



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:24 AM UTC

PDB ID : 8QNK / pdb_00008qnk
Title : OPR3 variant R283D in complex with NADPH4
Authors : Bijelic, A.; Macheroux, P.; Kerschbaumer, B.
Deposited on : 2023-09-27
Resolution : 1.91 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

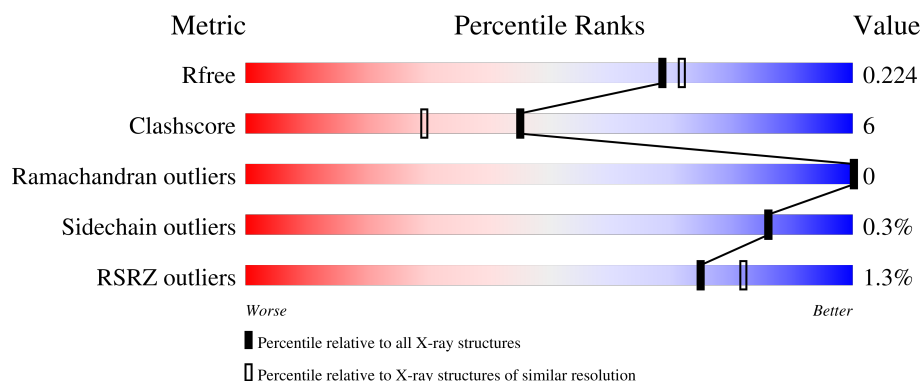
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 $\leq 5\%$. 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	402	
1	B	402	
1	C	402	
1	D	402	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12395 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 12-oxophytodienoate reductase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2898	1838	513	536	11			
1	B	375	Total	C	N	O	S	0	0	0
			2886	1834	509	532	11			
1	C	359	Total	C	N	O	S	0	0	0
			2754	1750	486	507	11			
1	D	356	Total	C	N	O	S	0	0	0
			2704	1721	473	499	11			

There are 28 discrepancies between the modelled and reference sequences:

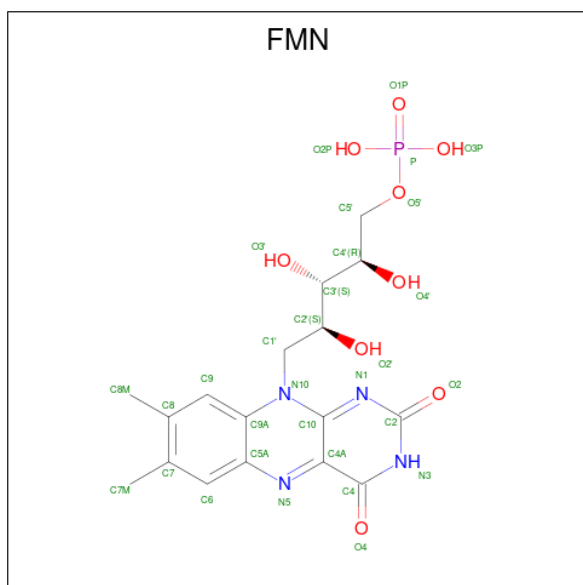
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q9FEW9
A	-4	HIS	-	expression tag	UNP Q9FEW9
A	-3	HIS	-	expression tag	UNP Q9FEW9
A	-2	HIS	-	expression tag	UNP Q9FEW9
A	-1	HIS	-	expression tag	UNP Q9FEW9
A	0	HIS	-	expression tag	UNP Q9FEW9
A	283	ASP	ARG	variant	UNP Q9FEW9
B	-5	HIS	-	expression tag	UNP Q9FEW9
B	-4	HIS	-	expression tag	UNP Q9FEW9
B	-3	HIS	-	expression tag	UNP Q9FEW9
B	-2	HIS	-	expression tag	UNP Q9FEW9
B	-1	HIS	-	expression tag	UNP Q9FEW9
B	0	HIS	-	expression tag	UNP Q9FEW9
B	283	ASP	ARG	variant	UNP Q9FEW9
C	-5	HIS	-	expression tag	UNP Q9FEW9
C	-4	HIS	-	expression tag	UNP Q9FEW9
C	-3	HIS	-	expression tag	UNP Q9FEW9
C	-2	HIS	-	expression tag	UNP Q9FEW9
C	-1	HIS	-	expression tag	UNP Q9FEW9
C	0	HIS	-	expression tag	UNP Q9FEW9
C	283	ASP	ARG	variant	UNP Q9FEW9

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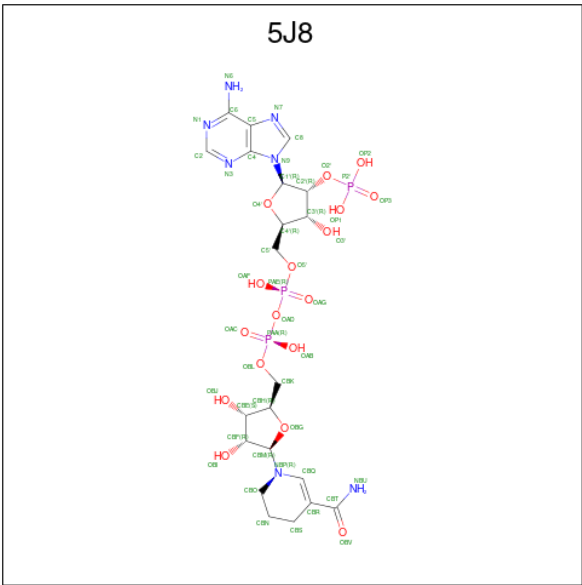
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP Q9FEW9
D	-4	HIS	-	expression tag	UNP Q9FEW9
D	-3	HIS	-	expression tag	UNP Q9FEW9
D	-2	HIS	-	expression tag	UNP Q9FEW9
D	-1	HIS	-	expression tag	UNP Q9FEW9
D	0	HIS	-	expression tag	UNP Q9FEW9
D	283	ASP	ARG	variant	UNP Q9FEW9

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



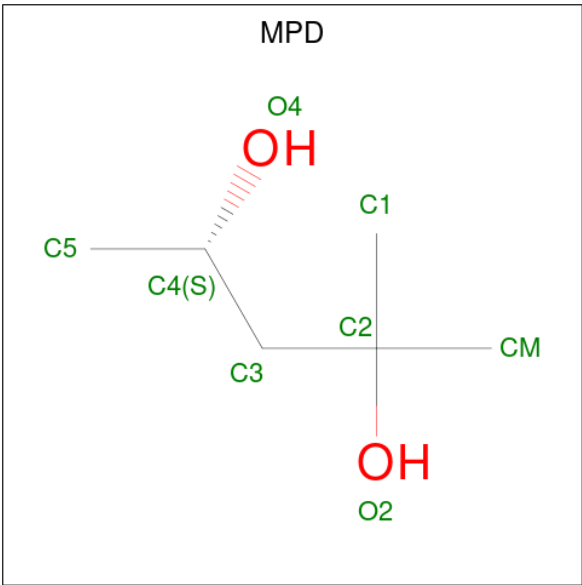
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is [[(2R,3S,4R,5R)-5-(5-aminocarbonyl-3,4-dihydro-2H-pyridin-1-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2R,3R,4R,5R)-5-(6-aminopurin-9-yl)-3-oxidanyl-4-phosphonooxy-oxolan-2-yl]methyl hydrogen phosphate (CCD ID: 5J8) (formula: $C_{21}H_{32}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).

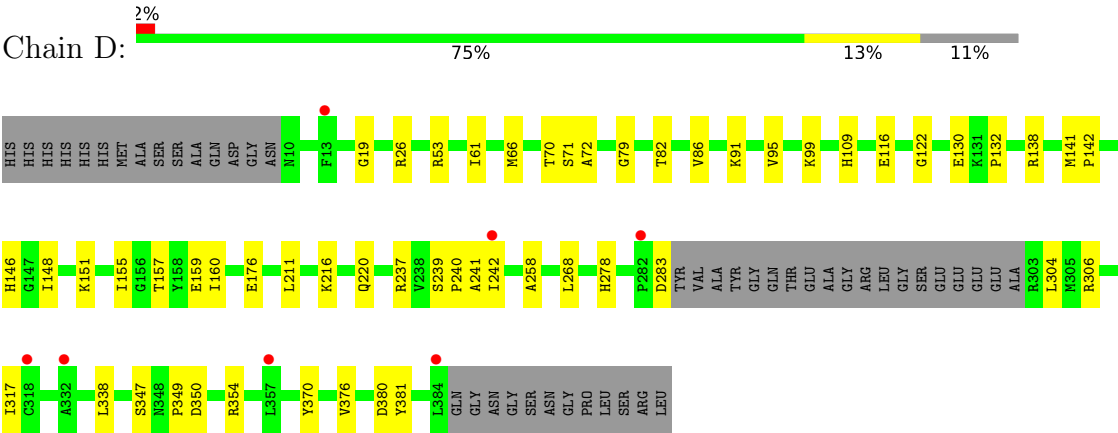


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	310	Total 310	O 310	0	0
5	B	285	Total 285	O 285	0	0
5	C	202	Total 202	O 202	0	0
5	D	128	Total 128	O 128	0	0

● Molecule 1: 12-oxophytodienoate reductase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.58Å 90.48Å 114.63Å 90.00° 110.02° 90.00°	Depositor
Resolution (Å)	35.90 – 1.91 35.90 – 1.91	Depositor EDS
% Data completeness (in resolution range)	95.5 (35.90-1.91) 95.5 (35.90-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.91Å)	Xtriage
Refinement program	PHENIX (dev_4761)	Depositor
R, R_{free}	0.195 , 0.222 0.199 , 0.224	Depositor DCC
R_{free} test set	5512 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12395	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5J8, FMN, MPD

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	0.35	1/2965 (0.0%)	0.56	1/4029 (0.0%)
1	B	0.31	0/2954	0.52	0/4016
1	C	0.37	0/2818	0.56	0/3835
1	D	0.27	0/2768	0.45	0/3771
All	All	0.33	1/11505 (0.0%)	0.52	1/15651 (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	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	THR	C-N	-6.08	1.22	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	MET	CG-SD-CE	-5.48	88.84	100.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	233	ARG	Sidechain
1	C	53	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2898	0	2847	26	0
1	B	2886	0	2833	39	0
1	C	2754	0	2690	28	0
1	D	2704	0	2618	38	0
2	A	31	0	19	4	0
2	B	31	0	19	2	0
2	C	31	0	19	2	0
2	D	31	0	19	1	0
3	A	48	0	0	0	0
3	C	48	0	0	2	0
4	A	8	0	14	4	0
5	A	310	0	0	7	1
5	B	285	0	0	9	1
5	C	202	0	0	8	0
5	D	128	0	0	8	0
All	All	12395	0	11078	132	2

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 6.

