



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:30 AM UTC

PDB ID : 7JW9 / pdb_00007jw9
Title : Ternary cocrystal structure of alkanesulfonate monooxygenase Msd from *Pseudomonas fluorescens*
Authors : Liew, J.J.M.; Dowling, D.P.
Deposited on : 2020-08-25
Resolution : 2.39 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

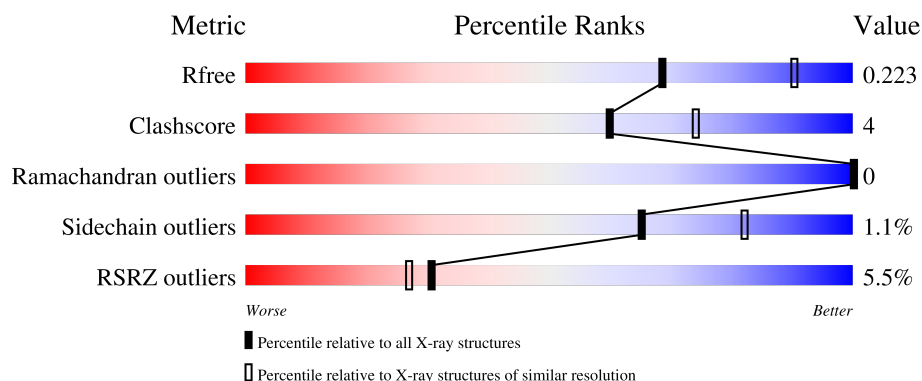
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	404	5% 81% 13% 6%
1	B	404	5% 84% 9% 6%
1	C	404	5% 84% 10% 6%
1	D	404	5% 82% 11% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12019 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 Alkanesulfonate monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	1	0
			2922	1854	517	546	5			
1	B	378	Total	C	N	O	S	0	1	0
			2940	1866	523	546	5			
1	C	378	Total	C	N	O	S	0	0	0
			2928	1859	520	544	5			
1	D	378	Total	C	N	O	S	0	2	0
			2946	1870	523	548	5			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP Q3K9A1
A	-21	GLY	-	expression tag	UNP Q3K9A1
A	-20	SER	-	expression tag	UNP Q3K9A1
A	-19	SER	-	expression tag	UNP Q3K9A1
A	-18	HIS	-	expression tag	UNP Q3K9A1
A	-17	HIS	-	expression tag	UNP Q3K9A1
A	-16	HIS	-	expression tag	UNP Q3K9A1
A	-15	HIS	-	expression tag	UNP Q3K9A1
A	-14	HIS	-	expression tag	UNP Q3K9A1
A	-13	HIS	-	expression tag	UNP Q3K9A1
A	-12	SER	-	expression tag	UNP Q3K9A1
A	-11	SER	-	expression tag	UNP Q3K9A1
A	-10	GLY	-	expression tag	UNP Q3K9A1
A	-9	LEU	-	expression tag	UNP Q3K9A1
A	-8	VAL	-	expression tag	UNP Q3K9A1
A	-7	PRO	-	expression tag	UNP Q3K9A1
A	-6	ARG	-	expression tag	UNP Q3K9A1
A	-5	GLY	-	expression tag	UNP Q3K9A1
A	-4	SER	-	expression tag	UNP Q3K9A1
A	-3	HIS	-	expression tag	UNP Q3K9A1
A	-2	MET	-	expression tag	UNP Q3K9A1

