Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:29 PM BST

PDB ID	:	6HMJ
Title	:	Structure of an RNA-binding Light-Oxygen-Voltage Receptor
Authors	:	Ziegler, T.; Moniot, S.; Moeglich, A.
Deposited on	:	2018-09-12
Resolution	:	2.51 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:

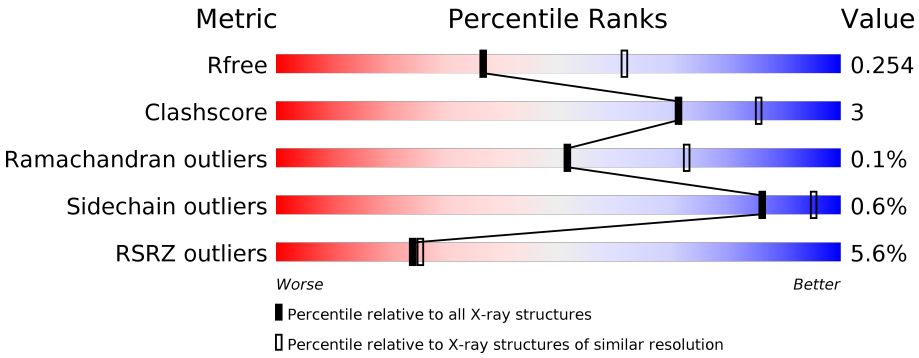
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.2

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 2.51 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	373	3% 91% 5% ·
1	B	373	6% 82% 12% 6%
1	C	373	5% 88% 7% 5%
1	D	373	8% 88% 6% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21802 atoms, of which 10756 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 Putative PAS/PAC sensor protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	359	Total	C	H	N	O	S	0	0	0
			5419	1701	2697	506	508	7			
1	B	352	Total	C	H	N	O	S	0	0	0
			5298	1660	2641	488	502	7			
1	C	355	Total	C	H	N	O	S	0	0	0
			5364	1686	2669	499	503	7			
1	D	353	Total	C	H	N	O	S	0	0	0
			5298	1661	2639	489	502	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	LEU	-	expression tag	UNP C8XJT7
A	367	GLU	-	expression tag	UNP C8XJT7
A	368	HIS	-	expression tag	UNP C8XJT7
A	369	HIS	-	expression tag	UNP C8XJT7
A	370	HIS	-	expression tag	UNP C8XJT7
A	371	HIS	-	expression tag	UNP C8XJT7
A	372	HIS	-	expression tag	UNP C8XJT7
A	373	HIS	-	expression tag	UNP C8XJT7
B	366	LEU	-	expression tag	UNP C8XJT7
B	367	GLU	-	expression tag	UNP C8XJT7
B	368	HIS	-	expression tag	UNP C8XJT7
B	369	HIS	-	expression tag	UNP C8XJT7
B	370	HIS	-	expression tag	UNP C8XJT7
B	371	HIS	-	expression tag	UNP C8XJT7
B	372	HIS	-	expression tag	UNP C8XJT7
B	373	HIS	-	expression tag	UNP C8XJT7
C	366	LEU	-	expression tag	UNP C8XJT7
C	367	GLU	-	expression tag	UNP C8XJT7
C	368	HIS	-	expression tag	UNP C8XJT7
C	369	HIS	-	expression tag	UNP C8XJT7
C	370	HIS	-	expression tag	UNP C8XJT7

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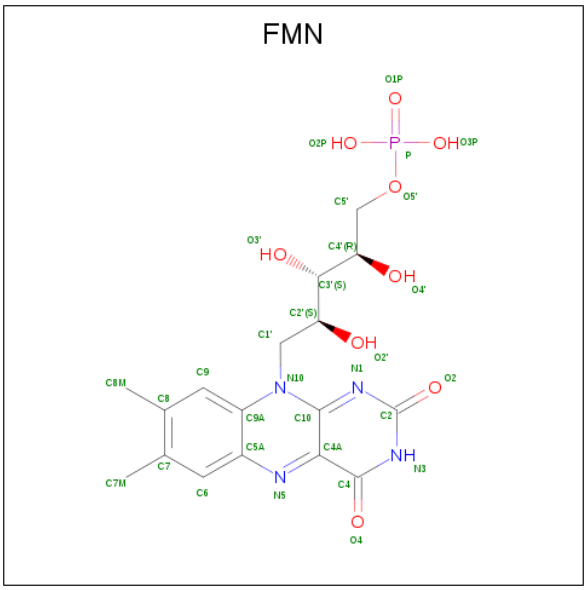
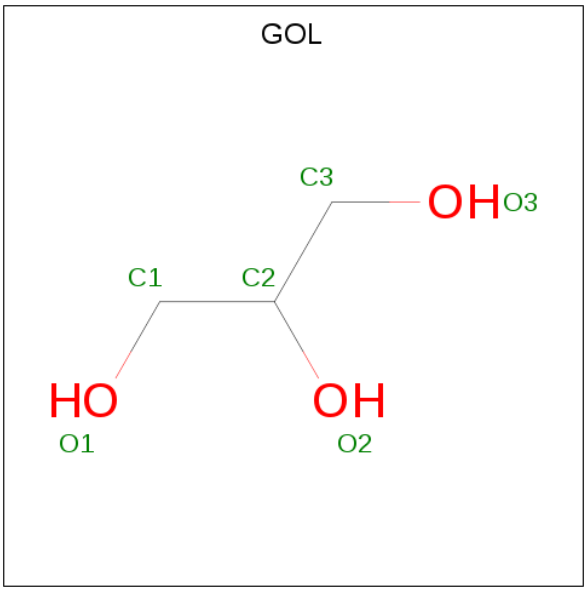
Chain	Residue	Modelled	Actual	Comment	Reference
C	371	HIS	-	expression tag	UNP C8XJT7
C	372	HIS	-	expression tag	UNP C8XJT7
C	373	HIS	-	expression tag	UNP C8XJT7
D	366	LEU	-	expression tag	UNP C8XJT7
D	367	GLU	-	expression tag	UNP C8XJT7
D	368	HIS	-	expression tag	UNP C8XJT7
D	369	HIS	-	expression tag	UNP C8XJT7
D	370	HIS	-	expression tag	UNP C8XJT7
D	371	HIS	-	expression tag	UNP C8XJT7
D	372	HIS	-	expression tag	UNP C8XJT7
D	373	HIS	-	expression tag	UNP C8XJT7

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



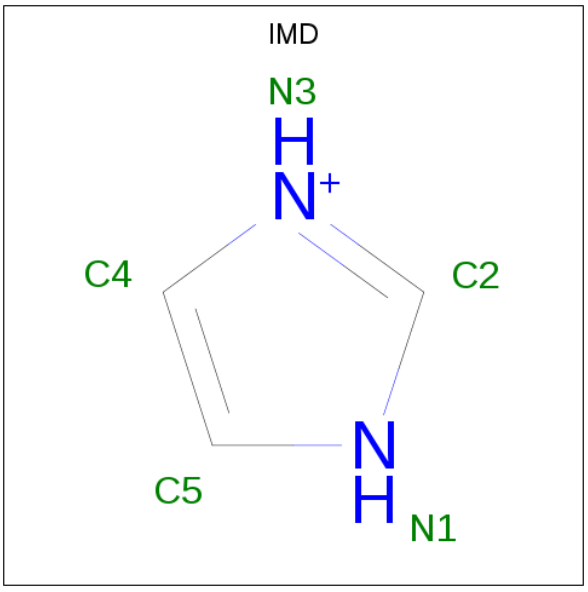
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			49	17	18	4	9	1		
2	B	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	C	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	D	1	Total	C	H	N	O	P	0	0
			49	17	18	4	9	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



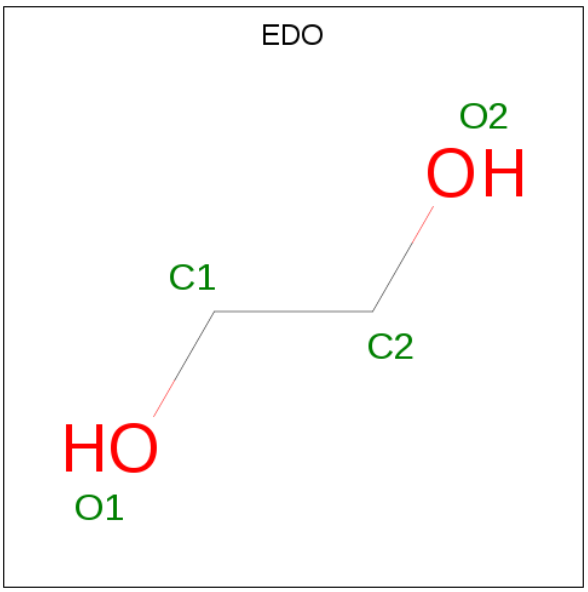
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 12 3 6 3	0	0
3	D	1	Total C H O 13 3 7 3	0	0
3	D	1	Total C H O 12 3 6 3	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H N 10 3 5 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C H O 10 2 6 2	0	0
5	D	1	Total C H O 10 2 6 2	0	0

- Molecule 6 is water.