All (132) 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:A:289:GLN:HG3	4:A:403:MPD:HM2	1.51	0.91
2:A:401:FMN:H5'2	1:B:289:GLN:HB2	1.57	0.86
1:C:324:ARG:NH2	5:C:502:HOH:O	1.95	0.79
3:C:402:5J8:OAC	5:C:503:HOH:O	2.02	0.76
1:C:324:ARG:NH1	5:C:501:HOH:O	1.86	0.75
1:A:300:GLU:OE2	5:A:502:HOH:O	2.05	0.74
1:B:17:LYS:HE3	5:B:610:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:GLU:OE2	5:C:505:HOH:O	2.11	0.68
1:B:51:GLU:OE1	5:B:501:HOH:O	2.12	0.68
1:B:91:LYS:NZ	5:B:506:HOH:O	2.25	0.68
1:B:324:ARG:HG3	1:B:355:ILE:HG23	1.78	0.66
1:D:176:GLU:OE2	5:D:504:HOH:O	2.14	0.65
1:D:283:ASP:OD1	5:D:503:HOH:O	2.14	0.65
1:A:130:GLU:OE2	5:A:503:HOH:O	2.14	0.64
1:D:157:THR:HA	1:D:160:ILE:HD12	1.81	0.61
4:A:403:MPD:H53	5:B:598:HOH:O	2.01	0.60
1:C:306:ARG:NH1	1:C:335:ASP:OD1	2.27	0.59
4:A:403:MPD:H51	1:B:190:TYR:OH	2.02	0.58
1:B:285:VAL:O	5:B:502:HOH:O	2.17	0.58
1:B:309:ARG:HG3	1:B:335:ASP:O	2.04	0.58
1:D:239:SER:HB2	1:D:242:ILE:HG13	1.86	0.57
1:B:48:GLU:O	1:B:52:GLN:HG3	2.04	0.57
1:A:165:GLU:OE2	1:A:168:ARG:NH2	2.37	0.57
1:C:203:ARG:HB2	1:C:208:GLY:HA3	1.87	0.56
1:B:112:ARG:HB3	1:B:127:SER:HB2	1.88	0.55
1:D:53:ARG:HG2	1:D:349:PRO:HA	1.87	0.55
1:A:373:ASP:OD2	5:A:504:HOH:O	2.18	0.55
1:A:32:MET:HE1	1:A:346:ILE:HG13	1.89	0.54
1:A:320:GLY:HA2	2:A:401:FMN:H5'1	1.90	0.54
1:D:141:MET:HE3	1:D:142:PRO:HD3	1.89	0.54
4:A:403:MPD:H52	4:A:403:MPD:H11	1.89	0.54
1:A:248:MET:HB2	5:A:581:HOH:O	2.07	0.54
1:D:317:ILE:HG12	1:D:338:LEU:HB2	1.89	0.54
1:B:13:PHE:CZ	1:B:356:LYS:HB2	2.43	0.53
1:D:216:LYS:O	1:D:220:GLN:HG3	2.08	0.53
1:C:325:GLU:H	1:C:325:GLU:CD	2.16	0.53
1:D:240:PRO:HG2	1:D:304:LEU:HD21	1.91	0.53
1:D:61:ILE:O	5:D:505:HOH:O	2.19	0.52
1:A:80:ILE:HD12	1:A:89:TRP:CD1	2.44	0.52
1:D:130:GLU:HB3	1:D:151:LYS:HE2	1.92	0.52
1:D:71:SER:HB2	1:D:109:HIS:HA	1.92	0.52
1:A:258:ALA:O	1:A:262:ARG:HG2	2.10	0.51
1:B:213:ASN:HA	1:B:216:LYS:HG3	1.91	0.51
1:B:11:PRO:HD2	1:B:328:ILE:HG23	1.92	0.51
1:B:219:THR:OG1	1:B:262:ARG:HG2	2.11	0.50
1:B:317:ILE:HG12	1:B:338:LEU:HB2	1.94	0.50
1:A:281:GLN:HB3	1:A:282:PRO:HD2	1.94	0.49
2:A:401:FMN:H4'	1:B:289:GLN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ARG:NH1	1:B:136:ARG:HB2	2.28	0.49
1:A:40:ASN:HA	1:A:77:VAL:O	2.12	0.49
1:A:19:GLY:HA3	5:A:611:HOH:O	2.13	0.48
1:C:112:ARG:HB3	1:C:127:SER:HB2	1.95	0.48
1:C:198:ASP:HB3	1:C:214:ARG:CZ	2.44	0.48
1:A:155:ILE:HB	1:A:159:GLU:HB3	1.96	0.48
1:B:66:MET:HB2	1:B:79:GLY:HA2	1.95	0.48
1:C:115:HIS:CE1	1:C:141:MET:HE1	2.49	0.47
1:B:32:MET:HA	2:B:401:FMN:N5	2.29	0.47
1:C:206:GLU:CG	5:C:505:HOH:O	2.63	0.47
1:B:309:ARG:NH1	5:B:509:HOH:O	2.31	0.47
1:C:306:ARG:HD3	1:C:335:ASP:OD1	2.14	0.47
1:C:206:GLU:HB2	1:C:216:LYS:HZ3	1.79	0.47
1:B:243:ASP:OD2	5:B:503:HOH:O	2.21	0.47
1:A:295:LEU:HD13	1:A:301:GLU:HA	1.96	0.46
1:C:66:MET:SD	1:C:72:ALA:HB2	2.55	0.46
1:C:366:ARG:NH2	3:C:402:5J8:OP1	2.48	0.46
1:D:211:LEU:HD13	1:D:258:ALA:HB2	1.97	0.46
1:B:253:LEU:HA	1:B:304:LEU:HD11	1.96	0.46
1:D:82:THR:O	1:D:86:VAL:HG23	2.16	0.46
1:B:71:SER:HB2	1:B:109:HIS:HA	1.98	0.45
1:D:99:LYS:HE3	1:D:99:LYS:HB3	1.79	0.45
1:A:244:HIS:CD2	1:B:290:THR:HB	2.52	0.45
1:C:11:PRO:HG3	1:C:332:ALA:HB2	1.97	0.45
1:D:66:MET:HB2	1:D:79:GLY:HA2	1.99	0.45
1:C:237:ARG:HA	1:C:278:HIS:O	2.17	0.45
1:D:132:PRO:HB3	1:D:151:LYS:HA	1.99	0.45
1:B:251:ASN:CG	1:B:254:SER:HB3	2.42	0.45
1:C:319:SER:OG	5:C:504:HOH:O	2.10	0.45
1:D:376:VAL:HA	1:D:380:ASP:OD2	2.16	0.45
1:B:40:ASN:HA	1:B:77:VAL:O	2.18	0.44
1:C:32:MET:HA	2:C:401:FMN:N5	2.32	0.44
1:B:233:ARG:NH2	5:B:512:HOH:O	2.38	0.44
1:A:324:ARG:O	1:A:328:ILE:HG13	2.17	0.44
1:C:324:ARG:HB3	1:C:325:GLU:OE2	2.18	0.44
1:D:268:LEU:HD12	1:D:268:LEU:HA	1.83	0.44
1:D:130:GLU:HG2	5:D:581:HOH:O	2.17	0.44
1:C:206:GLU:HG3	5:C:505:HOH:O	2.18	0.43
1:D:155:ILE:HB	1:D:159:GLU:HB2	1.99	0.43
1:B:323:THR:H	1:B:326:LEU:HB2	1.82	0.43
1:D:70:THR:OG1	5:D:506:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:ASP:OD1	1:D:350:ASP:N	2.52	0.43
1:D:19:GLY:HA3	5:D:525:HOH:O	2.18	0.43
1:B:347:SER:HA	1:B:381:TYR:CG	2.54	0.43
1:C:165:GLU:CD	1:C:168:ARG:HH21	2.27	0.43
1:D:350:ASP:O	1:D:354:ARG:HG3	2.19	0.43
1:D:138:ARG:HB3	1:D:146:HIS:HB3	2.00	0.42
1:A:347:SER:HB3	1:A:364:TYR:HB3	2.00	0.42
1:B:32:MET:HA	2:B:401:FMN:C5A	2.48	0.42
1:D:66:MET:SD	1:D:72:ALA:HB2	2.59	0.42
1:D:237:ARG:HA	1:D:278:HIS:O	2.19	0.42
1:A:212:ALA:HA	1:A:262:ARG:HH21	1.85	0.42
1:A:60:LEU:O	1:A:103:ILE:HA	2.19	0.42
1:C:51:GLU:HG3	1:C:99:LYS:HD2	2.02	0.42
1:C:155:ILE:HB	1:C:159:GLU:HB3	2.00	0.42
1:C:209:GLY:N	5:C:506:HOH:O	2.17	0.42
1:A:320:GLY:HA2	2:A:401:FMN:C5'	2.50	0.41
1:B:282:PRO:O	5:B:504:HOH:O	2.22	0.41
1:D:116:GLU:O	1:D:122:GLY:HA2	2.20	0.41
1:C:132:PRO:HB3	1:C:151:LYS:HA	2.02	0.41
1:D:26:ARG:NH1	5:D:501:HOH:O	1.96	0.41
1:D:370:TYR:CE1	2:D:401:FMN:HM71	2.56	0.41
1:A:265:LYS:HE3	5:A:543:HOH:O	2.21	0.41
1:B:242:ILE:HG22	1:B:244:HIS:H	1.86	0.41
1:D:148:ILE:HG13	5:D:540:HOH:O	2.20	0.41
1:A:223:GLN:NE2	5:A:517:HOH:O	2.49	0.41
1:D:141:MET:HE3	1:D:141:MET:HA	2.02	0.41
1:B:139:ILE:HB	1:B:149:TYR:CE1	2.56	0.41
1:C:325:GLU:CD	1:C:325:GLU:N	2.79	0.41
1:C:370:TYR:CE1	2:C:401:FMN:HM71	2.56	0.41
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.86	0.41
1:D:241:ALA:C	1:D:242:ILE:HG12	2.46	0.41
1:A:21:PHE:CE1	1:A:180:ASP:HB3	2.55	0.41
1:D:211:LEU:HA	1:D:211:LEU:HD23	1.86	0.41
1:D:306:ARG:HD2	1:D:306:ARG:HA	1.67	0.41
1:D:347:SER:HA	1:D:381:TYR:CG	2.56	0.41
1:A:237:ARG:HA	1:A:278:HIS:O	2.21	0.41
1:B:211:LEU:HD11	1:B:255:LEU:HA	2.03	0.41
1:D:91:LYS:O	1:D:95:VAL:HG23	2.20	0.41
1:C:261:GLU:O	1:C:265:LYS:HG3	2.22	0.40
1:B:131:LYS:HB2	1:B:131:LYS:HE3	1.87	0.40
1:A:146:HIS:ND1	1:B:296:GLY:N	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:LEU:HA	1:B:304:LEU:CD1	2.52	0.40
1:B:368:THR:HB	1:B:377:GLY:HA3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:703:HOH:O	5:B:710:HOH:O[2_746]	2.07	0.13
5:A:571:HOH:O	5:A:736:HOH:O[2_646]	2.10	0.10

