
1	C	352	VAL	3.8
1	G	334	ILE	3.7
1	E	237	VAL	3.5
1	B	77	VAL	3.3
1	H	84	ALA	3.3
1	G	168	GLY	3.1
1	F	95	ALA	3.1
1	F	97	PHE	3.1
1	H	323	TRP	3.1
1	F	85	ALA	3.0
1	F	215	ALA	2.9
1	F	57	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	238	GLY	2.8
1	G	118	ALA	2.8
1	A	237	VAL	2.8
1	F	84	ALA	2.7
1	E	81	ALA	2.7
1	B	97	PHE	2.7
1	G	346	SER	2.7
1	F	166	ALA	2.7
1	G	177	LEU	2.7
1	G	179	ALA	2.7
1	F	237	VAL	2.7
1	G	50	ALA	2.7
1	B	314	LEU	2.6
1	G	216	GLY	2.6
1	G	338	ASP	2.6
1	E	80	ALA	2.6
1	H	316	PHE	2.6
1	E	216	GLY	2.6
1	E	197	THR	2.6
1	E	215	ALA	2.5
1	H	95	ALA	2.5
1	E	236	GLN	2.5
1	B	293	ALA	2.5
1	G	215	ALA	2.5
1	C	353	GLU	2.5
1	F	348	PRO	2.4
1	E	218	ILE	2.4
1	A	18	ALA	2.4
1	D	142	LEU	2.4
1	D	333	ALA	2.4
1	B	215	ALA	2.4
1	F	81	ALA	2.4
1	F	216	GLY	2.4
1	F	235	VAL	2.4
1	G	146	SER	2.4
1	D	179	ALA	2.3
1	G	142	LEU	2.3
1	F	218	ILE	2.3
1	F	94	PHE	2.3
1	H	81	ALA	2.3
1	D	1	MET	2.3
1	B	316	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	168	GLY	2.3
1	F	80	ALA	2.3
1	H	97	PHE	2.3
1	G	197	THR	2.3
1	E	60	SER	2.3
1	D	94	PHE	2.2
1	B	177	LEU	2.2
1	F	236	GLN	2.2
1	H	50	ALA	2.2
1	F	16	ILE	2.2
1	C	19	PRO	2.2
1	E	209	GLU	2.2
1	E	217	GLY	2.2
1	G	347	LEU	2.2
1	A	236	GLN	2.1
1	D	95	ALA	2.1
1	F	18	ALA	2.1
1	D	92	PRO	2.1
1	C	260	ASP	2.1
1	B	173	ILE	2.1
1	G	84	ALA	2.1
1	A	181	GLY	2.1
1	G	176	GLY	2.1
1	D	81	ALA	2.1
1	F	53	ALA	2.1
1	B	98	ASN	2.1
1	F	119	GLU	2.1
1	E	2	PRO	2.0
1	A	238	GLY	2.0
1	A	179	ALA	2.0
1	F	349	SER	2.0
1	C	10	GLY	2.0
1	C	215	ALA	2.0
1	F	176	GLY	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 carbohydrates in this entry.