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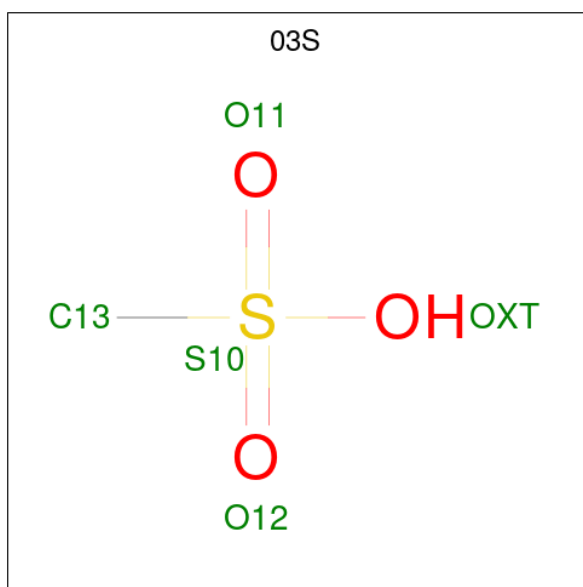
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP Q3K9A1
A	0	SER	-	expression tag	UNP Q3K9A1
B	-22	MET	-	initiating methionine	UNP Q3K9A1
B	-21	GLY	-	expression tag	UNP Q3K9A1
B	-20	SER	-	expression tag	UNP Q3K9A1
B	-19	SER	-	expression tag	UNP Q3K9A1
B	-18	HIS	-	expression tag	UNP Q3K9A1
B	-17	HIS	-	expression tag	UNP Q3K9A1
B	-16	HIS	-	expression tag	UNP Q3K9A1
B	-15	HIS	-	expression tag	UNP Q3K9A1
B	-14	HIS	-	expression tag	UNP Q3K9A1
B	-13	HIS	-	expression tag	UNP Q3K9A1
B	-12	SER	-	expression tag	UNP Q3K9A1
B	-11	SER	-	expression tag	UNP Q3K9A1
B	-10	GLY	-	expression tag	UNP Q3K9A1
B	-9	LEU	-	expression tag	UNP Q3K9A1
B	-8	VAL	-	expression tag	UNP Q3K9A1
B	-7	PRO	-	expression tag	UNP Q3K9A1
B	-6	ARG	-	expression tag	UNP Q3K9A1
B	-5	GLY	-	expression tag	UNP Q3K9A1
B	-4	SER	-	expression tag	UNP Q3K9A1
B	-3	HIS	-	expression tag	UNP Q3K9A1
B	-2	MET	-	expression tag	UNP Q3K9A1
B	-1	ALA	-	expression tag	UNP Q3K9A1
B	0	SER	-	expression tag	UNP Q3K9A1
C	-22	MET	-	initiating methionine	UNP Q3K9A1
C	-21	GLY	-	expression tag	UNP Q3K9A1
C	-20	SER	-	expression tag	UNP Q3K9A1
C	-19	SER	-	expression tag	UNP Q3K9A1
C	-18	HIS	-	expression tag	UNP Q3K9A1
C	-17	HIS	-	expression tag	UNP Q3K9A1
C	-16	HIS	-	expression tag	UNP Q3K9A1
C	-15	HIS	-	expression tag	UNP Q3K9A1
C	-14	HIS	-	expression tag	UNP Q3K9A1
C	-13	HIS	-	expression tag	UNP Q3K9A1
C	-12	SER	-	expression tag	UNP Q3K9A1
C	-11	SER	-	expression tag	UNP Q3K9A1
C	-10	GLY	-	expression tag	UNP Q3K9A1
C	-9	LEU	-	expression tag	UNP Q3K9A1
C	-8	VAL	-	expression tag	UNP Q3K9A1
C	-7	PRO	-	expression tag	UNP Q3K9A1
C	-6	ARG	-	expression tag	UNP Q3K9A1