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	374/402 (93%)	360 (96%)	14 (4%)	0	100	100
1	B	373/402 (93%)	361 (97%)	12 (3%)	0	100	100
1	C	355/402 (88%)	344 (97%)	11 (3%)	0	100	100
1	D	352/402 (88%)	339 (96%)	13 (4%)	0	100	100
All	All	1454/1608 (90%)	1404 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	301/328 (92%)	300 (100%)	1 (0%)	86	86
1	B	299/328 (91%)	298 (100%)	1 (0%)	86	86
1	C	285/328 (87%)	284 (100%)	1 (0%)	84	83
1	D	277/328 (84%)	277 (100%)	0	100	100
All	All	1162/1312 (89%)	1159 (100%)	3 (0%)	86	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	PHE
1	B	345	PHE
1	C	345	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	B	22	ASN
1	B	223	GLN
1	D	43	GLN
1	D	119	GLN
1	D	362	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FMN	C	401	-	33,33,33	1.12	2 (6%)	48,50,50	1.24	6 (12%)
3	5J8	A	402	-	52,52,52	4.38	30 (57%)	68,80,80	2.85	16 (23%)
2	FMN	B	401	-	33,33,33	1.11	2 (6%)	48,50,50	1.80	11 (22%)
2	FMN	D	401	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	7 (14%)
4	MPD	A	403	-	7,7,7	0.46	0	9,10,10	0.74	0
2	FMN	A	401	-	33,33,33	1.11	2 (6%)	48,50,50	1.55	11 (22%)
3	5J8	C	402	-	52,52,52	4.30	30 (57%)	68,80,80	2.75	14 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	C	401	-	-	1/18/18/18	0/3/3/3
3	5J8	A	402	-	-	12/34/77/77	0/5/5/5
2	FMN	B	401	-	-	5/18/18/18	0/3/3/3
2	FMN	D	401	-	-	6/18/18/18	0/3/3/3
4	MPD	A	403	-	-	4/5/5/5	-
2	FMN	A	401	-	-	2/18/18/18	0/3/3/3
3	5J8	C	402	-	-	10/34/77/77	0/5/5/5

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	5J8	C3'-C2'	-12.94	1.24	1.53
3	C	402	5J8	C3'-C2'	-12.51	1.25	1.53
3	A	402	5J8	CBE-CBF	-10.57	1.24	1.53
3	C	402	5J8	CBE-CBF	-10.52	1.24	1.53
3	A	402	5J8	PAE-OAD	9.81	1.70	1.59
3	C	402	5J8	CBO-NBP	9.33	1.62	1.46
3	A	402	5J8	CBO-NBP	9.14	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	5J8	PAE-OAD	9.11	1.69	1.59
3	A	402	5J8	CBQ-CBR	8.60	1.58	1.35
3	C	402	5J8	CBQ-CBR	8.38	1.58	1.35
3	A	402	5J8	PAA-OAD	8.37	1.68	1.59
3	C	402	5J8	PAA-OAD	8.09	1.68	1.59
3	A	402	5J8	CBS-CBR	-7.11	1.37	1.50
3	C	402	5J8	CBS-CBR	-6.94	1.38	1.50
3	A	402	5J8	C3'-C4'	5.95	1.68	1.53
3	C	402	5J8	C3'-C4'	5.92	1.68	1.53
3	A	402	5J8	O4'-C4'	-5.72	1.32	1.45
3	A	402	5J8	CBT-NBU	5.71	1.49	1.33
3	C	402	5J8	CBT-NBU	5.57	1.49	1.33
3	C	402	5J8	O4'-C4'	-5.54	1.32	1.45
3	A	402	5J8	C1'-N9	-5.39	1.31	1.46
3	C	402	5J8	C1'-N9	-5.12	1.32	1.46
3	A	402	5J8	OBG-CBM	-5.12	1.30	1.42
3	C	402	5J8	OBG-CBM	-5.11	1.30	1.42
3	C	402	5J8	O4'-C1'	4.16	1.51	1.42
3	A	402	5J8	OBJ-CBE	3.96	1.52	1.43
3	C	402	5J8	P2'-O2'	3.96	1.66	1.59
3	C	402	5J8	OBJ-CBE	3.95	1.52	1.43
3	C	402	5J8	CBN-CBO	-3.93	1.38	1.51
3	A	402	5J8	CBN-CBO	-3.93	1.38	1.51
2	C	401	FMN	C4A-N5	3.77	1.38	1.30
3	A	402	5J8	O4'-C1'	3.75	1.50	1.42
2	A	401	FMN	C4A-N5	3.71	1.38	1.30
3	C	402	5J8	C2'-C1'	3.61	1.62	1.53
3	A	402	5J8	C2'-C1'	3.56	1.61	1.53
2	B	401	FMN	C4A-N5	3.56	1.38	1.30
3	A	402	5J8	CBK-CBH	-3.54	1.40	1.51
2	D	401	FMN	C4A-N5	3.51	1.38	1.30
3	A	402	5J8	CBF-CBM	3.49	1.64	1.53
3	C	402	5J8	CBF-CBM	3.25	1.63	1.53
3	C	402	5J8	OBG-CBH	2.96	1.51	1.45
3	A	402	5J8	C5-C4	-2.95	1.33	1.39
2	C	401	FMN	C10-N1	2.88	1.39	1.33
3	C	402	5J8	CBK-CBH	-2.88	1.42	1.51
3	A	402	5J8	C4-N9	-2.85	1.31	1.37
3	A	402	5J8	P2'-O2'	2.83	1.64	1.59
3	A	402	5J8	C8-N9	-2.73	1.32	1.37
2	D	401	FMN	C10-N1	2.69	1.38	1.33
2	B	401	FMN	C10-N1	2.69	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	5J8	CBN-CBS	2.66	1.60	1.52
3	C	402	5J8	CBN-CBS	2.61	1.60	1.52
3	A	402	5J8	OBV-CBT	-2.60	1.18	1.24
3	C	402	5J8	CBE-CBH	2.59	1.59	1.53
3	C	402	5J8	C5-C4	-2.56	1.34	1.39
2	A	401	FMN	C10-N1	2.52	1.38	1.33
3	C	402	5J8	C6-N6	2.52	1.40	1.34
3	C	402	5J8	C8-N9	-2.43	1.33	1.37
3	C	402	5J8	C4-N9	-2.43	1.32	1.37
3	A	402	5J8	C6-N6	2.33	1.40	1.34
3	C	402	5J8	OBI-CBF	2.27	1.48	1.43
3	C	402	5J8	C8-N7	2.27	1.36	1.31
3	A	402	5J8	CBE-CBH	2.20	1.58	1.53
3	A	402	5J8	O3'-C3'	2.20	1.48	1.43
3	C	402	5J8	O3'-C3'	2.15	1.48	1.43
3	A	402	5J8	CBQ-NBP	2.14	1.42	1.35
3	A	402	5J8	OBI-CBF	2.13	1.48	1.43
3	C	402	5J8	CBQ-NBP	2.11	1.42	1.35
3	A	402	5J8	C5-C6	-2.08	1.35	1.41