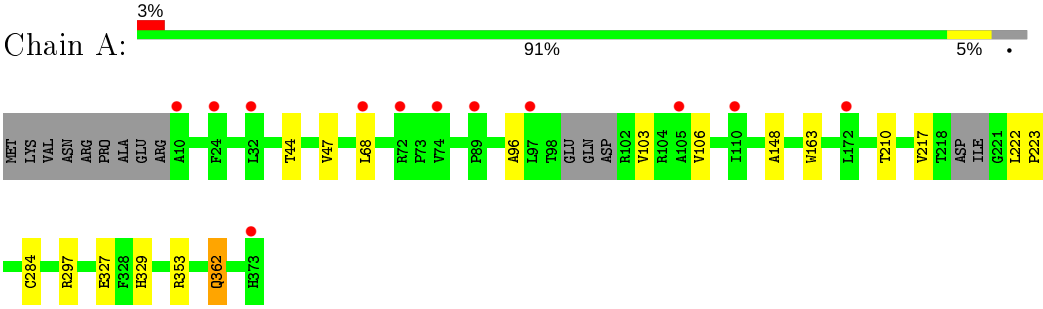
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	58	Total O 58 58	0	0
6	B	25	Total O 25 25	0	0
6	C	37	Total O 37 37	0	0
6	D	38	Total O 38 38	0	0

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.

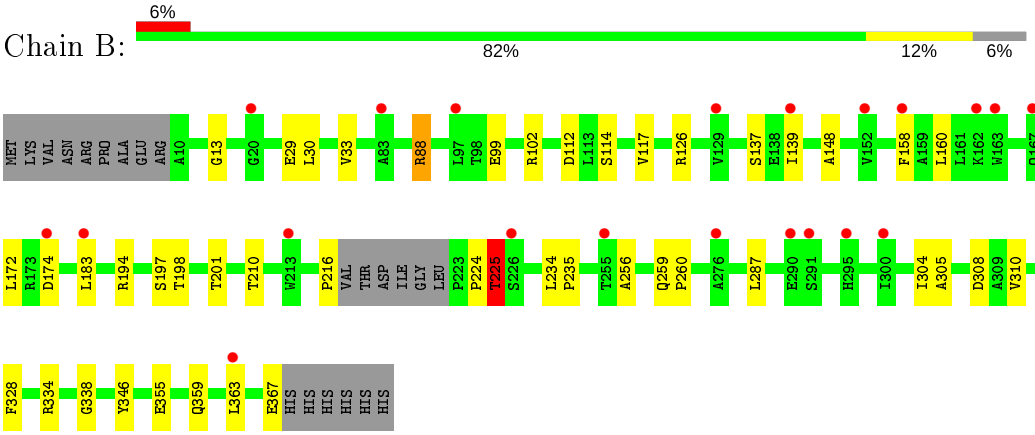
- Molecule 1: Putative PAS/PAC sensor protein

Chain A:



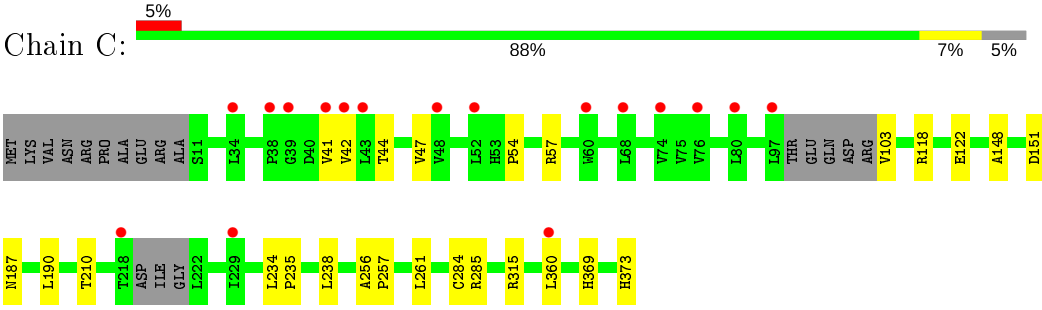
- Molecule 1: Putative PAS/PAC sensor protein

Chain B:



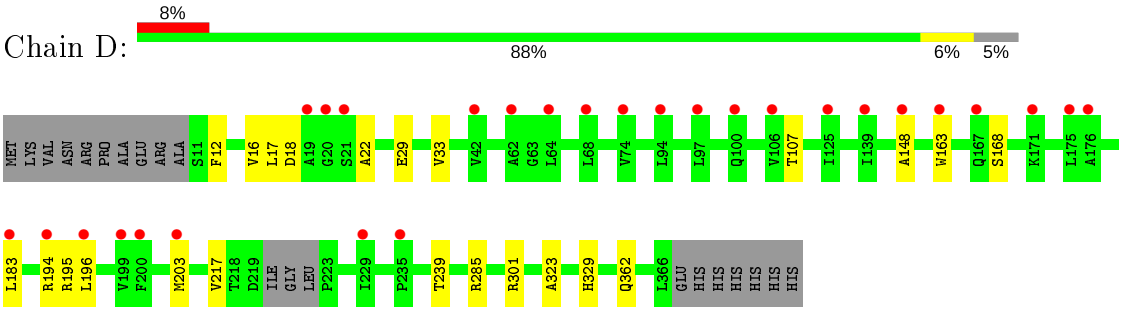
- Molecule 1: Putative PAS/PAC sensor protein

Chain C:



- Molecule 1: Putative PAS/PAC sensor protein

Chain D:


8%
88%
6%
5%
MET LYS VAL ASN ARG PRO ALA GLU ARG ALA S11 F12 V16 L17 D18 A19 G20 S21 A22 E29 V33 V42 A62 G63 L64 L68 V74 L94 L97 Q100 V106 T107 I125 I139 A148 W163 Q167 S168 K171 L175 A176
L183 R194 R195 L196 V199 F200 M203 V217 T218 D219 ILE GLY LEU P223 I229 P235 T239 R285 R301 A323 H329 Q362 L366 GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.01Å 150.34Å 219.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.13 – 2.51 150.34 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.7 (71.13-2.51) 98.8 (150.34-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.52Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.243 , 0.254 0.242 , 0.254	Depositor DCC
R_{free} test set	3753 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21802	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, IMD, EDO

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	0.25	0/2777	0.45	0/3785
1	B	0.25	0/2707	0.48	0/3691
1	C	0.24	0/2750	0.44	0/3749
1	D	0.25	0/2709	0.46	0/3695
All	All	0.25	0/10943	0.46	0/14920

There are no bond length outliers.

There are no bond angle outliers.