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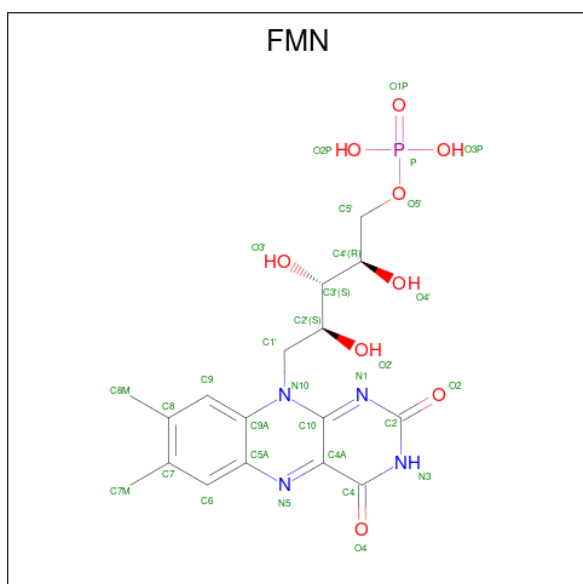
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q3K9A1
C	-4	SER	-	expression tag	UNP Q3K9A1
C	-3	HIS	-	expression tag	UNP Q3K9A1
C	-2	MET	-	expression tag	UNP Q3K9A1
C	-1	ALA	-	expression tag	UNP Q3K9A1
C	0	SER	-	expression tag	UNP Q3K9A1
D	-22	MET	-	initiating methionine	UNP Q3K9A1
D	-21	GLY	-	expression tag	UNP Q3K9A1
D	-20	SER	-	expression tag	UNP Q3K9A1
D	-19	SER	-	expression tag	UNP Q3K9A1
D	-18	HIS	-	expression tag	UNP Q3K9A1
D	-17	HIS	-	expression tag	UNP Q3K9A1
D	-16	HIS	-	expression tag	UNP Q3K9A1
D	-15	HIS	-	expression tag	UNP Q3K9A1
D	-14	HIS	-	expression tag	UNP Q3K9A1
D	-13	HIS	-	expression tag	UNP Q3K9A1
D	-12	SER	-	expression tag	UNP Q3K9A1
D	-11	SER	-	expression tag	UNP Q3K9A1
D	-10	GLY	-	expression tag	UNP Q3K9A1
D	-9	LEU	-	expression tag	UNP Q3K9A1
D	-8	VAL	-	expression tag	UNP Q3K9A1
D	-7	PRO	-	expression tag	UNP Q3K9A1
D	-6	ARG	-	expression tag	UNP Q3K9A1
D	-5	GLY	-	expression tag	UNP Q3K9A1
D	-4	SER	-	expression tag	UNP Q3K9A1
D	-3	HIS	-	expression tag	UNP Q3K9A1
D	-2	MET	-	expression tag	UNP Q3K9A1
D	-1	ALA	-	expression tag	UNP Q3K9A1
D	0	SER	-	expression tag	UNP Q3K9A1

- Molecule 2 is methanesulfonic acid (CCD ID: 03S) (formula: CH₄O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			5	1	3	1		
2	B	1	Total	C	O	S	0	0
			5	1	3	1		
2	C	1	Total	C	O	S	0	0
			5	1	3	1		
2	D	1	Total	C	O	S	0	0
			5	1	3	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

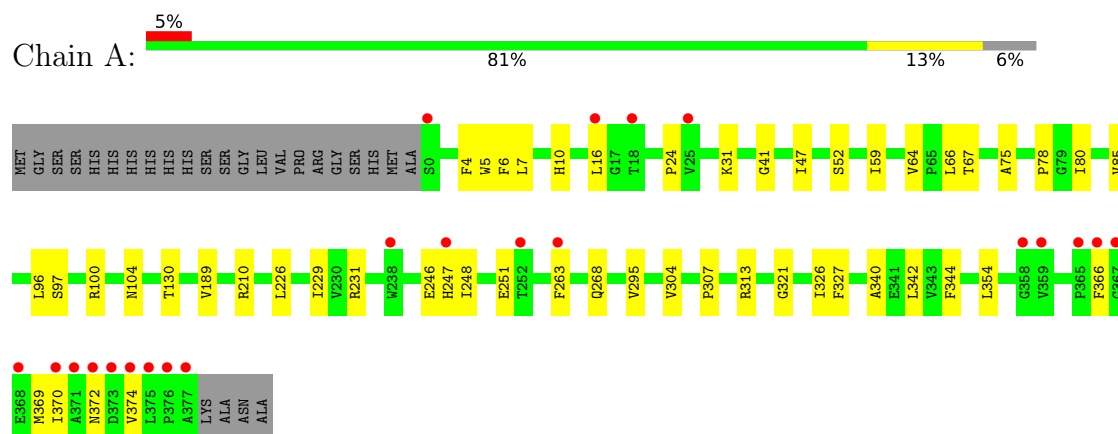
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total	O	0	0
			34	34		
5	B	27	Total	O	0	0
			27	27		
5	C	39	Total	O	0	0
			39	39		
5	D	38	Total	O	0	0
			38	38		