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	5J8	C4-N9-C8	12.30	118.66	105.74
3	C	402	5J8	C4-N9-C8	11.94	118.27	105.74
3	A	402	5J8	N9-C8-N7	-9.46	100.52	113.94
3	C	402	5J8	N9-C8-N7	-9.23	100.83	113.94
3	A	402	5J8	N6-C6-N1	-7.11	102.53	118.38
3	C	402	5J8	N6-C6-N1	-7.05	102.68	118.38
2	B	401	FMN	C5'-C4'-C3'	-6.89	99.23	112.22
3	C	402	5J8	C1'-N9-C8	-6.73	112.16	127.09
3	A	402	5J8	C1'-N9-C8	-6.65	112.35	127.09
3	C	402	5J8	N3-C4-N9	5.72	136.90	127.17
3	A	402	5J8	N3-C4-N9	5.72	136.89	127.17
3	A	402	5J8	N3-C2-N1	-5.60	120.10	128.58
3	C	402	5J8	N3-C2-N1	-5.58	120.14	128.58
2	B	401	FMN	O5'-P-O1P	4.70	119.15	106.44
3	A	402	5J8	C5-C4-N9	-4.35	101.07	105.81
3	C	402	5J8	C5-C4-N9	-4.13	101.31	105.81
3	A	402	5J8	P2'-O2'-C2'	-4.01	112.71	123.43
3	A	402	5J8	C5-C6-N1	3.99	127.63	117.51
3	C	402	5J8	C5-C6-N1	3.93	127.48	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	5J8	C5-N7-C8	3.90	109.58	103.45
3	C	402	5J8	C5-N7-C8	3.80	109.43	103.45
3	C	402	5J8	C5-C4-N3	-3.58	121.79	126.72
3	C	402	5J8	C2-N3-C4	3.52	120.42	111.83
3	A	402	5J8	C2-N3-C4	3.47	120.31	111.83
3	A	402	5J8	C5-C4-N3	-3.40	122.04	126.72
2	A	401	FMN	C5'-C4'-C3'	2.99	117.85	112.22
2	A	401	FMN	C4A-C10-N10	2.97	120.74	116.48
2	B	401	FMN	C4-N3-C2	-2.91	120.48	125.64
2	A	401	FMN	C4-N3-C2	-2.90	120.49	125.64
2	A	401	FMN	C4'-C3'-C2'	-2.81	108.89	113.57
2	C	401	FMN	C10-C4A-N5	-2.78	119.13	124.81
2	D	401	FMN	C4A-C10-N10	2.77	120.44	116.48
3	A	402	5J8	O4'-C1'-C2'	-2.74	101.88	106.59
2	C	401	FMN	C4-N3-C2	-2.68	120.88	125.64
2	A	401	FMN	O5'-P-O1P	2.67	113.66	106.44
2	A	401	FMN	C10-C4A-N5	-2.66	119.37	124.81
3	C	402	5J8	C5-C6-N6	2.65	129.84	123.29
3	A	402	5J8	C5-C6-N6	2.64	129.83	123.29
2	B	401	FMN	C4A-C10-N10	2.61	120.22	116.48
2	A	401	FMN	O3P-P-O5'	-2.55	100.01	106.67
2	D	401	FMN	C4-N3-C2	-2.55	121.12	125.64
2	B	401	FMN	C10-C4A-N5	-2.53	119.65	124.81
2	C	401	FMN	C4A-C10-N10	2.52	120.09	116.48
2	D	401	FMN	C10-C4A-N5	-2.50	119.71	124.81
2	C	401	FMN	C9A-C5A-N5	-2.48	119.82	122.45
2	C	401	FMN	C4A-C4-N3	2.46	119.51	113.25
2	B	401	FMN	C4A-C4-N3	2.44	119.46	113.25
2	B	401	FMN	O4-C4-C4A	-2.41	120.18	126.53
2	D	401	FMN	C4A-C4-N3	2.35	119.23	113.25
3	A	402	5J8	C4'-O4'-C1'	-2.34	104.29	109.47
2	D	401	FMN	O4-C4-C4A	-2.30	120.45	126.53
2	A	401	FMN	O2P-P-O5'	2.27	112.58	106.67
2	B	401	FMN	O3P-P-O5'	-2.23	100.85	106.67
3	C	402	5J8	CBH-OBG-CBM	-2.23	104.55	109.47
2	A	401	FMN	C4A-C4-N3	2.21	118.88	113.25
2	A	401	FMN	O4-C4-C4A	-2.18	120.77	126.53
2	C	401	FMN	C4A-C10-N1	-2.18	119.24	124.59
3	A	402	5J8	C6-C5-C4	-2.15	114.25	117.18
2	B	401	FMN	C9A-C5A-N5	-2.07	120.25	122.45
2	B	401	FMN	O3'-C3'-C2'	2.05	113.60	108.93
2	D	401	FMN	C9A-C5A-N5	-2.04	120.29	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FMN	C1'-C2'-C3'	2.04	115.19	109.66
3	C	402	5J8	C6-C5-C4	-2.03	114.40	117.18
2	B	401	FMN	C4A-C10-N1	-2.01	119.67	124.59
2	A	401	FMN	C5A-C9A-N10	2.00	119.78	117.97

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	FMN	O4'-C4'-C5'-O5'
2	B	401	FMN	C5'-O5'-P-O1P
2	B	401	FMN	C5'-O5'-P-O2P
2	B	401	FMN	C5'-O5'-P-O3P
3	A	402	5J8	CBF-CBM-NBP-CBO
3	A	402	5J8	C5'-O5'-PAE-OAD
3	A	402	5J8	C5'-O5'-PAE-OAG
3	A	402	5J8	C5'-O5'-PAE-OAF
3	C	402	5J8	OBG-CBM-NBP-CBQ
4	A	403	MPD	C2-C3-C4-O4
4	A	403	MPD	C2-C3-C4-C5
2	D	401	FMN	C2'-C3'-C4'-O4'
2	D	401	FMN	C2'-C3'-C4'-C5'
3	C	402	5J8	C3'-C2'-O2'-P2'
2	D	401	FMN	O3'-C3'-C4'-O4'
2	D	401	FMN	O3'-C3'-C4'-C5'
3	A	402	5J8	CBF-CBM-NBP-CBQ
2	B	401	FMN	C3'-C4'-C5'-O5'
3	C	402	5J8	O4'-C4'-C5'-O5'
2	A	401	FMN	C4'-C5'-O5'-P
3	A	402	5J8	CBE-CBH-CBK-OBL
3	C	402	5J8	C3'-C4'-C5'-O5'
3	C	402	5J8	PAE-OAD-PAA-OBL
3	C	402	5J8	C2'-C1'-N9-C8
3	A	402	5J8	OBG-CBM-NBP-CBQ
2	C	401	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C5'-O5'-P-O1P
2	D	401	FMN	C5'-O5'-P-O1P
3	C	402	5J8	C1'-C2'-O2'-P2'
3	A	402	5J8	C2'-O2'-P2'-OP1
3	A	402	5J8	OBG-CBH-CBK-OBL
3	C	402	5J8	CBQ-CBR-CBT-NBU
3	A	402	5J8	C2'-O2'-P2'-OP3