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	2722	2697	2697	15	0
1	B	2657	2641	2641	30	0
1	C	2695	2669	2669	19	0
1	D	2659	2639	2639	15	0
2	A	31	18	19	1	0
2	B	31	19	19	1	0
2	C	31	19	19	1	0
2	D	31	18	19	2	0
3	A	6	6	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	12	13	16	0	0
4	B	5	5	5	0	0
5	C	4	6	6	0	0
5	D	4	6	6	0	0
6	A	58	0	0	2	0
6	B	25	0	0	2	0
6	C	37	0	0	0	0
6	D	38	0	0	0	0
All	All	11046	10756	10763	75	0

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

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:SER:OG	1:D:203:MET:O	1.98	0.81
1:B:171:LYS:NZ	1:B:174:ASP:OD2	2.16	0.76
1:D:194:ARG:NH1	1:D:323:ALA:O	2.22	0.73
1:B:33:VAL:O	1:B:88:ARG:NH2	2.22	0.72
1:C:42:VAL:CG1	1:C:47:VAL:HG21	2.22	0.69
1:D:301:ARG:NH1	2:D:401:FMN:O3P	2.28	0.67
1:A:297:ARG:NH1	6:A:502:HOH:O	2.28	0.66
1:B:29:GLU:OE2	1:B:29:GLU:N	2.29	0.65
1:C:42:VAL:HG12	1:C:47:VAL:HG21	1.80	0.64
1:C:369:HIS:O	1:C:373:HIS:N	2.33	0.61
1:C:41:VAL:HG13	1:C:41:VAL:O	2.01	0.60
1:A:297:ARG:NE	2:A:400:FMN:O1P	2.33	0.59
1:B:88:ARG:NH1	1:B:112:ASP:OD2	2.35	0.58
1:C:118:ARG:NH2	1:C:122:GLU:OE2	2.36	0.58
1:A:327:GLU:OE1	1:A:353:ARG:NH2	2.36	0.57
1:D:285:ARG:NE	2:D:401:FMN:O1P	2.30	0.56
1:C:285:ARG:NH1	2:C:400:FMN:O2P	2.39	0.55
1:B:210:THR:HG22	1:B:210:THR:O	2.06	0.55
1:B:305:ALA:N	6:B:503:HOH:O	2.41	0.54
1:B:194:ARG:NH1	1:B:323:ALA:O	2.42	0.53
1:D:163:TRP:CE2	1:D:362:GLN:NE2	2.77	0.52
1:D:29:GLU:O	1:D:33:VAL:HG23	2.09	0.52
1:B:183:LEU:O	1:B:183:LEU:HD23	2.11	0.51
1:D:217:VAL:HG21	1:D:329:HIS:CD2	2.46	0.51
1:C:187:ASN:HB3	1:C:190:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLN:OE1	1:B:304:ILE:HG21	2.12	0.49
1:B:328:PHE:HA	1:B:346:TYR:O	2.13	0.49
1:B:210:THR:CG2	1:B:210:THR:O	2.62	0.48
1:D:183:LEU:HD22	1:D:196:LEU:HD21	1.95	0.48
1:C:238:LEU:HD13	1:D:239:THR:HA	1.96	0.48
1:B:114:SER:O	1:B:117:VAL:HG12	2.14	0.48
1:A:210:THR:O	1:A:210:THR:HG22	2.12	0.47
1:C:151:ASP:OD1	1:D:195:ARG:NH2	2.40	0.46
1:B:139:ILE:HD12	1:B:172:LEU:HG	1.98	0.46
1:C:210:THR:HG22	1:C:210:THR:O	2.15	0.46
1:B:224:PRO:O	1:B:225:THR:HG22	2.16	0.45
1:B:234:LEU:N	1:B:235:PRO:HD2	2.32	0.45
1:A:103:VAL:HG13	1:A:103:VAL:O	2.16	0.44
1:B:210:THR:HG23	1:B:315:ARG:HD2	2.00	0.44
1:A:163:TRP:NE1	1:A:362:GLN:OE1	2.48	0.44
1:B:334:ARG:NH1	1:B:338:GLY:O	2.50	0.44
1:A:148:ALA:HB3	1:B:148:ALA:HB3	2.00	0.44
1:B:160:LEU:HG	1:B:363:LEU:HD21	2.00	0.44
1:A:270:ARG:NH1	6:A:511:HOH:O	2.51	0.43
1:B:197:SER:O	1:B:201:THR:HG23	2.18	0.43
1:D:12:PHE:C	1:D:33:VAL:HG21	2.38	0.43
1:C:103:VAL:O	1:C:103:VAL:HG13	2.19	0.43
1:A:217:VAL:HG21	1:A:329:HIS:NE2	2.34	0.43
1:C:256:ALA:HB1	1:C:257:PRO:HD2	2.01	0.42
1:B:194:ARG:O	1:B:198:THR:HG23	2.19	0.42
1:C:44:THR:HB	1:C:47:VAL:HG23	2.01	0.42
1:C:54:PRO:HA	1:C:57:ARG:HD2	2.00	0.42
1:A:210:THR:O	1:A:210:THR:CG2	2.67	0.42
1:B:13:GLY:HA3	1:B:30:LEU:HA	2.01	0.42
1:C:148:ALA:HB3	1:D:148:ALA:HB3	2.01	0.42
1:D:16:VAL:HG22	1:D:107:THR:HG22	2.02	0.42
1:A:261:LEU:HD21	1:A:284:CYS:SG	2.60	0.42
1:C:210:THR:CG2	1:C:210:THR:O	2.67	0.42
1:B:99:GLU:N	1:B:102:ARG:O	2.48	0.41
1:D:17:LEU:HD21	1:D:22:ALA:HA	2.01	0.41
1:B:126:ARG:NH1	6:B:505:HOH:O	2.53	0.41
1:B:287:LEU:HD12	2:B:400:FMN:C4	2.50	0.41
1:B:216:PRO:HA	1:B:310:VAL:HA	2.02	0.41
1:B:355:GLU:O	1:B:359:GLN:HG2	2.20	0.41
1:C:261:LEU:HD13	1:C:284:CYS:SG	2.60	0.41
1:D:17:LEU:HD23	1:D:18:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HG	1:A:223:PRO:HD2	2.03	0.41
1:B:224:PRO:O	1:B:225:THR:CB	2.69	0.41
1:C:152:VAL:HG12	1:C:360:LEU:HD21	2.03	0.41
1:C:234:LEU:N	1:C:235:PRO:HD2	2.36	0.41
1:B:367:GLU:N	1:B:367:GLU:OE1	2.48	0.40
1:A:68:LEU:HD23	1:A:106:VAL:HG23	2.03	0.40
1:B:256:ALA:HB3	1:B:260:PRO:HD2	2.02	0.40
1:A:44:THR:OG1	1:A:47:VAL:HG23	2.21	0.40
1:A:96:ALA:HB1	1:A:103:VAL:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	353/373 (95%)	350 (99%)	3 (1%)	0	100 100
1	B	348/373 (93%)	345 (99%)	2 (1%)	1 (0%)	41 61
1	C	349/373 (94%)	342 (98%)	7 (2%)	0	100 100
1	D	349/373 (94%)	347 (99%)	2 (1%)	0	100 100
All	All	1399/1492 (94%)	1384 (99%)	14 (1%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	225	THR

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	281/295 (95%)	280 (100%)	1 (0%)	91 97
1	B	274/295 (93%)	269 (98%)	5 (2%)	59 81
1	C	279/295 (95%)	278 (100%)	1 (0%)	91 97
1	D	274/295 (93%)	274 (100%)	0	100 100
All	All	1108/1180 (94%)	1101 (99%)	7 (1%)	86 95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	GLN
1	B	88	ARG
1	B	137	SER
1	B	158	PHE
1	B	225	THR
1	B	308	ASP
1	C	315	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