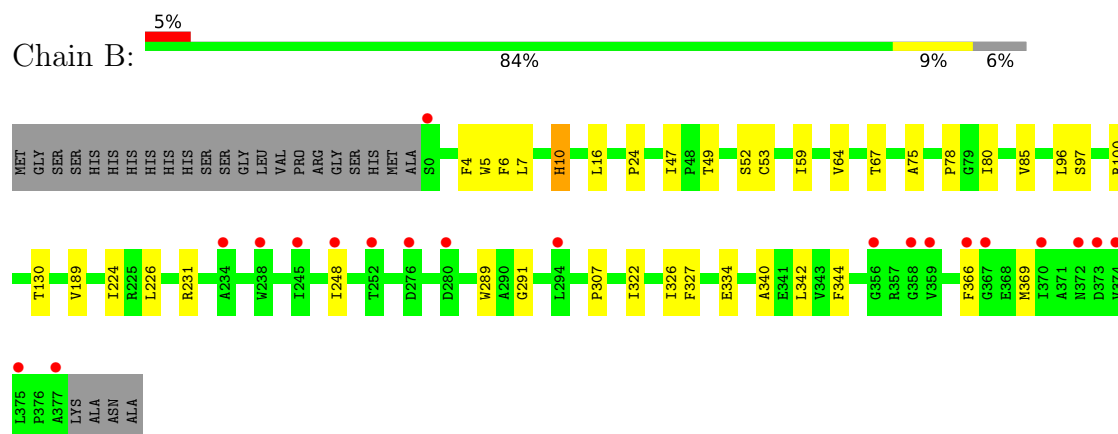
3 Residue-property plots [i](#)

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.

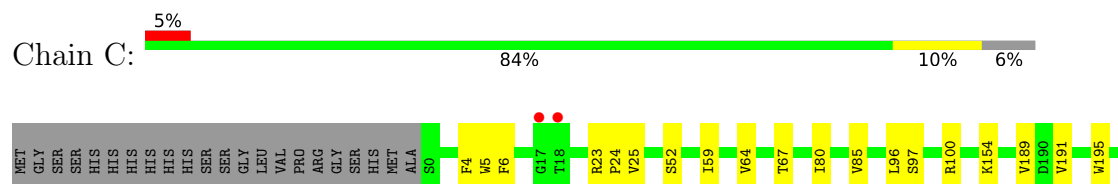
- Molecule 1: Alkanesulfonate monooxygenase