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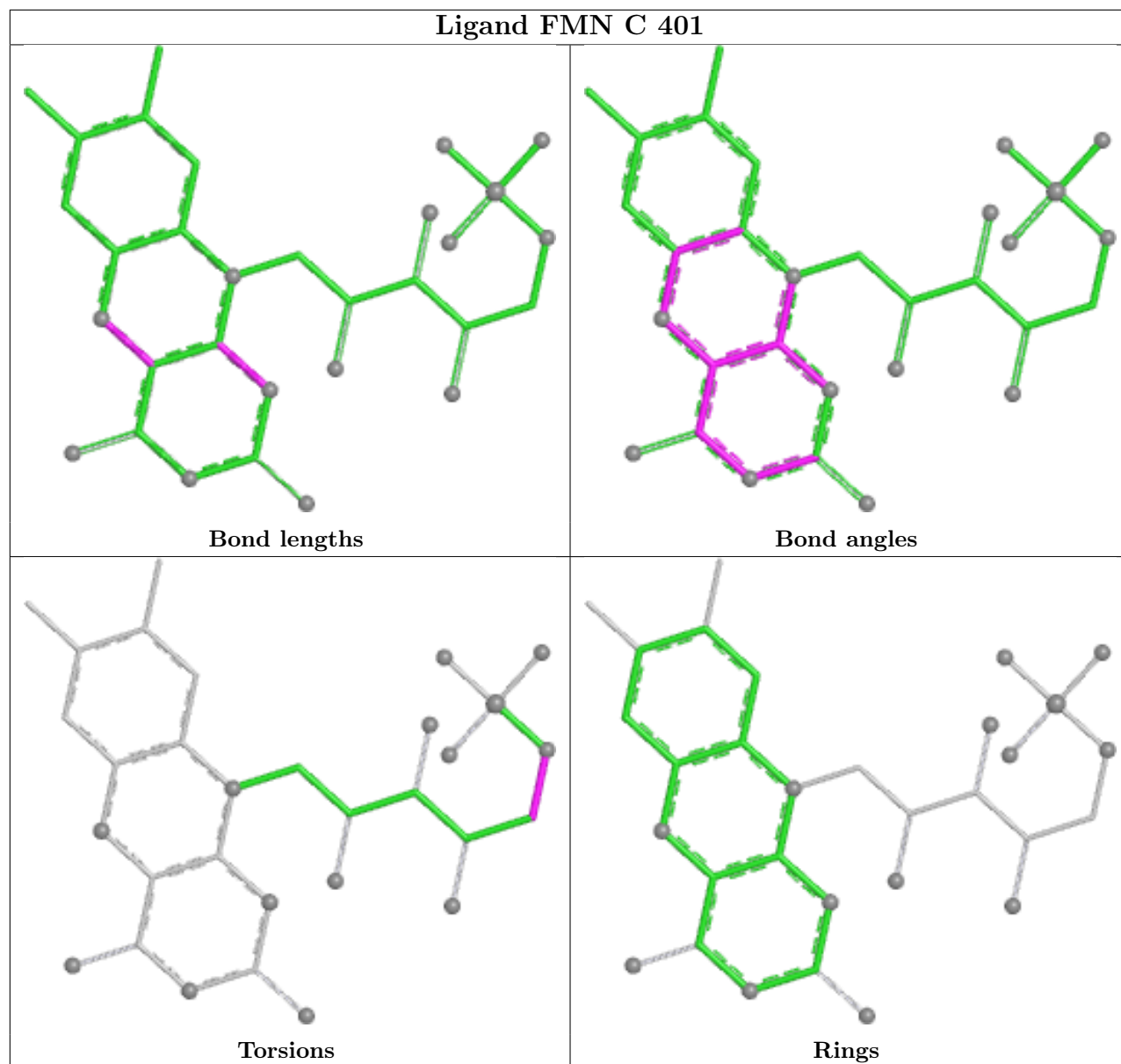
Mol	Chain	Res	Type	Atoms
2	D	401	FMN	C4'-C5'-O5'-P
3	A	402	5J8	CBH-CBK-OBL-PAA
4	A	403	MPD	O2-C2-C3-C4
3	A	402	5J8	C2'-O2'-P2'-OP2
4	A	403	MPD	C1-C2-C3-C4
3	C	402	5J8	C2'-O2'-P2'-OP3
3	C	402	5J8	CBQ-CBR-CBT-OBV

There are no ring outliers.

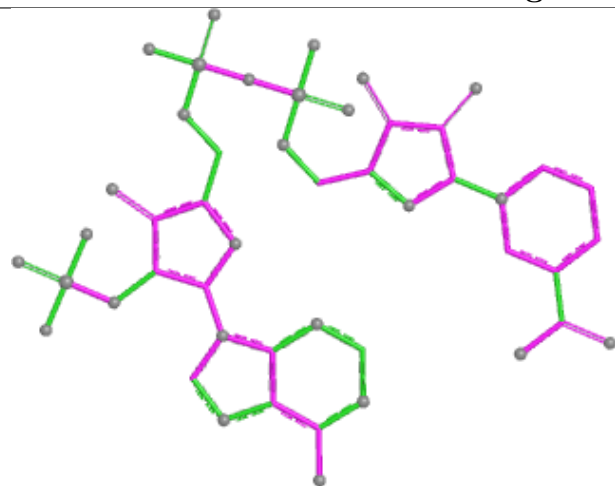
6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	FMN	2	0
2	B	401	FMN	2	0
2	D	401	FMN	1	0
4	A	403	MPD	4	0
2	A	401	FMN	4	0
3	C	402	5J8	2	0

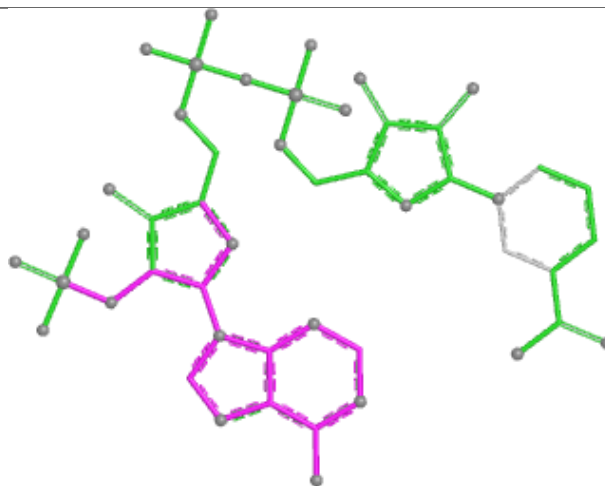
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