10 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	A	401	-	5,5,5	0.85	0	5,5,5	1.05	0
5	EDO	D	403	-	3,3,3	0.48	0	2,2,2	0.24	0
2	FMN	D	401	-	31,33,33	2.26	5 (16%)	40,50,50	2.28	8 (20%)
4	IMD	B	401	-	3,5,5	0.42	0	4,5,5	0.60	0
3	GOL	D	402	-	5,5,5	0.91	0	5,5,5	1.00	0
2	FMN	A	400	-	31,33,33	2.22	5 (16%)	40,50,50	2.40	8 (20%)
2	FMN	B	400	-	31,33,33	2.24	5 (16%)	40,50,50	2.18	7 (17%)
2	FMN	C	400	-	31,33,33	2.23	5 (16%)	40,50,50	2.41	7 (17%)
3	GOL	D	404	-	5,5,5	0.89	0	5,5,5	1.01	0
5	EDO	C	401	-	3,3,3	0.48	0	2,2,2	0.28	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	A	401	-	-	0/4/4/4	-
5	EDO	D	403	-	-	0/1/1/1	-
2	FMN	D	401	-	-	5/18/18/18	0/3/3/3
4	IMD	B	401	-	-	-	0/1/1/1
3	GOL	D	402	-	-	2/4/4/4	-
2	FMN	A	400	-	-	3/18/18/18	0/3/3/3
2	FMN	B	400	-	-	0/18/18/18	0/3/3/3
2	FMN	C	400	-	-	3/18/18/18	0/3/3/3
3	GOL	D	404	-	-	2/4/4/4	-
5	EDO	C	401	-	-	0/1/1/1	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FMN	C4A-C10	9.53	1.48	1.38
2	B	400	FMN	C4A-C10	9.42	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	FMN	C4A-C10	9.39	1.48	1.38
2	C	400	FMN	C4A-C10	9.33	1.48	1.38
2	D	401	FMN	C4-C4A	4.30	1.48	1.41
2	B	400	FMN	C4-C4A	4.20	1.48	1.41
2	A	400	FMN	C4-C4A	3.99	1.48	1.41
2	C	400	FMN	C4-C4A	3.96	1.48	1.41
2	B	400	FMN	C9A-C5A	3.68	1.49	1.42
2	A	400	FMN	C9A-C5A	3.67	1.49	1.42
2	C	400	FMN	C9A-C5A	3.67	1.49	1.42
2	D	401	FMN	C9A-C5A	3.65	1.49	1.42
2	C	400	FMN	C8-C7	3.37	1.49	1.40
2	B	400	FMN	C8-C7	3.34	1.49	1.40
2	D	401	FMN	C8-C7	3.32	1.49	1.40
2	A	400	FMN	C8-C7	3.32	1.49	1.40
2	D	401	FMN	C9A-N10	3.10	1.42	1.38
2	C	400	FMN	C9A-N10	3.03	1.42	1.38
2	A	400	FMN	C9A-N10	2.86	1.42	1.38
2	B	400	FMN	C9A-N10	2.86	1.42	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	400	FMN	C4-N3-C2	8.96	122.70	115.14
2	A	400	FMN	C4-N3-C2	8.90	122.66	115.14
2	D	401	FMN	C4-N3-C2	8.40	122.23	115.14
2	B	400	FMN	C4-N3-C2	8.03	121.92	115.14
2	C	400	FMN	C1'-N10-C9A	7.38	124.10	118.29
2	A	400	FMN	C1'-N10-C9A	7.06	123.85	118.29
2	D	401	FMN	C1'-N10-C9A	6.57	123.46	118.29
2	B	400	FMN	C1'-N10-C9A	5.83	122.89	118.29
2	A	400	FMN	C4-C4A-C10	-5.36	116.40	119.95
2	C	400	FMN	C4-C4A-C10	-5.07	116.60	119.95
2	B	400	FMN	C4-C4A-C10	-4.88	116.72	119.95
2	D	401	FMN	C4-C4A-C10	-4.74	116.81	119.95
2	B	400	FMN	C4A-N5-C5A	4.09	120.86	116.77
2	D	401	FMN	C4A-N5-C5A	4.04	120.80	116.77
2	C	400	FMN	C4A-C4-N3	-3.82	118.21	123.43
2	A	400	FMN	C4A-C4-N3	-3.77	118.28	123.43
2	D	401	FMN	C4A-C4-N3	-3.75	118.30	123.43
2	A	400	FMN	C4A-N5-C5A	3.71	120.48	116.77
2	C	400	FMN	C4A-N5-C5A	3.53	120.30	116.77
2	B	400	FMN	C4A-C4-N3	-3.43	118.74	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	400	FMN	C9A-N10-C10	-3.11	117.83	121.91
2	B	400	FMN	C4-C4A-N5	3.05	122.08	118.60
2	A	400	FMN	C4-C4A-N5	3.00	122.03	118.60
2	A	400	FMN	C5'-C4'-C3'	-3.00	106.42	112.20
2	D	401	FMN	C9A-N10-C10	-2.95	118.04	121.91
2	D	401	FMN	C4-C4A-N5	2.95	121.97	118.60
2	C	400	FMN	C4-C4A-N5	2.89	121.90	118.60
2	A	400	FMN	C9A-N10-C10	-2.81	118.22	121.91
2	B	400	FMN	C9A-N10-C10	-2.76	118.29	121.91
2	D	401	FMN	O3P-P-O2P	2.26	116.27	107.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	FMN	C5'-O5'-P-O2P
2	D	401	FMN	C5'-O5'-P-O3P
3	D	402	GOL	C1-C2-C3-O3
2	A	400	FMN	C3'-C4'-C5'-O5'
2	A	400	FMN	O4'-C4'-C5'-O5'
2	C	400	FMN	C3'-C4'-C5'-O5'
3	D	404	GOL	O1-C1-C2-C3
3	D	402	GOL	O2-C2-C3-O3
3	D	404	GOL	O1-C1-C2-O2
2	D	401	FMN	C5'-O5'-P-O1P
2	A	400	FMN	C4'-C5'-O5'-P
2	D	401	FMN	C3'-C4'-C5'-O5'
2	C	400	FMN	O4'-C4'-C5'-O5'
2	D	401	FMN	C4'-C5'-O5'-P
2	C	400	FMN	C4'-C5'-O5'-P

There are no ring outliers.

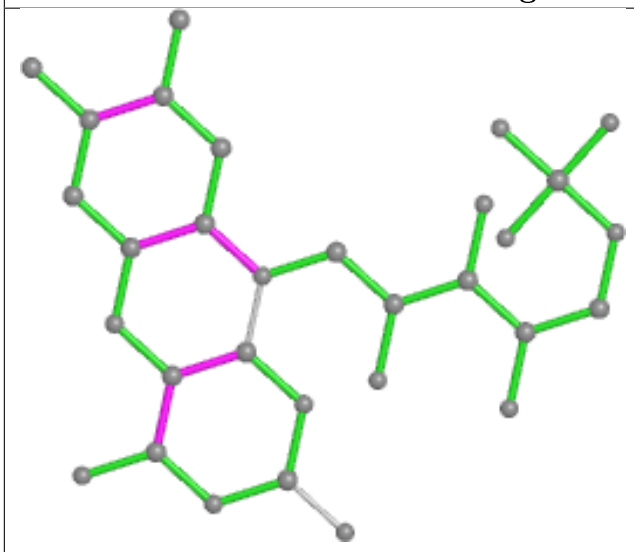
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	FMN	2	0
2	A	400	FMN	1	0
2	B	400	FMN	1	0
2	C	400	FMN	1	0

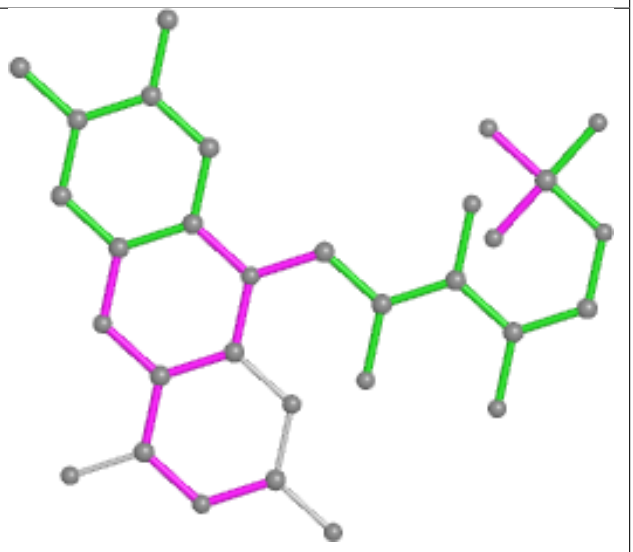
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