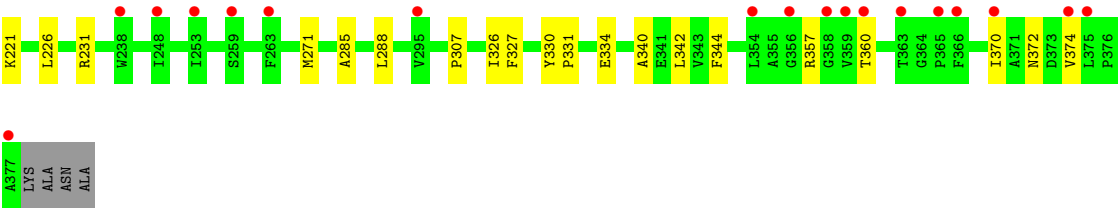


- Molecule 1: Alkanesulfonate monooxygenase

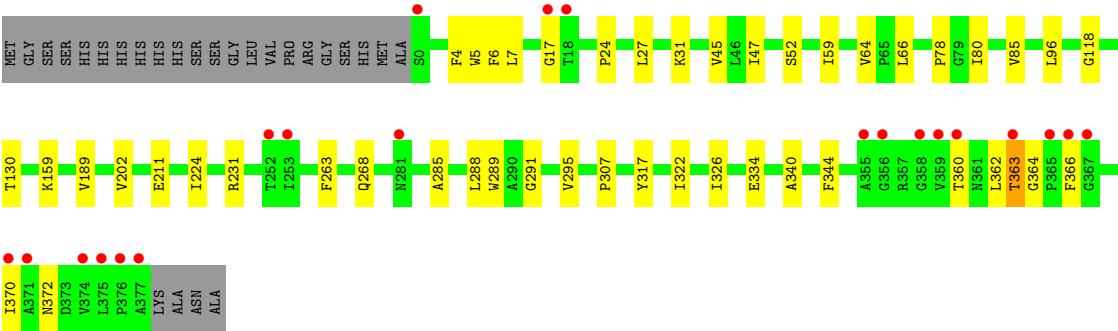
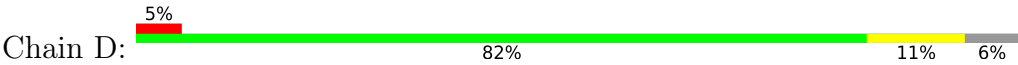


- Molecule 1: Alkanesulfonate monooxygenase





● Molecule 1: Alkanesulfonate monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	92.47Å 92.47Å 320.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.24 – 2.39 46.24 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.24-2.39) 99.6 (46.24-2.39)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.184 , 0.221 0.186 , 0.223	Depositor DCC
R_{free} test set	3032 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12019	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 03S, FMN, NA

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	0.10	0/2996	0.28	0/4078
1	B	0.09	0/3014	0.27	0/4097
1	C	0.09	0/2999	0.27	0/4077
1	D	0.09	0/3023	0.27	0/4109
All	All	0.09	0/12032	0.27	0/16361

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 [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	2922	0	2858	35	0
1	B	2940	0	2902	27	0
1	C	2928	0	2885	28	0
1	D	2946	0	2908	33	0
2	A	5	0	3	0	0
2	B	5	0	3	0	0
2	C	5	0	3	0	0
2	D	5	0	3	0	0
3	A	31	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	19	0	0
3	C	31	0	19	0	0
3	D	31	0	19	0	0
4	A	1	0	0	0	0
5	A	34	0	0	0	0
5	B	27	0	0	0	0
5	C	39	0	0	0	0
5	D	38	0	0	1	0
All	All	12019	0	11641	102	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 4.