6.4 Ligands (i)

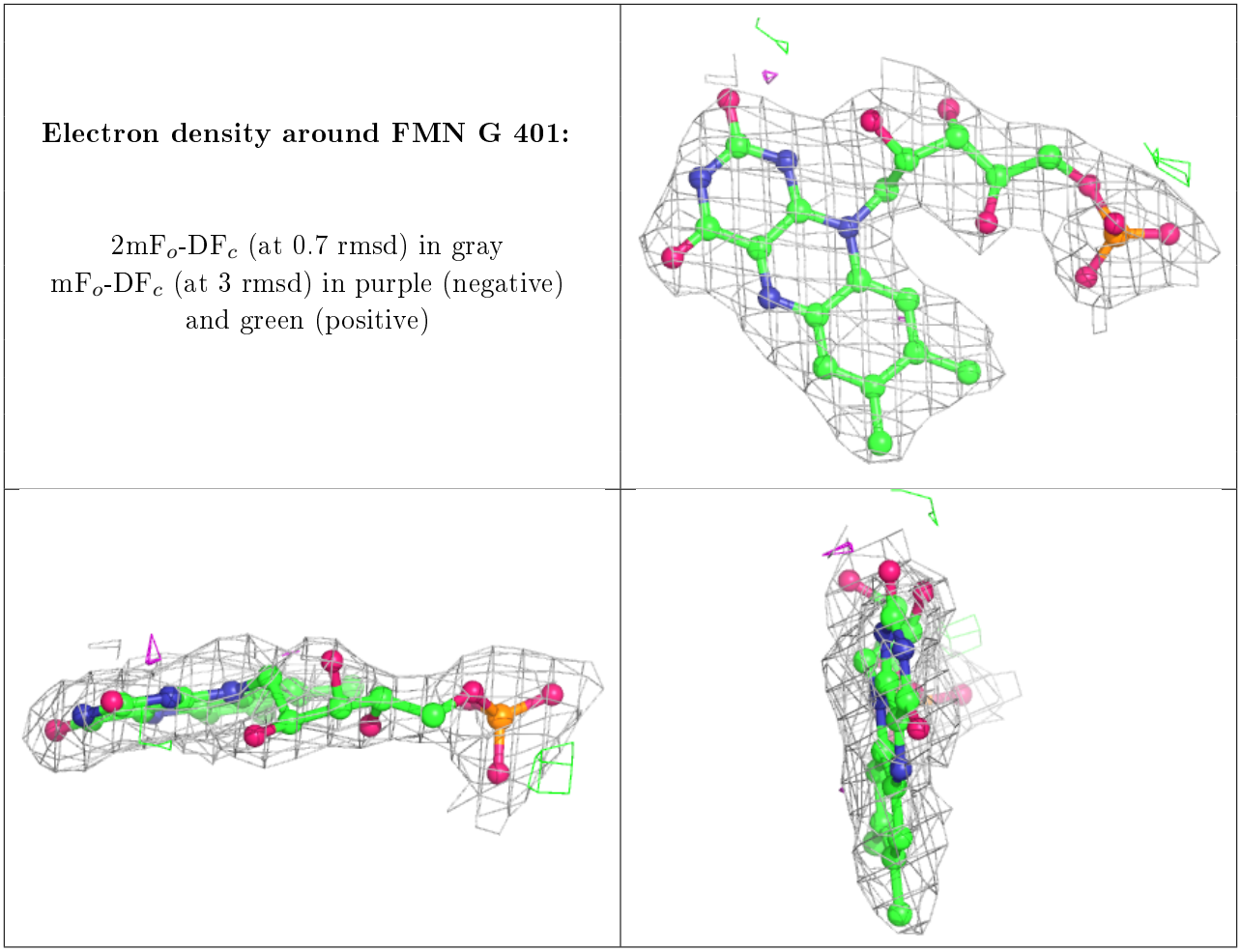
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	GOL	E	402	6/6	0.84	0.31	53,62,68,76	0
3	GOL	F	402	6/6	0.85	0.36	58,83,85,104	0
3	GOL	A	402	6/6	0.86	0.38	43,56,60,66	0
3	GOL	G	402	6/6	0.87	0.39	58,65,66,69	0
2	FMN	G	401	31/31	0.94	0.25	33,53,60,64	0
2	FMN	E	401	31/31	0.94	0.26	28,47,56,59	0
2	FMN	F	401	31/31	0.96	0.22	27,58,65,68	0
2	FMN	B	401	31/31	0.96	0.23	33,52,68,70	0
2	FMN	H	401	31/31	0.96	0.24	22,44,55,60	0
2	FMN	A	401	31/31	0.97	0.27	26,42,49,50	0
2	FMN	C	401	31/31	0.97	0.21	30,42,53,60	0
2	FMN	D	401	31/31	0.97	0.23	28,49,60,64	0