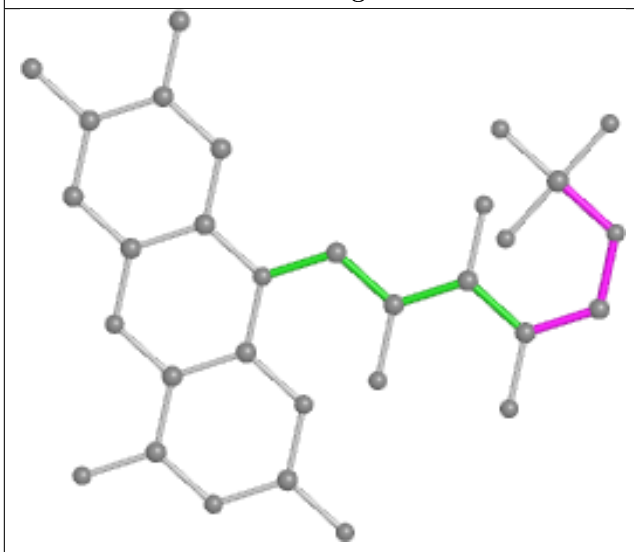
Ligand FMN D 401



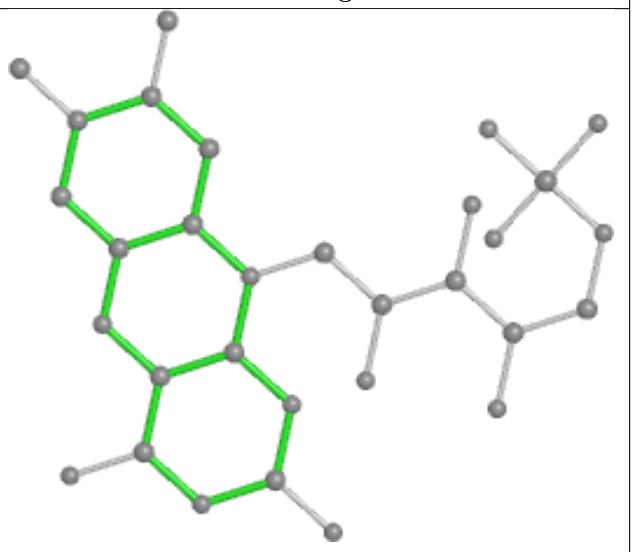
Bond lengths



Bond angles

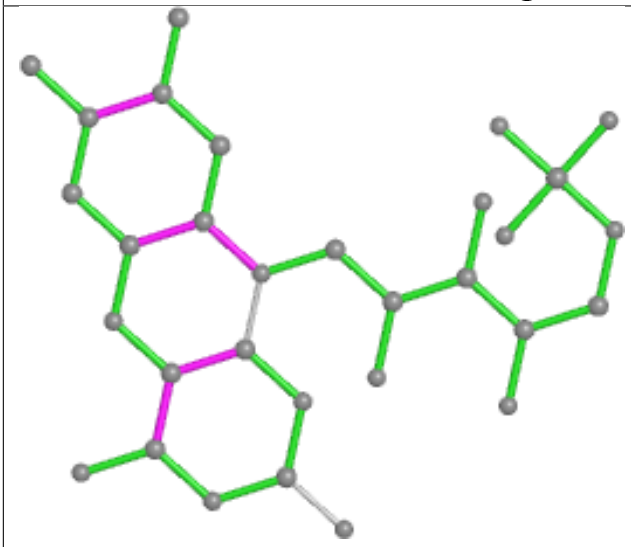


Torsions

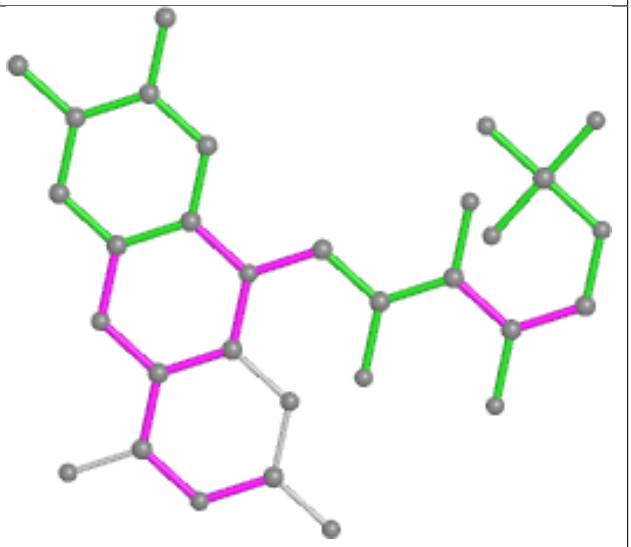


Rings

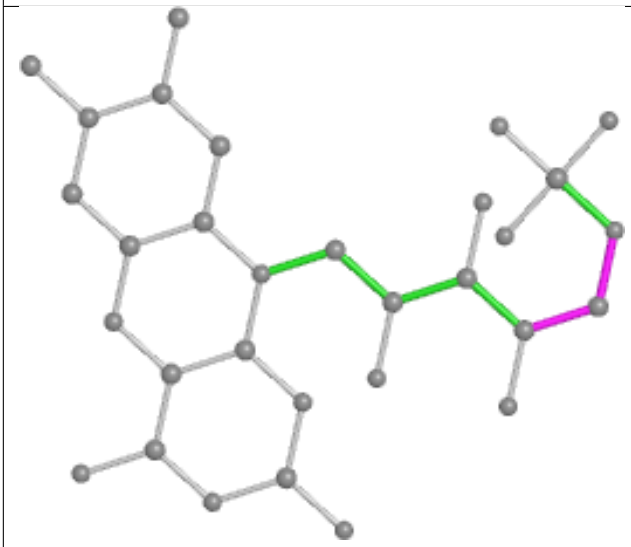
Ligand FMN A 400



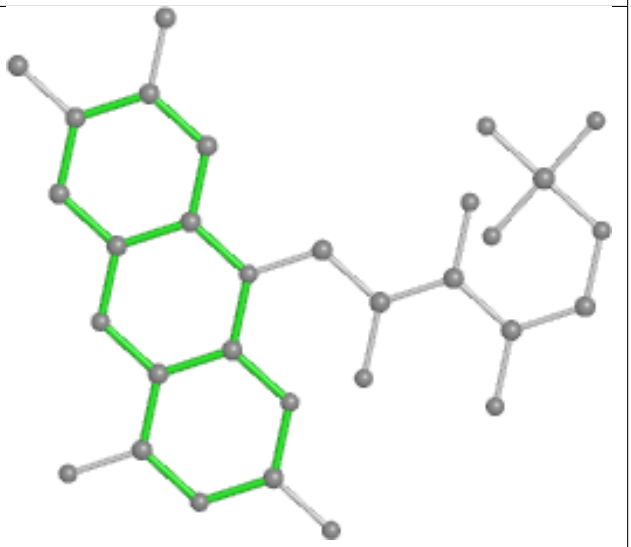
Bond lengths



Bond angles

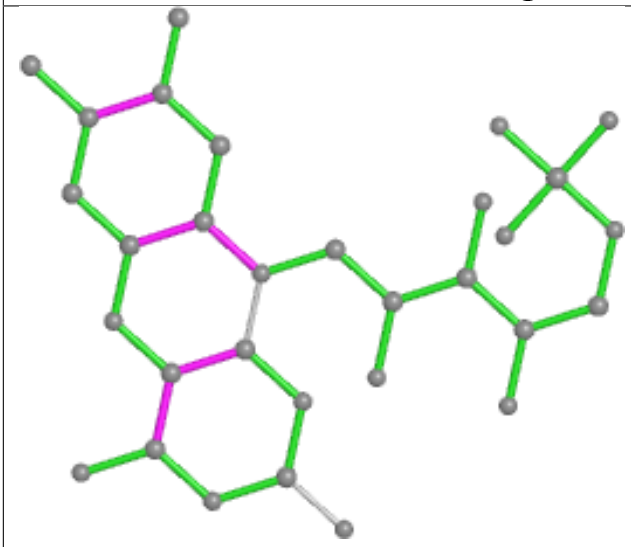


Torsions

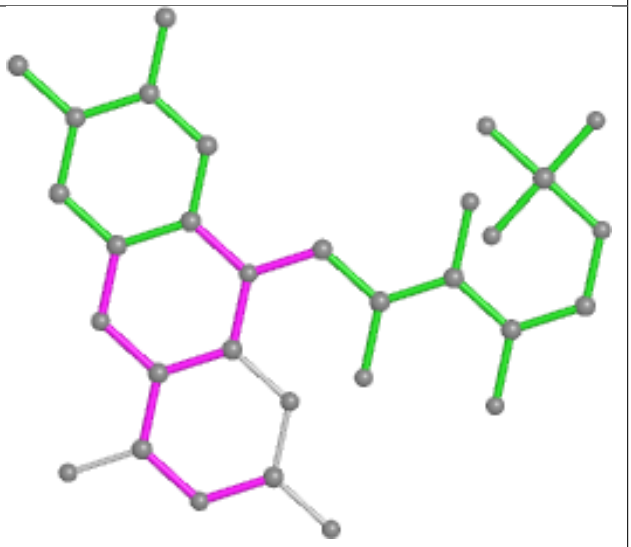


Rings

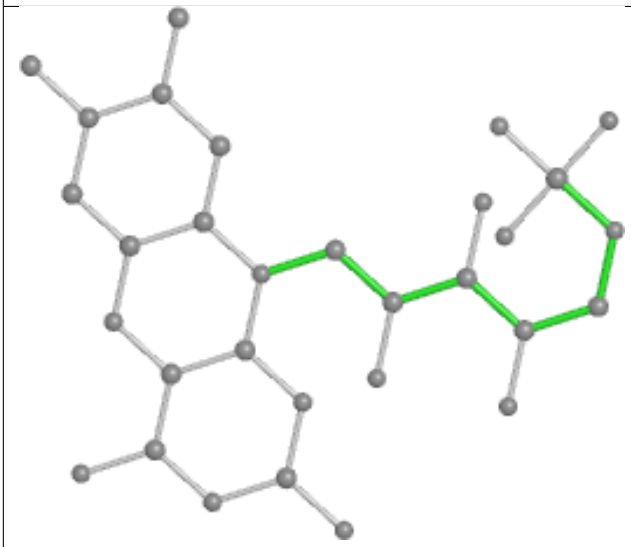
Ligand FMN B 400



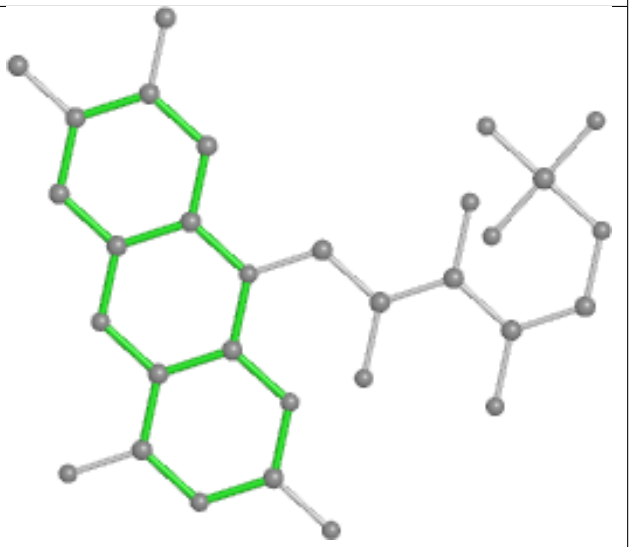
Bond lengths



Bond angles

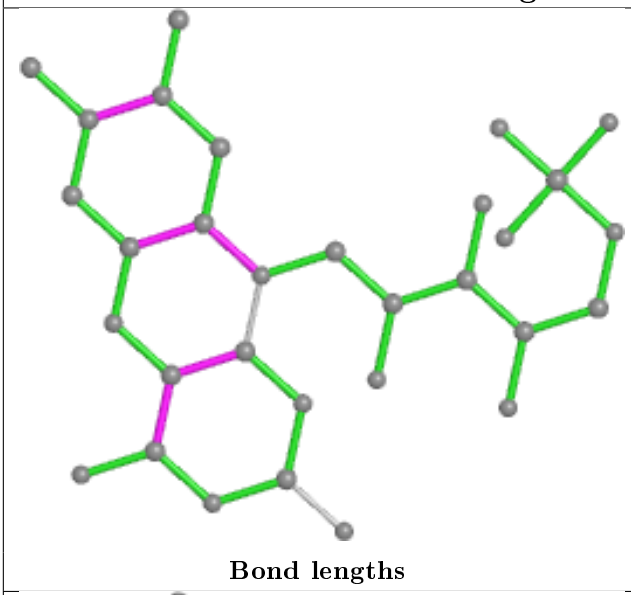


Torsions

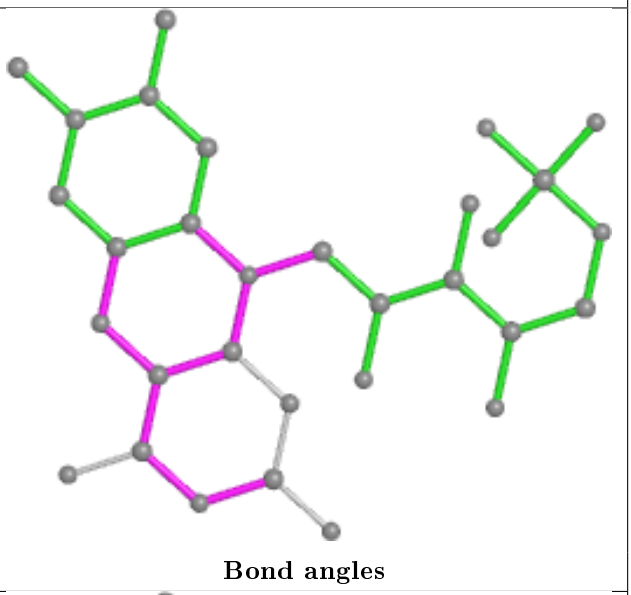


Rings

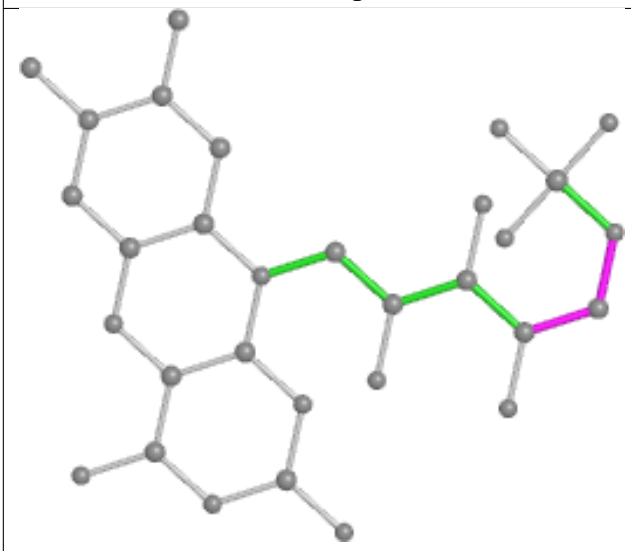
Ligand FMN C 400



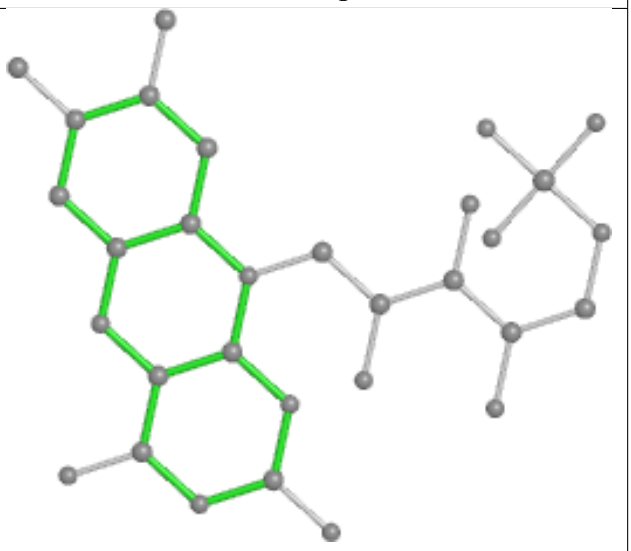
Bond lengths



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	359/373 (96%)	0.57	12 (3%)	46	50	44, 68, 120, 149	0
1	B	352/373 (94%)	0.66	22 (6%)	20	21	52, 89, 129, 165	0
1	C	355/373 (95%)	0.69	18 (5%)	28	29	43, 75, 125, 157	0
1	D	353/373 (94%)	0.66	28 (7%)	12	12	47, 76, 118, 151	0