All (102) 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:85:VAL:HG21	1:B:80:ILE:HD12	1.72	0.72
1:A:80:ILE:HD13	1:B:85:VAL:HG21	1.77	0.65
1:A:210:ARG:HH22	1:A:321:GLY:HA3	1.62	0.65
1:A:372:ASN:HA	1:D:52:SER:HB3	1.78	0.64
1:C:59:ILE:HD13	1:D:96:LEU:HD11	1.80	0.64
1:D:360:THR:HG22	1:D:362:LEU:H	1.64	0.62
1:A:31:LYS:HD3	1:A:66:LEU:HD13	1.81	0.62
1:A:59:ILE:HD13	1:B:96:LEU:HD11	1.81	0.62
1:C:85:VAL:HG21	1:D:80:ILE:HD13	1.84	0.60
1:D:263:PHE:HD2	1:D:268:GLN:HG2	1.69	0.58
1:A:370:ILE:HD11	1:D:17:GLY:HA2	1.86	0.58
1:A:96:LEU:HD11	1:B:59:ILE:HD13	1.86	0.57
1:B:78:PRO:HG2	1:B:130:THR:HG23	1.88	0.55
1:A:370:ILE:HD12	1:D:295:VAL:HB	1.89	0.55
1:D:317:TYR:HB3	1:D:322:ILE:HD12	1.88	0.55
1:D:159:LYS:NZ	5:D:502:HOH:O	2.40	0.54
1:C:96:LEU:HD22	1:D:27:LEU:HB2	1.89	0.54
1:C:96:LEU:HD11	1:D:59:ILE:HD13	1.90	0.53
1:C:4:PHE:HB2	1:C:326:ILE:HA	1.91	0.53
1:A:78:PRO:HG2	1:A:130:THR:HG23	1.91	0.53
1:D:340:ALA:O	1:D:344:PHE:HB2	2.09	0.52
1:C:370:ILE:HB	1:C:374:VAL:HB	1.92	0.52
1:B:231:ARG:O	1:B:307:PRO:HD3	2.10	0.51
1:C:357:ARG:NH2	1:C:360:THR:O	2.43	0.51
1:A:16:LEU:HB2	1:A:248:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PHE:HD2	1:A:268:GLN:HG2	1.76	0.51
1:B:97:SER:O	1:B:100:ARG:HD3	2.11	0.51
1:C:80:ILE:HD13	1:D:85:VAL:HG21	1.92	0.51
1:C:285:ALA:HB3	1:C:288:LEU:HB3	1.92	0.51
1:B:340:ALA:O	1:B:344:PHE:HB2	2.11	0.50
1:B:369:MET:HG3	1:C:52:SER:HB2	1.94	0.50
1:A:251:GLU:OE1	1:A:251:GLU:N	2.39	0.50
1:C:340:ALA:O	1:C:344:PHE:HB2	2.12	0.49
1:B:4:PHE:HB2	1:B:326:ILE:HA	1.94	0.49
1:A:340:ALA:O	1:A:344:PHE:HB2	2.12	0.49
1:A:52:SER:HB3	1:D:372:ASN:HA	1.94	0.49
1:D:202:VAL:HG11	1:D:322:ILE:HD11	1.94	0.49
1:D:363:THR:OG1	1:D:364:GLY:N	2.45	0.48
1:D:78:PRO:HG2	1:D:130:THR:HG23	1.95	0.48
1:A:41:GLY:HA3	1:A:354:LEU:HD13	1.96	0.48
1:A:97:SER:O	1:A:100:ARG:HD3	2.14	0.48
1:B:5:TRP:CD1	1:B:6:PHE:H	2.31	0.48
1:C:231:ARG:O	1:C:307:PRO:HD3	2.13	0.48
1:A:231:ARG:O	1:A:307:PRO:HD3	2.14	0.48
1:A:307:PRO:HG3	1:A:342:LEU:HB3	1.95	0.48
1:B:16:LEU:HB2	1:B:248:ILE:HD11	1.96	0.48
1:B:5:TRP:CG	1:B:6:PHE:H	2.33	0.47
1:C:334:GLU:N	1:C:334:GLU:OE1	2.46	0.47
1:A:5:TRP:CD1	1:A:6:PHE:H	2.31	0.47
1:A:295:VAL:HG13	1:D:370:ILE:HG23	1.97	0.47
1:D:285:ALA:HB3	1:D:288:LEU:HB3	1.96	0.47
1:D:289:TRP:CZ2	1:D:291:GLY:HA3	2.49	0.47
1:A:4:PHE:HB2	1:A:326:ILE:HA	1.96	0.47
1:A:5:TRP:CG	1:A:6:PHE:H	2.32	0.47
1:B:7:LEU:HD12	1:B:47:ILE:HG12	1.97	0.47
1:B:224:ILE:HB	1:B:322:ILE:HD13	1.97	0.47
1:A:246:GLU:HG3	1:A:247:HIS:CD2	2.51	0.46