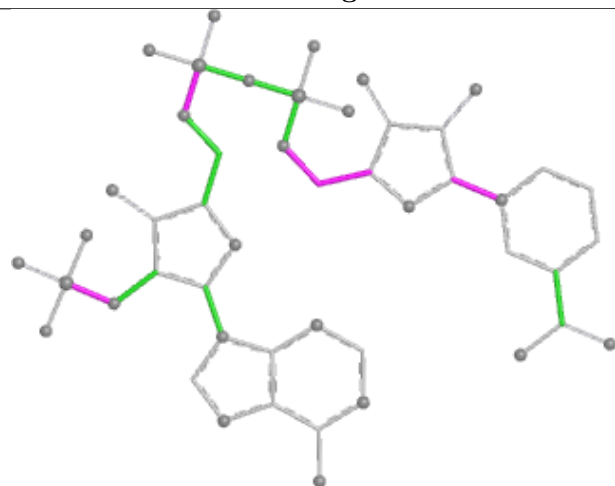
Ligand 5J8 A 402



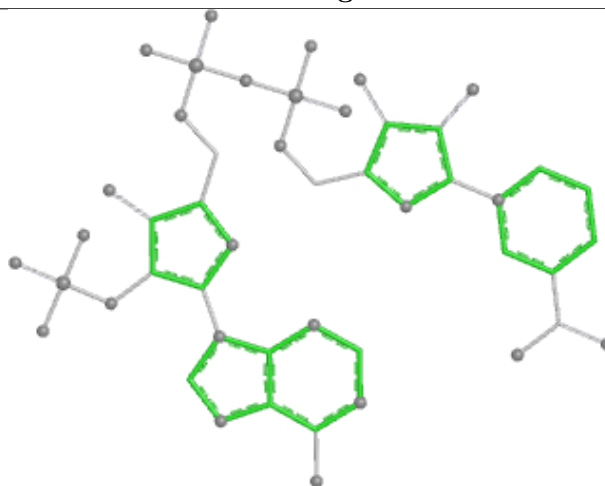
Bond lengths



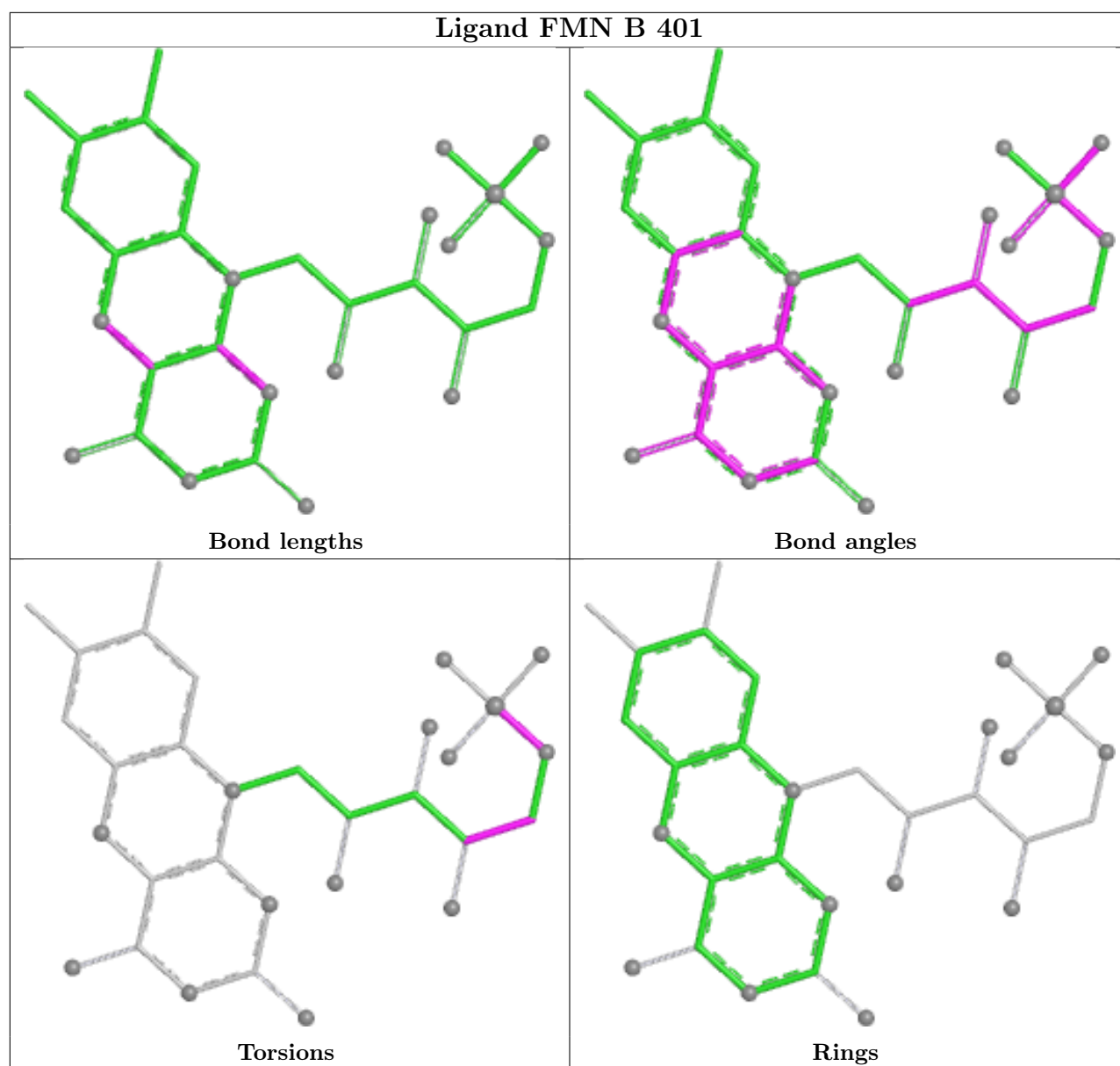
Bond angles

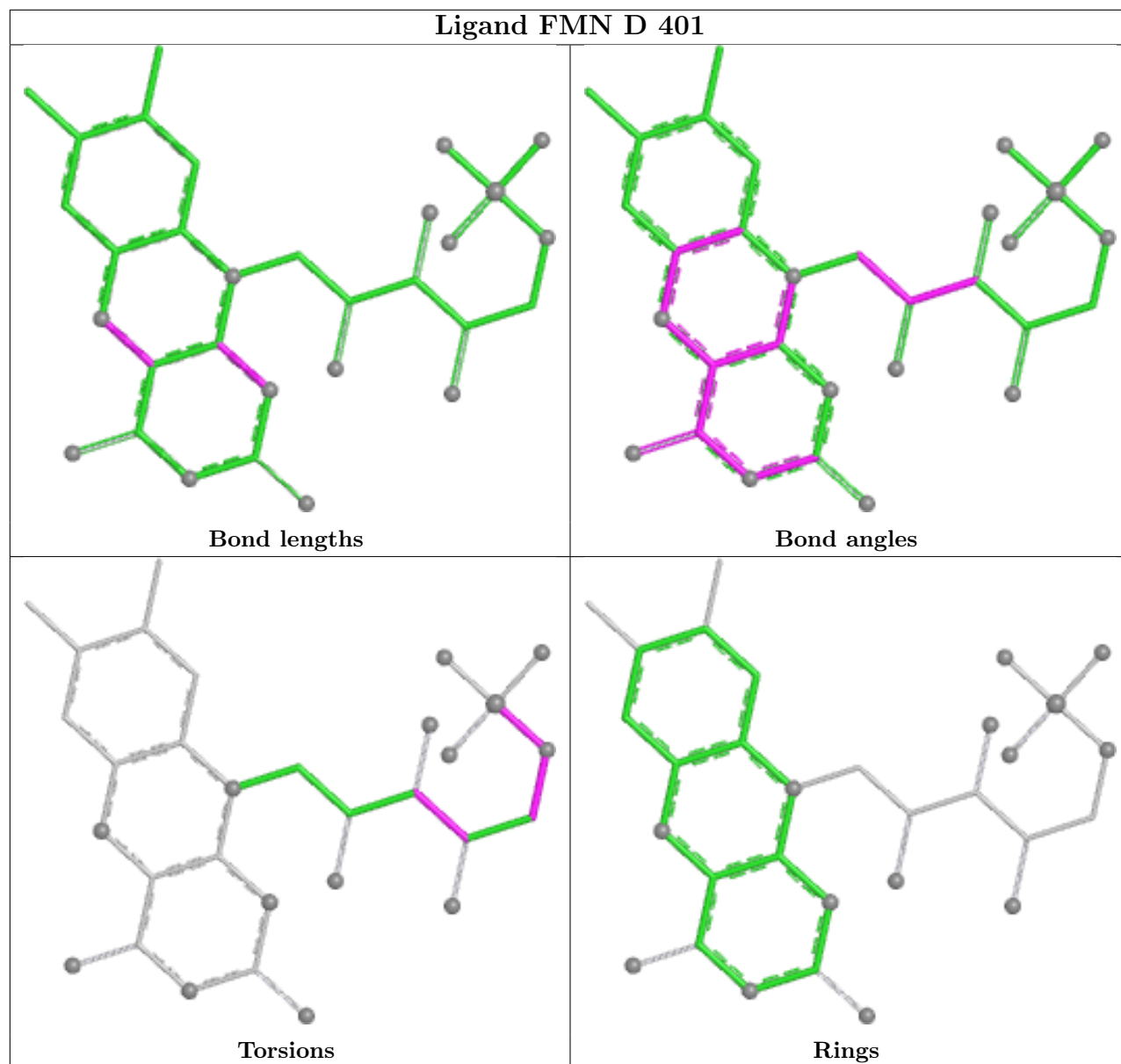


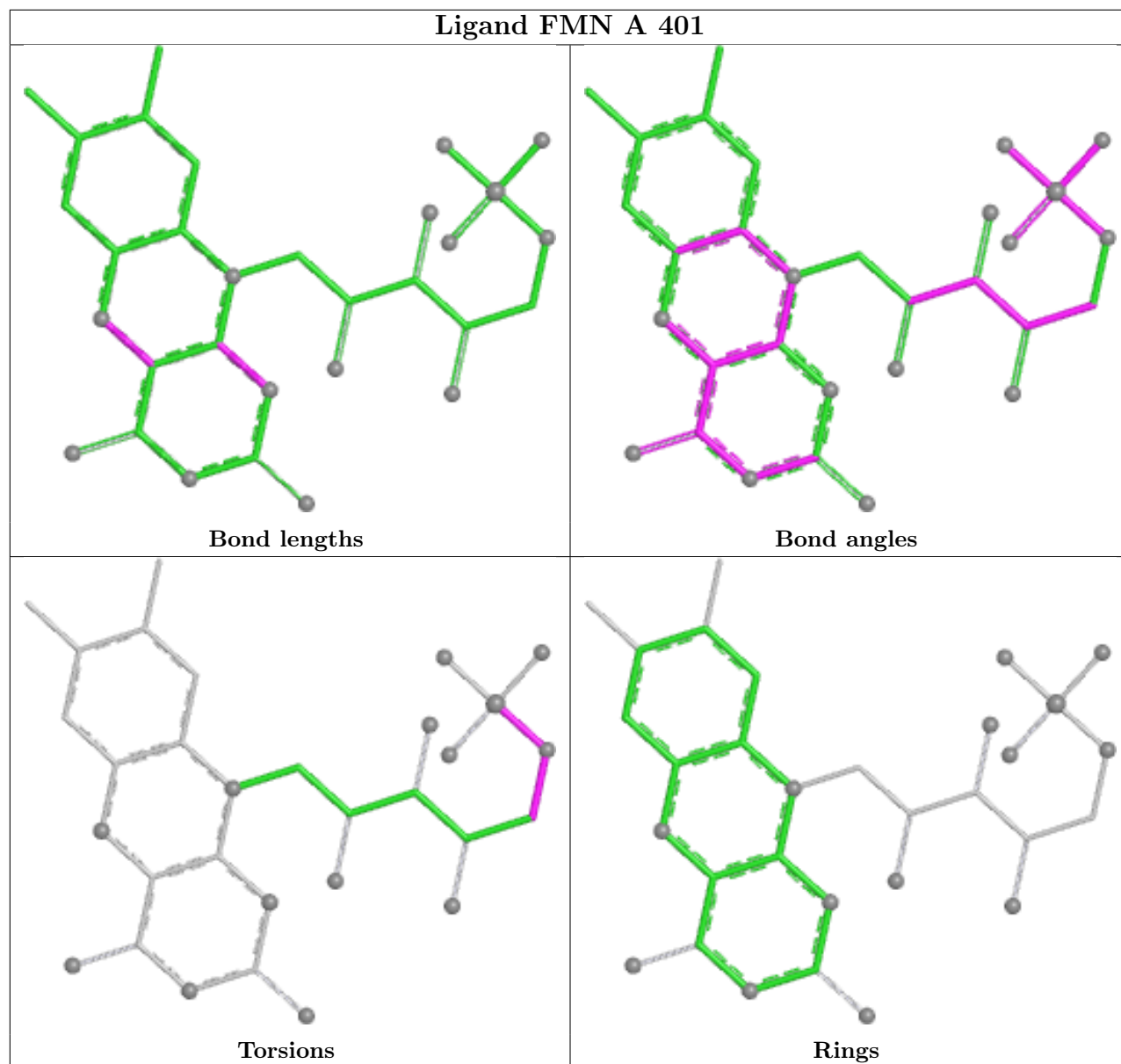
Torsions

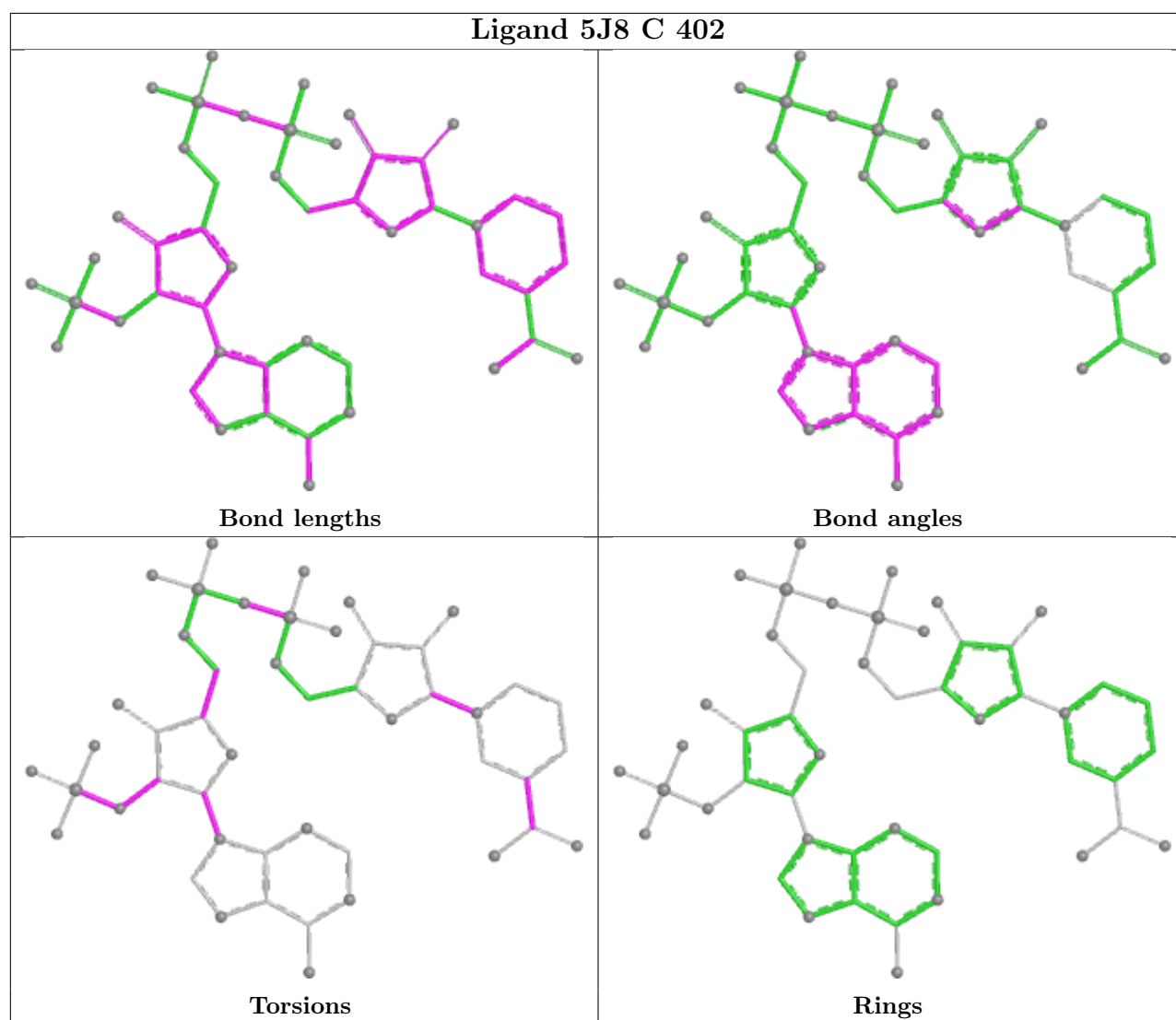


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	376/402 (93%)	-0.10	2 (0%) 87 91	16, 25, 37, 52	0
1	B	375/402 (93%)	0.03	4 (1%) 78 84	19, 28, 42, 49	0
1	C	359/402 (89%)	0.19	6 (1%) 69 75	22, 32, 45, 58	0
1	D	356/402 (88%)	0.72	7 (1%) 65 71	33, 43, 55, 64	0
All	All	1466/1608 (91%)	0.20	19 (1%) 75 82	16, 32, 49, 64	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	384	LEU	4.0
1	C	209	GLY	3.3
1	A	287	TYR	3.2
1	D	318	CYS	2.8
1	C	284	TYR	2.7
1	C	123	ALA	2.6
1	D	242	ILE	2.5
1	B	158	TYR	2.4
1	D	332	ALA	2.4
1	A	9	ASN	2.4