All	All	1419/1492 (95%)	0.65	80 (5%)	24	25	43, 76, 124, 165	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	GLY	6.3
1	C	42	VAL	5.6
1	B	169	ASN	4.7
1	A	10	ALA	4.3
1	B	167	GLN	4.1
1	B	163	TRP	3.9
1	C	97	LEU	3.7
1	D	68	LEU	3.5
1	B	97	LEU	3.5
1	C	41	VAL	3.3
1	D	196	LEU	3.2
1	B	226	SER	3.1
1	A	68	LEU	3.1
1	C	43	LEU	3.0
1	A	74	VAL	3.0
1	C	52	LEU	3.0
1	B	255	THR	2.9
1	D	21	SER	2.9
1	D	97	LEU	2.9
1	D	229	ILE	2.9
1	C	38	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	203	MET	2.8
1	B	20	GLY	2.7
1	B	152	VAL	2.7
1	B	83	ALA	2.7
1	A	172	LEU	2.7
1	C	229	ILE	2.7
1	D	235	PRO	2.6
1	C	48	VAL	2.6
1	D	194	ARG	2.6
1	D	176	ALA	2.6
1	C	80	LEU	2.6
1	C	74	VAL	2.5
1	B	363	LEU	2.5
1	D	74	VAL	2.5
1	B	300	ILE	2.5
1	D	94	LEU	2.5
1	A	373	HIS	2.5
1	B	290	GLU	2.5
1	C	76	VAL	2.5
1	D	199	VAL	2.5
1	A	24	PHE	2.4
1	D	100	GLN	2.4
1	D	19	ALA	2.4
1	B	158	PHE	2.4
1	D	139	ILE	2.4
1	C	60	TRP	2.4
1	A	110	ILE	2.3
1	C	218	THR	2.3
1	D	175	LEU	2.3
1	B	129	VAL	2.3
1	B	213	TRP	2.3
1	B	295	HIS	2.3
1	A	32	LEU	2.3
1	C	172	LEU	2.3
1	D	125	ILE	2.2
1	B	183	LEU	2.2
1	A	97	LEU	2.2
1	D	106	VAL	2.2
1	D	64	LEU	2.2
1	B	291	SER	2.2
1	C	68	LEU	2.1
1	B	276	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	62	ALA	2.1