1:B:226:LEU:O	1:B:327:PHE:HA	2.16	0.46
1:D:231:ARG:O	1:D:307:PRO:HD3	2.16	0.45
1:D:4:PHE:HB2	1:D:326:ILE:HA	1.98	0.45
1:C:307:PRO:HG3	1:C:342:LEU:HB3	1.99	0.45
1:A:7:LEU:HD12	1:A:47:ILE:HG12	1.98	0.45
1:D:224:ILE:HB	1:D:322:ILE:HD13	1.97	0.45
1:A:366:PHE:HE1	1:D:24:PRO:HD3	1.81	0.45
1:B:67:THR:OG1	1:B:100:ARG:NH2	2.50	0.45
1:C:97:SER:O	1:C:100:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:TRP:CG	1:D:6:PHE:H	2.34	0.44
1:C:5:TRP:CG	1:C:6:PHE:H	2.35	0.44
1:C:191:VAL:HG22	1:C:221:LYS:HB2	1.99	0.44
1:B:10:HIS:HB3	1:B:53:CYS:SG	2.57	0.44
1:B:334:GLU:N	1:B:334:GLU:OE1	2.47	0.44
1:D:5:TRP:CD1	1:D:6:PHE:H	2.35	0.44
1:B:24:PRO:HG3	1:C:357:ARG:HA	1.99	0.43
1:D:7:LEU:HD12	1:D:47:ILE:HG12	1.99	0.43
1:B:289:TRP:CZ2	1:B:291:GLY:HA3	2.54	0.43
1:C:5:TRP:CD1	1:C:6:PHE:H	2.37	0.43
1:D:5:TRP:HB3	1:D:45:VAL:HG12	2.00	0.43
1:B:307:PRO:HG3	1:B:342:LEU:HB3	2.01	0.43
1:C:67:THR:OG1	1:C:100:ARG:NH2	2.51	0.43
1:A:67:THR:OG1	1:A:100:ARG:NH2	2.52	0.43
1:C:195:TRP:HB3	1:C:271:MET:HE3	2.01	0.43
1:A:229:ILE:HB	1:A:304:VAL:HG22	2.01	0.42
1:C:23:ARG:NH2	1:C:334:GLU:OE2	2.27	0.42
1:B:52:SER:HB3	1:C:372:ASN:HA	2.01	0.42
1:B:334:GLU:HG3	1:C:334:GLU:HG3	2.01	0.42
1:A:370:ILE:HB	1:A:374:VAL:HB	2.00	0.42
1:C:226:LEU:O	1:C:327:PHE:HA	2.19	0.42
1:D:31:LYS:HD3	1:D:66:LEU:HD13	2.01	0.42
1:A:369:MET:HE3	1:A:369:MET:HB3	1.96	0.41
1:D:334:GLU:OE1	1:D:334:GLU:N	2.51	0.41
1:B:49:THR:HB	1:B:75:ALA:HB3	2.02	0.41
1:D:263:PHE:CD2	1:D:268:GLN:HG2	2.51	0.41
3:A:402:FMN:HM71	3:A:402:FMN:HM83	1.84	0.41
1:A:75:ALA:HA	1:A:104:ASN:O	2.21	0.41
1:B:366:PHE:HE1	1:C:24:PRO:HD3	1.86	0.41
1:A:24:PRO:HD3	1:D:366:PHE:HE1	1.86	0.40
1:C:330:TYR:HA	1:C:331:PRO:HA	1.95	0.40
1:A:226:LEU:O	1:A:327:PHE:HA	2.20	0.40
1:A:248:ILE:HD13	1:A:295:VAL:HG21	2.02	0.40
1:C:154:LYS:O	1:D:118:GLY:HA2	2.22	0.40
1:A:313:ARG:HA	1:A:313:ARG:HD3	1.93	0.40
1:B:369:MET:HE3	1:B:369:MET:HB3	1.96	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	377/404 (93%)	364 (97%)	13 (3%)	0	100	100
1	B	377/404 (93%)	367 (97%)	10 (3%)	0	100	100
1	C	376/404 (93%)	363 (96%)	13 (4%)	0	100	100
1	D	378/404 (94%)	367 (97%)	11 (3%)	0	100	100
All	All	1508/1616 (93%)	1461 (97%)	47 (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	298/321 (93%)	295 (99%)	3 (1%)	68	84
1	B	302/321 (94%)	299 (99%)	3 (1%)	68	84
1	C	300/321 (94%)	297 (99%)	3 (1%)	68	84
1	D	303/321 (94%)	299 (99%)	4 (1%)	61	80
All	All	1203/1284 (94%)	1190 (99%)	13 (1%)	65	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	64	VAL