1	D	357	LEU	2.3
1	B	209	GLY	2.3
1	B	248	MET	2.3
1	C	302	ALA	2.2
1	D	282	PRO	2.1
1	C	243	ASP	2.1
1	B	227	SER	2.1
1	C	283	ASP	2.0
1	D	13	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

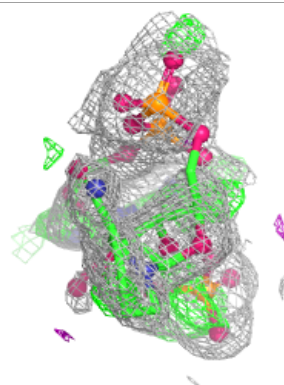
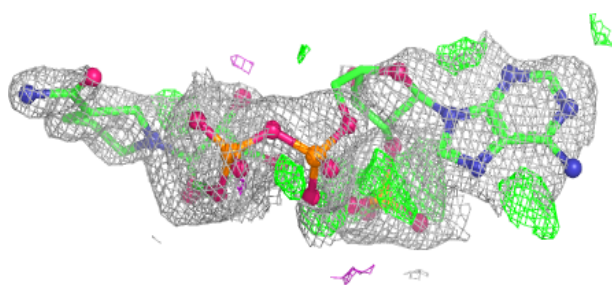
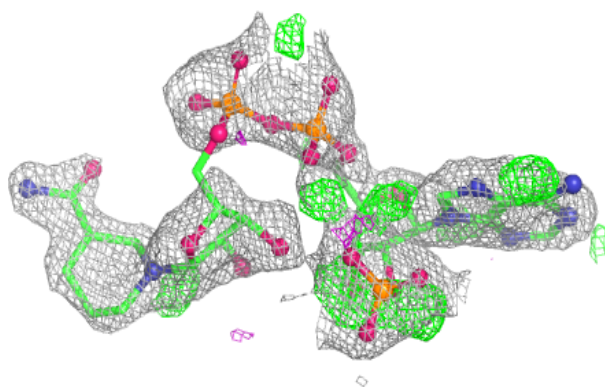
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	5J8	A	402	48/48	0.80	0.15	28,39,53,57	48
4	MPD	A	403	8/8	0.85	0.15	27,29,37,38	0
3	5J8	C	402	48/48	0.88	0.10	21,51,56,64	0
2	FMN	D	401	31/31	0.92	0.08	31,36,42,46	0
2	FMN	B	401	31/31	0.95	0.07	20,23,28,35	0
2	FMN	A	401	31/31	0.96	0.07	15,18,24,26	0
2	FMN	C	401	31/31	0.96	0.06	20,24,26,28	0

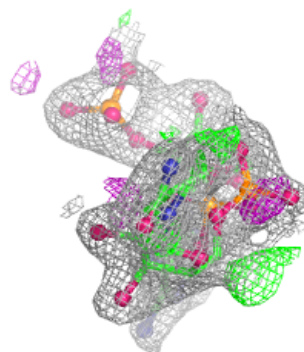
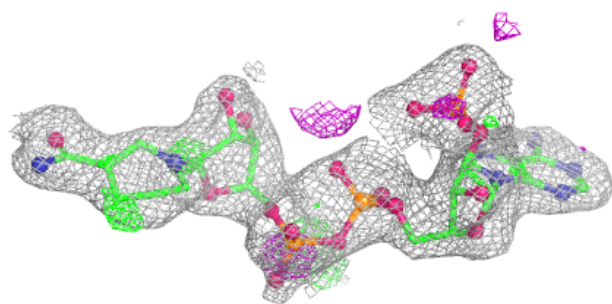
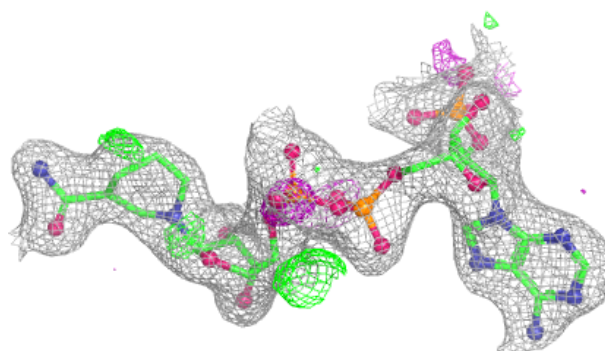
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5J8 A 402:

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

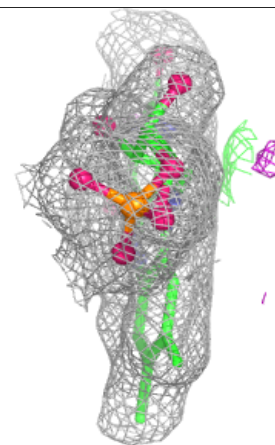
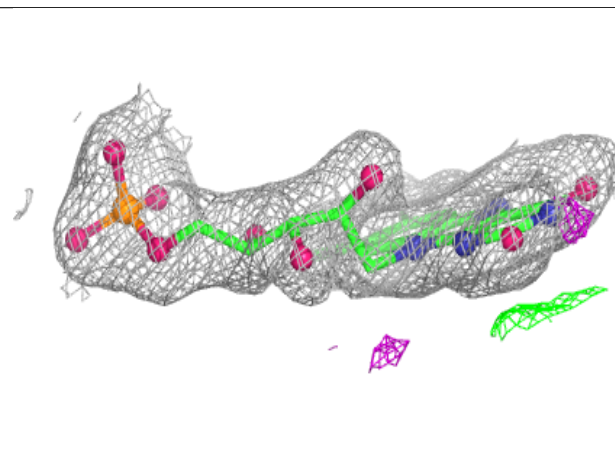
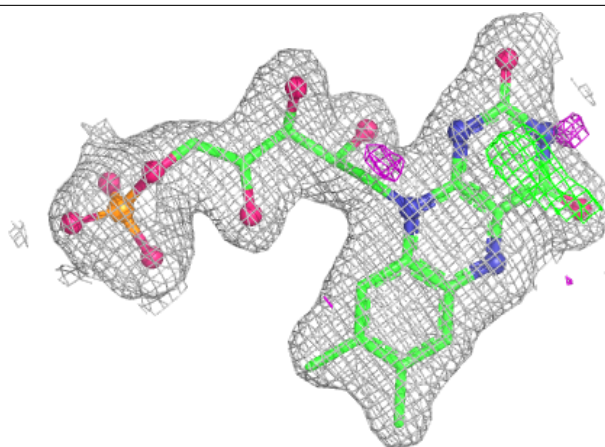
**Electron density around 5J8 C 402:**

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



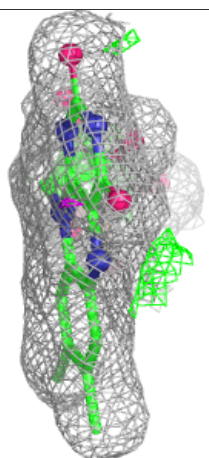
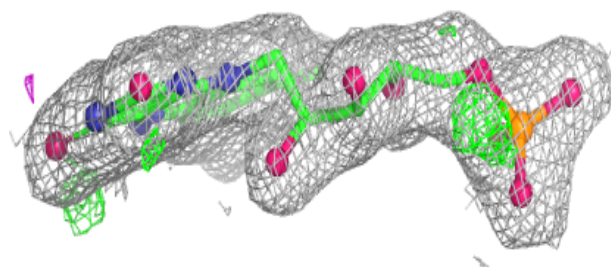
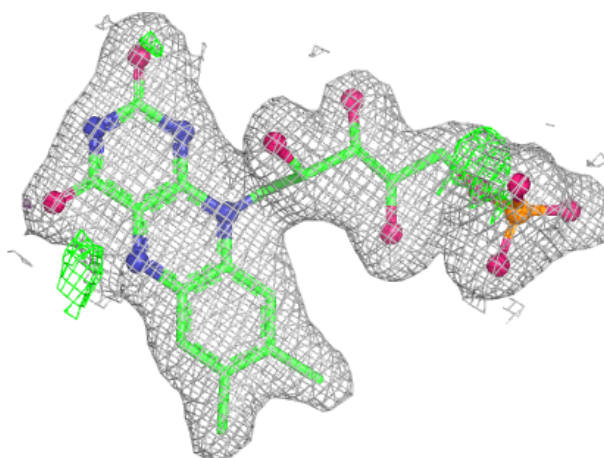
Electron density around FMN D 401:

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



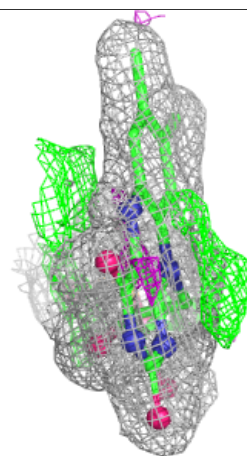
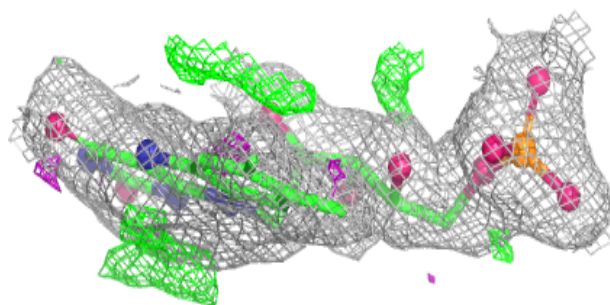
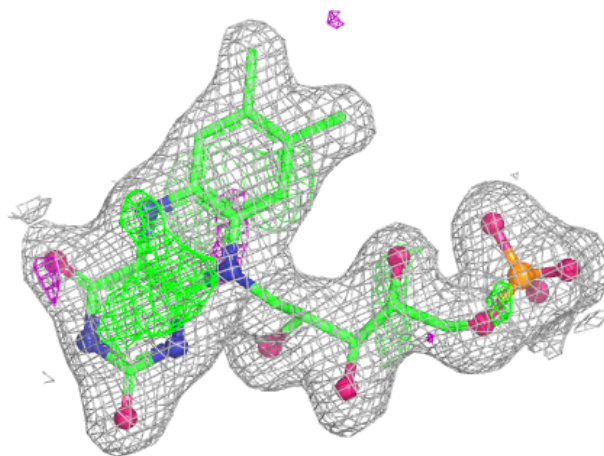
Electron density around FMN B 401:

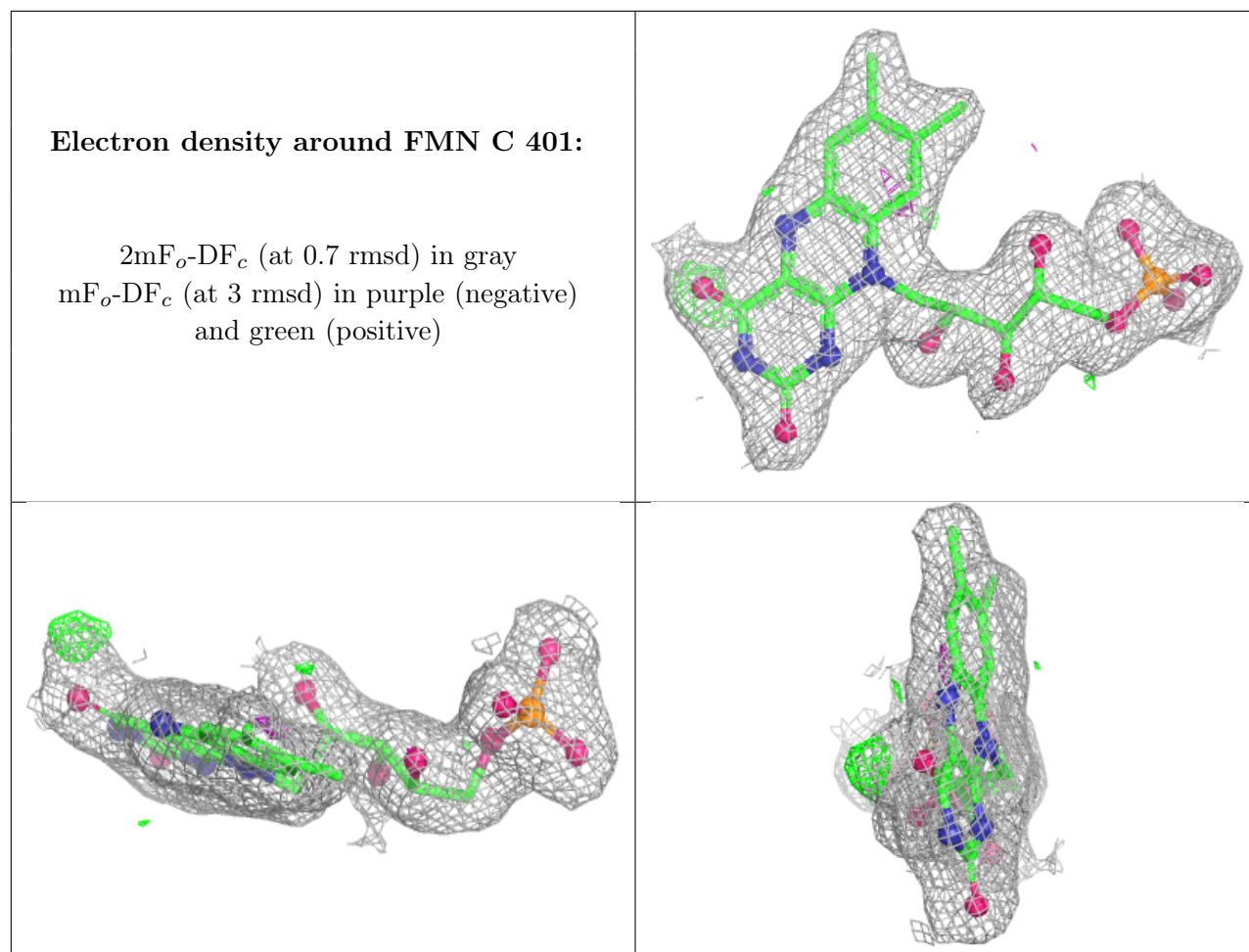
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.