1	D	148	ALA	2.1
1	C	34	LEU	2.1
1	B	162	LYS	2.1
1	B	139	ILE	2.1
1	D	163	TRP	2.1
1	D	167	GLN	2.1
1	D	20	GLY	2.1
1	D	171	LYS	2.1
1	B	174	ASP	2.0
1	D	42	VAL	2.0
1	C	360	LEU	2.0
1	A	105	ALA	2.0
1	A	72	ARG	2.0
1	D	183	LEU	2.0
1	D	200	PHE	2.0
1	A	89	PRO	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	EDO	D	403	4/4	0.59	0.19	86,104,104,104	0
3	GOL	D	404	6/6	0.80	0.27	83,85,102,102	0
2	FMN	B	400	31/31	0.88	0.19	82,92,110,111	0
5	EDO	C	401	4/4	0.89	0.17	73,87,89,89	0
3	GOL	A	401	6/6	0.95	0.18	65,67,80,81	0
4	IMD	B	401	5/5	0.95	0.15	86,86,104,104	0

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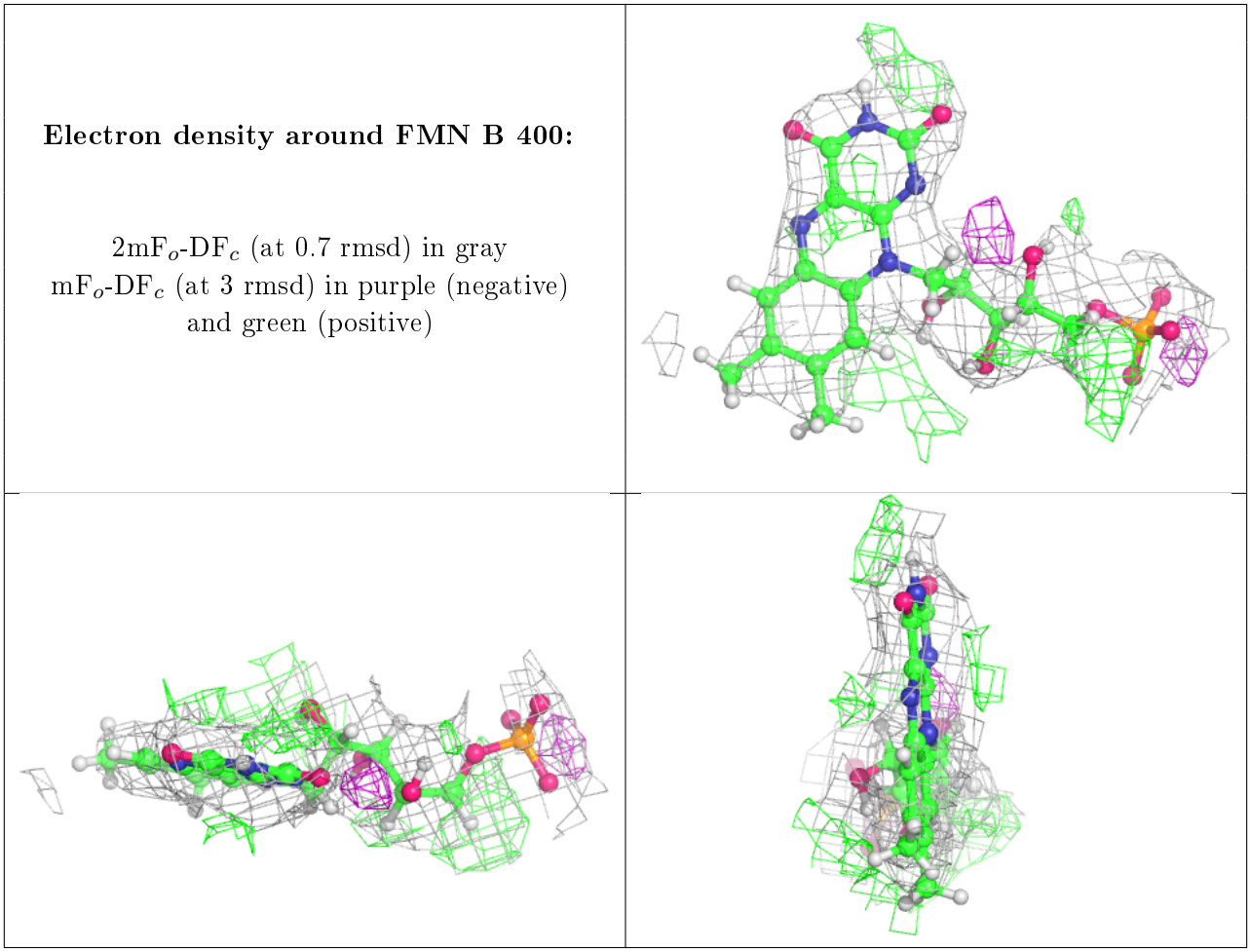
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	D	402	6/6	0.95	0.16	59,61,74,74	0
2	FMN	C	400	31/31	0.96	0.17	61,68,81,83	0
2	FMN	A	400	31/31	0.96	0.20	51,55,66,68	0
2	FMN	D	401	31/31	0.96	0.22	47,56,67,68	0

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.

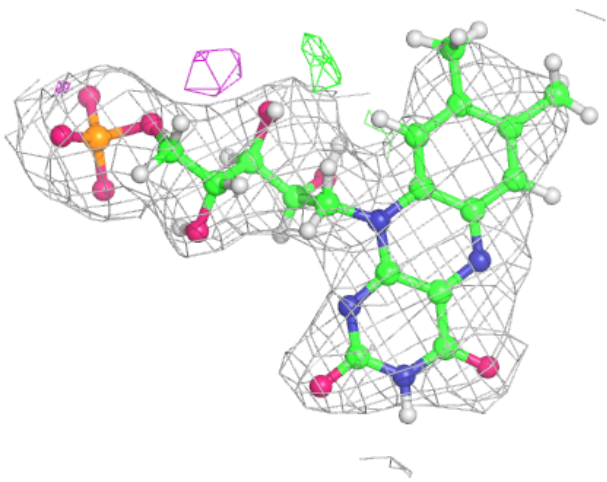
Electron density around FMN B 400:

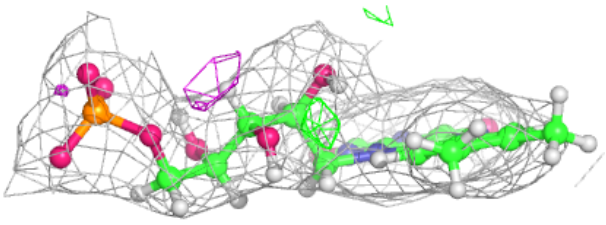
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