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

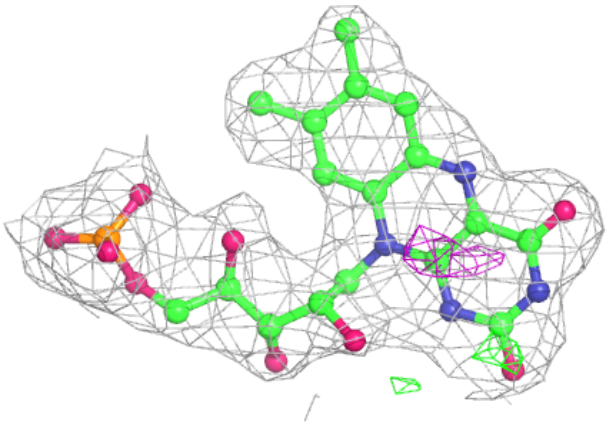
Electron density around FMN G 401:

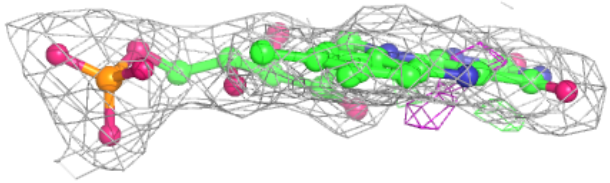
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

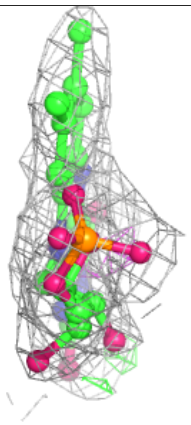


Electron density around FMN E 401:

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

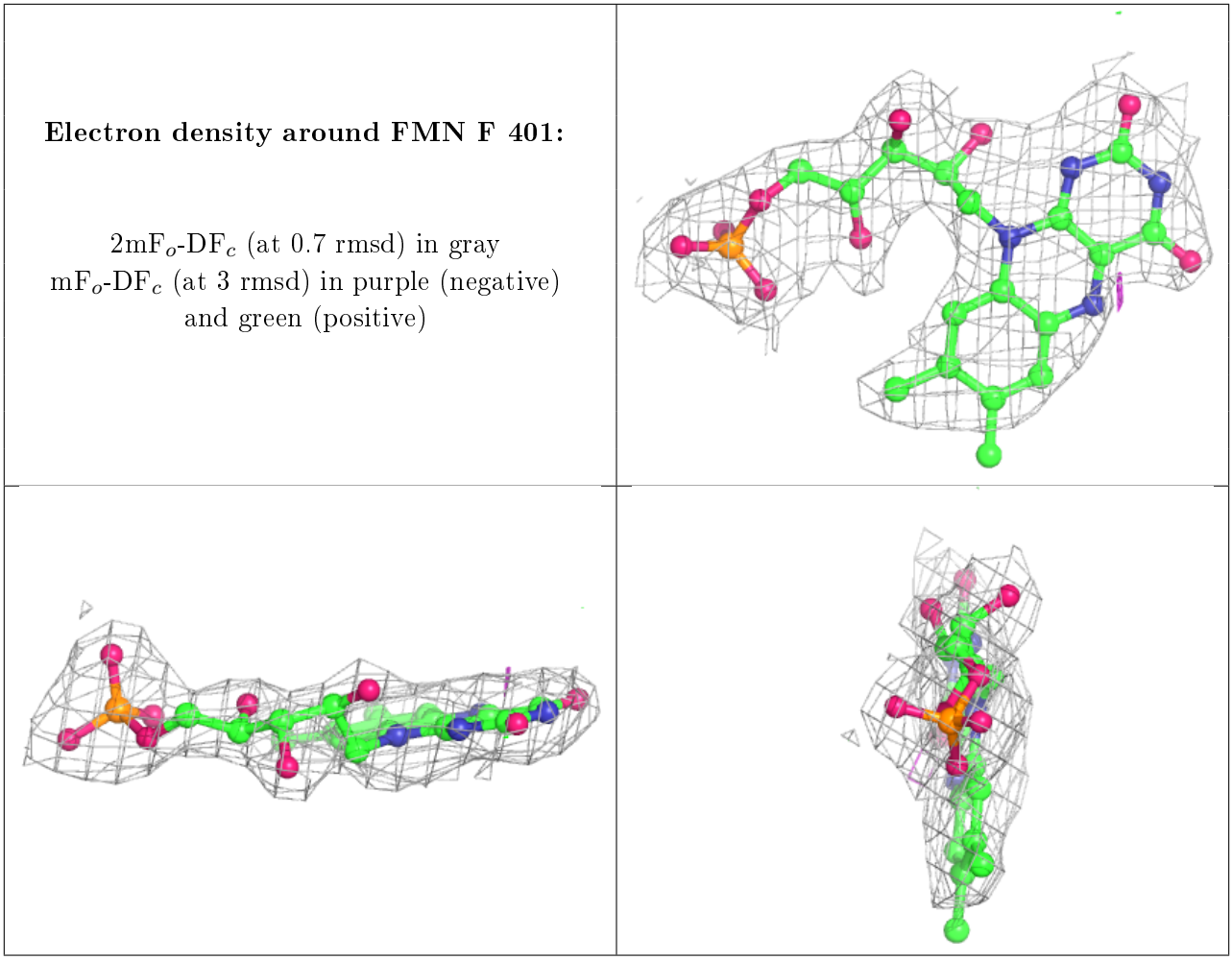






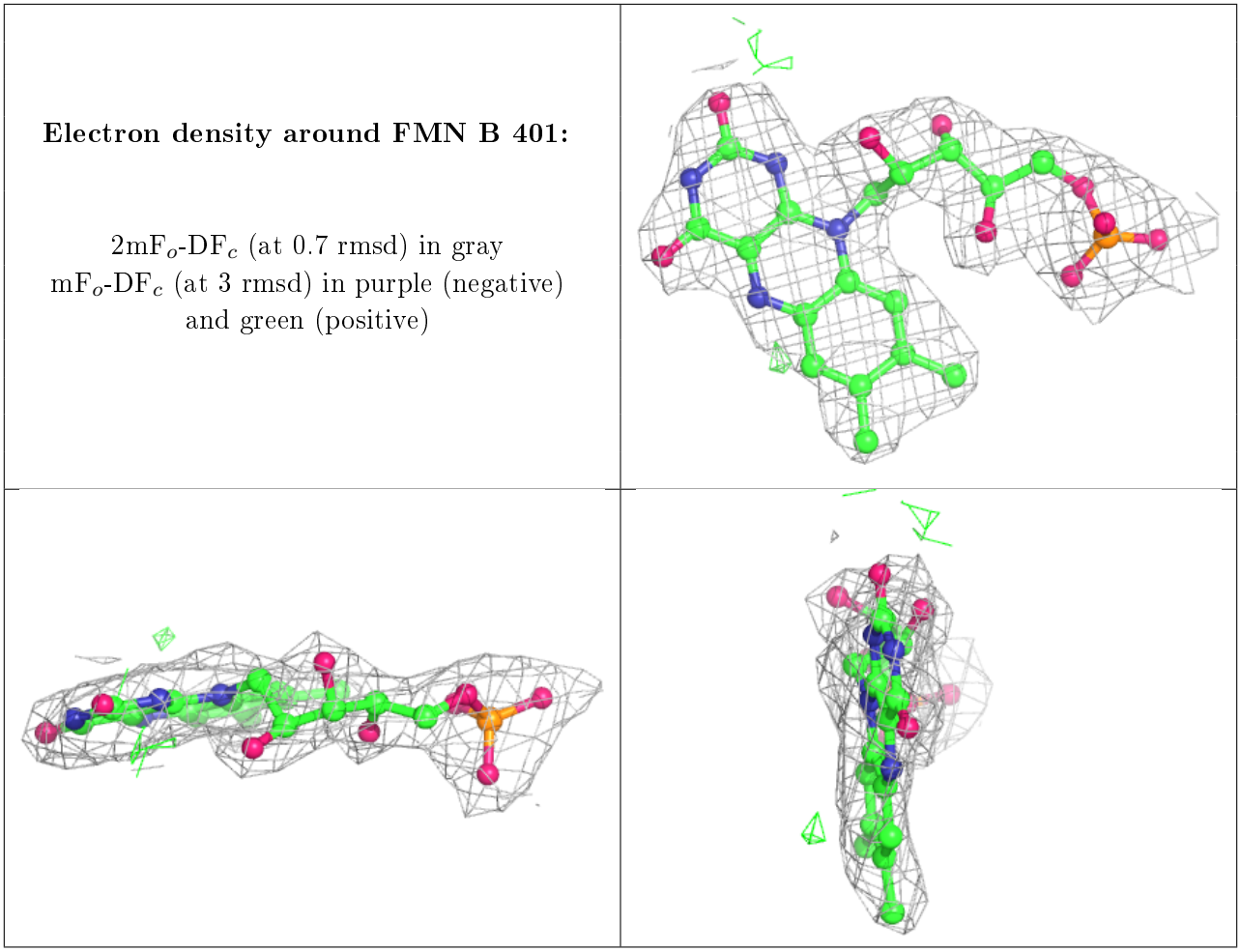
Electron density around FMN F 401:

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



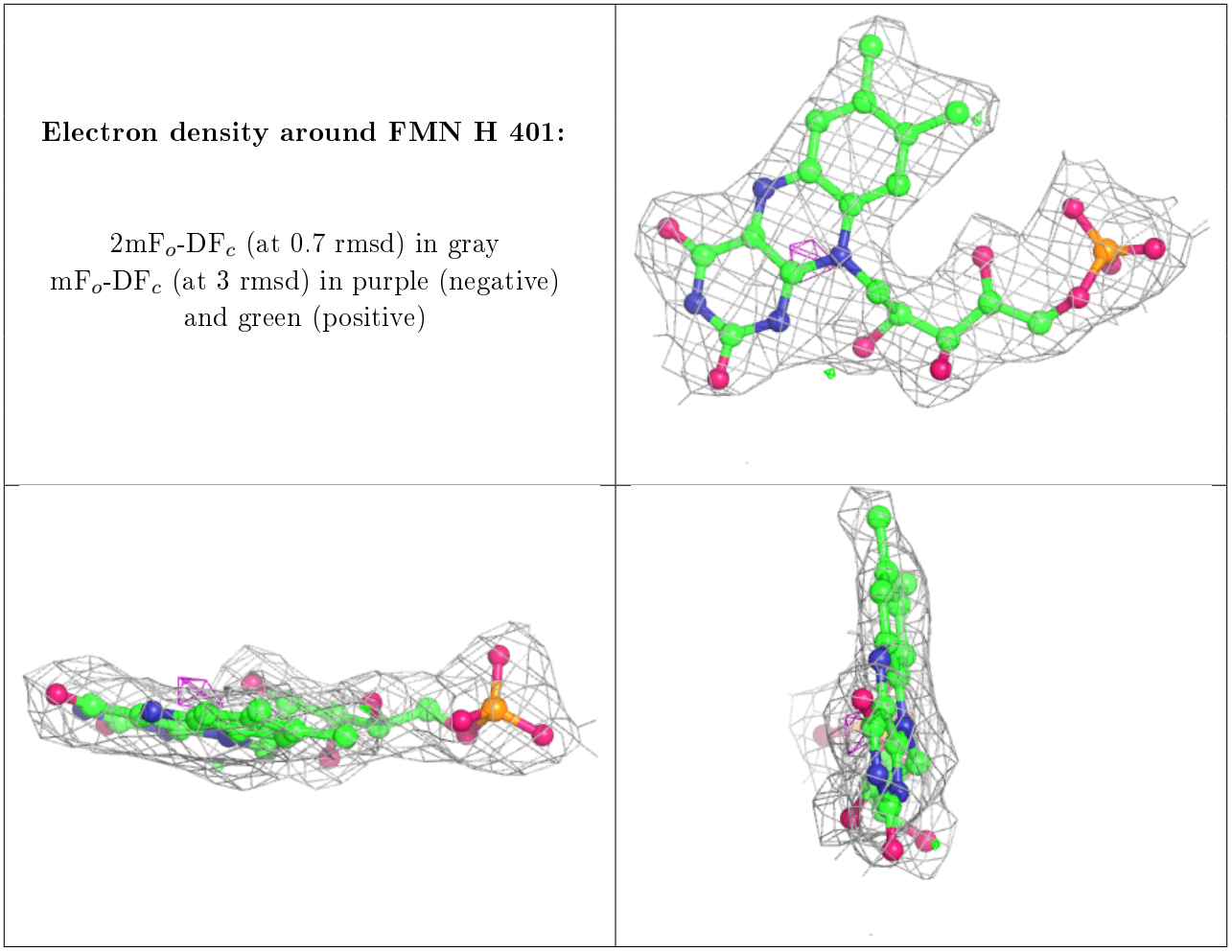
Electron density around FMN B 401:

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



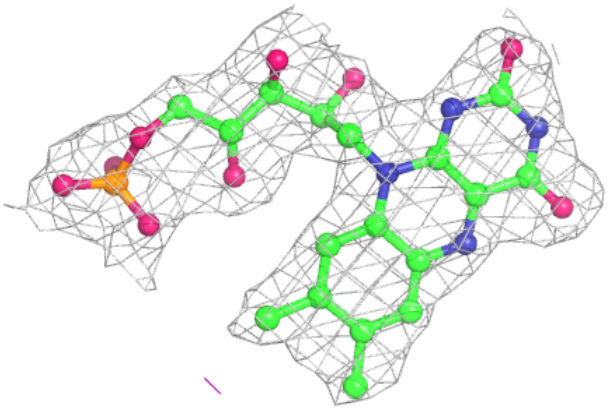
Electron density around FMN H 401:

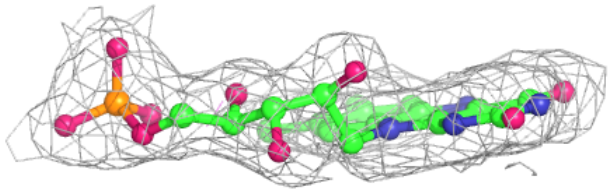
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

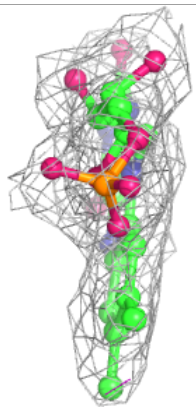


Electron density around FMN A 401:

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

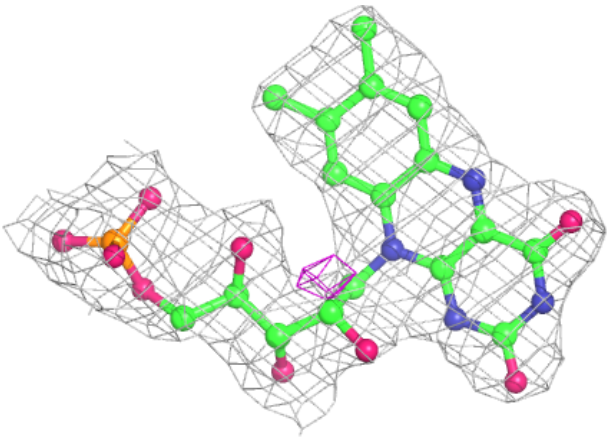


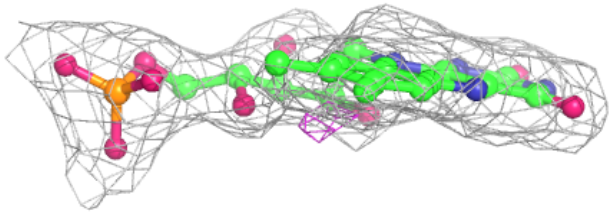


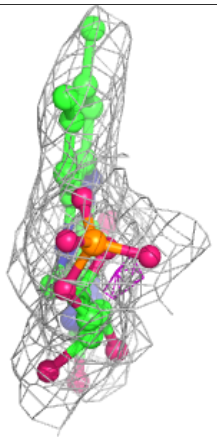


Electron density around FMN C 401:

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

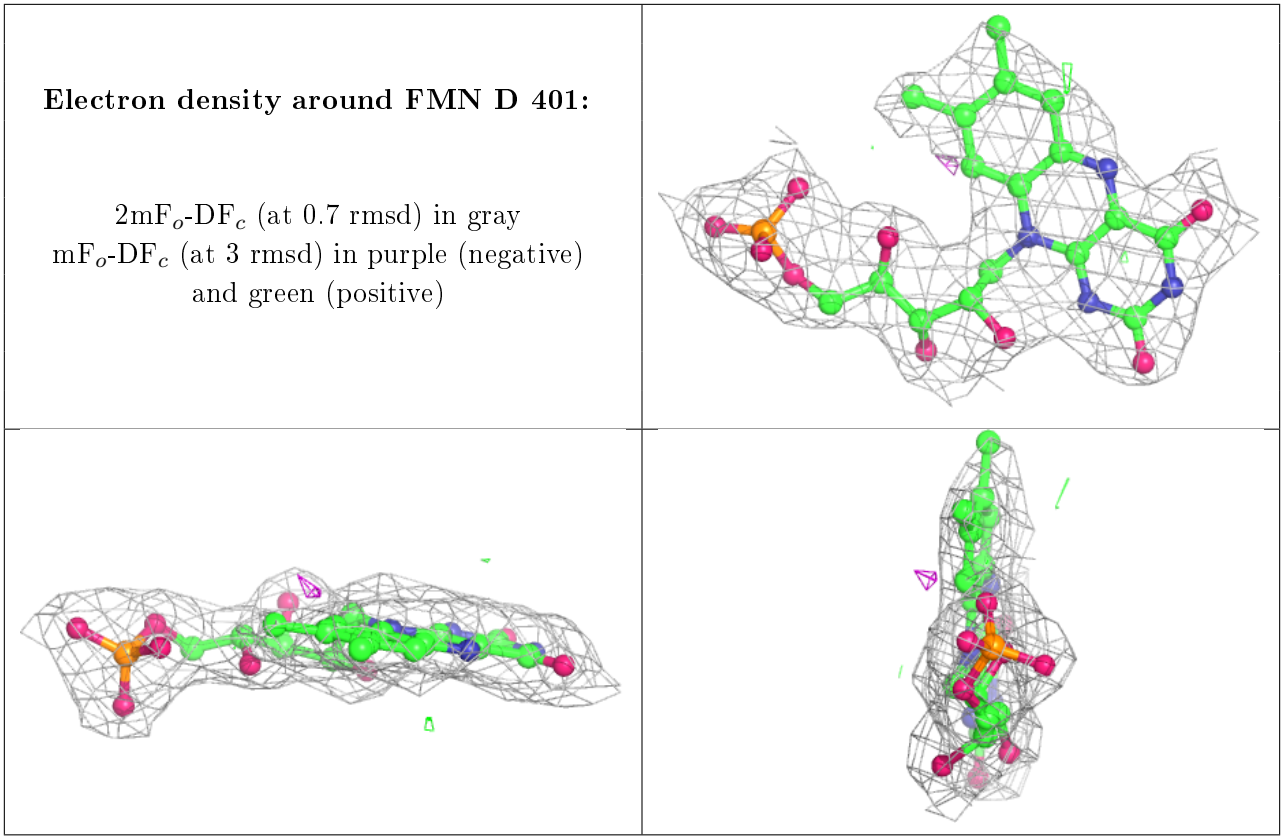






Electron density around FMN D 401:

$2mF_o$-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.