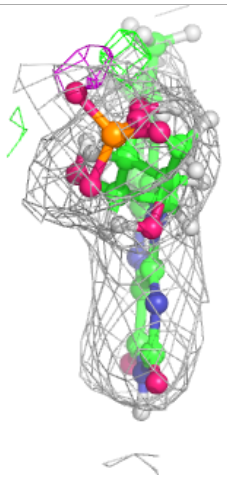


Electron density around FMN C 400:

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

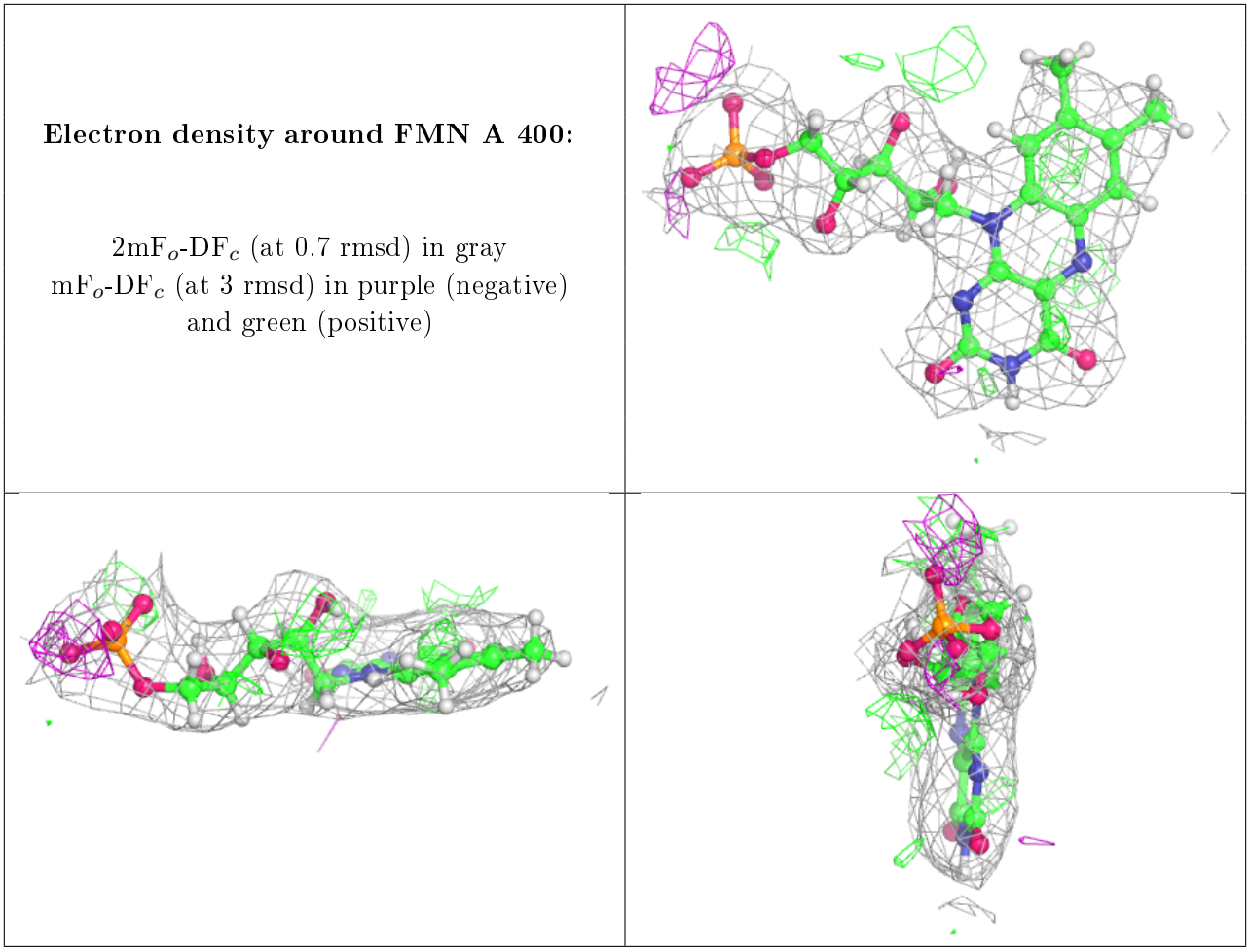






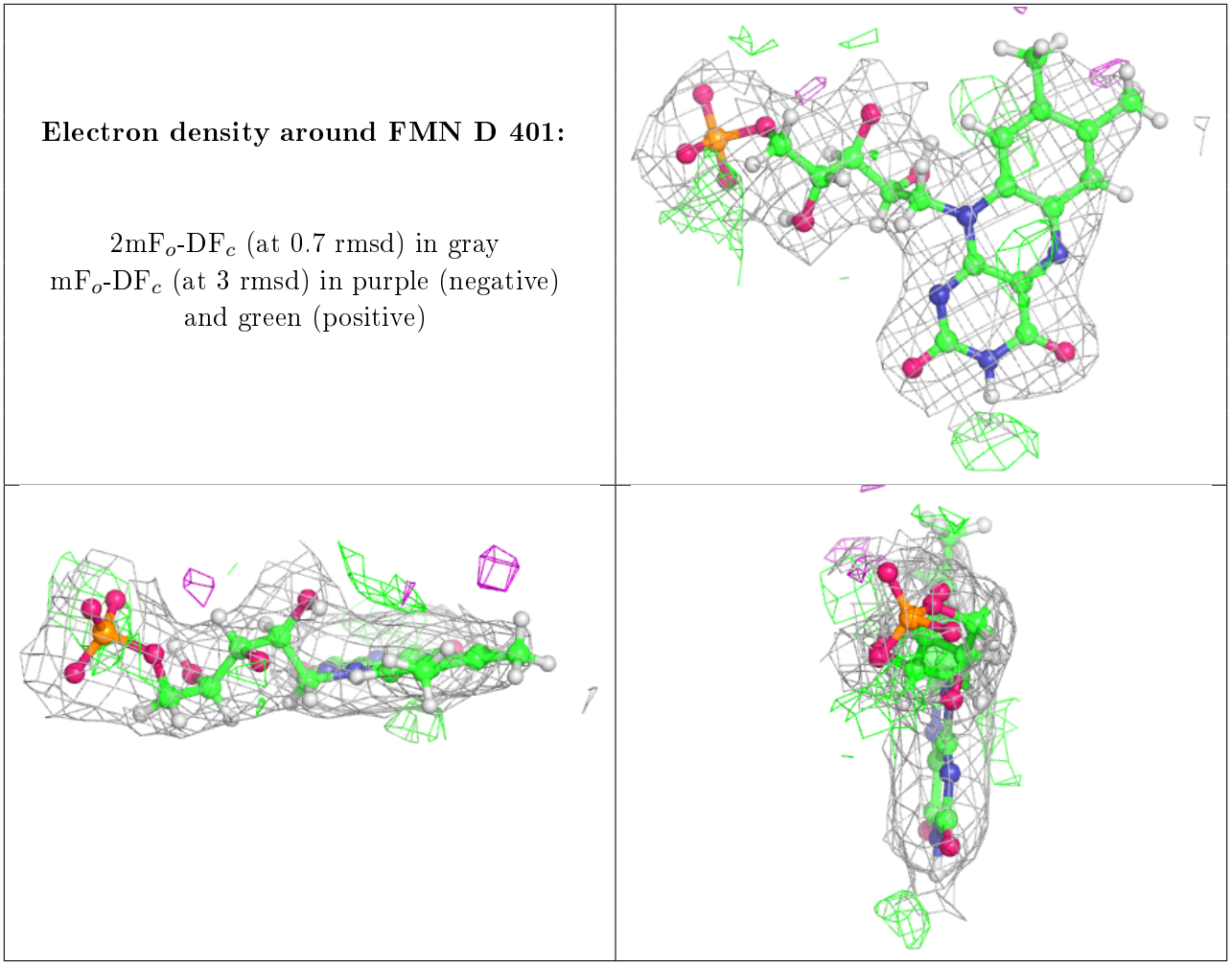
Electron density around FMN A 400:

$2mF_o$-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.