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Mol	Chain	Res	Type
1	A	189	VAL
1	B	10	HIS
1	B	64	VAL
1	B	189	VAL
1	C	25	VAL
1	C	64	VAL
1	C	189	VAL
1	D	64	VAL
1	D	189	VAL
1	D	211	GLU
1	D	363	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	ASN
1	A	361	ASN
1	C	20	GLN
1	C	247	HIS
1	D	43	HIS

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](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	FMN	B	402	-	33,33,33	1.11	3 (9%)	48,50,50	1.26	9 (18%)
2	03S	B	401	-	4,4,4	0.55	0	6,6,6	0.46	0
3	FMN	A	402	-	33,33,33	1.10	3 (9%)	48,50,50	1.26	8 (16%)
2	03S	D	401	-	4,4,4	0.55	0	6,6,6	0.47	0
3	FMN	D	402	-	33,33,33	1.11	3 (9%)	48,50,50	1.25	8 (16%)
2	03S	A	401	-	4,4,4	0.55	0	6,6,6	0.47	0
3	FMN	C	402	-	33,33,33	1.11	3 (9%)	48,50,50	1.26	8 (16%)
2	03S	C	401	-	4,4,4	0.55	0	6,6,6	0.47	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	FMN	B	402	-	-	6/18/18/18	0/3/3/3
3	FMN	C	402	-	-	4/18/18/18	0/3/3/3
3	FMN	D	402	-	-	3/18/18/18	0/3/3/3
3	FMN	A	402	-	-	3/18/18/18	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	FMN	C5A-N5	-2.87	1.34	1.39
3	D	402	FMN	C5A-N5	-2.83	1.34	1.39
3	C	402	FMN	C5A-N5	-2.77	1.34	1.39
3	A	402	FMN	C5A-N5	-2.76	1.34	1.39
3	B	402	FMN	C6-C7	-2.35	1.36	1.39
3	D	402	FMN	C6-C7	-2.29	1.36	1.39
3	C	402	FMN	C6-C7	-2.27	1.36	1.39
3	A	402	FMN	C6-C7	-2.17	1.36	1.39
3	C	402	FMN	C2-N3	-2.11	1.34	1.39
3	A	402	FMN	C2-N3	-2.10	1.34	1.39
3	B	402	FMN	C2-N3	-2.08	1.34	1.39
3	D	402	FMN	C2-N3	-2.06	1.34	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	FMN	C4-C4A-N5	2.86	122.16	118.21
3	C	402	FMN	C4-C4A-N5	2.69	121.92	118.21
3	D	402	FMN	C4-C4A-N5	2.63	121.84	118.21
3	B	402	FMN	C4A-C10-N1	-2.62	118.17	124.59
3	B	402	FMN	C4-N3-C2	-2.55	121.11	125.64
3	C	402	FMN	C4A-C10-N1	-2.55	118.33	124.59
3	B	402	FMN	C4-C4A-N5	2.55	121.73	118.21
3	C	402	FMN	C4-N3-C2	-2.54	121.13	125.64
3	D	402	FMN	C4A-C10-N1	-2.54	118.37	124.59
3	A	402	FMN	C5A-C9A-N10	2.53	120.26	117.97
3	C	402	FMN	C5A-C9A-N10	2.53	120.26	117.97
3	D	402	FMN	C4-N3-C2	-2.53	121.16	125.64
3	B	402	FMN	C5A-C9A-N10	2.50	120.23	117.97
3	A	402	FMN	C4-N3-C2	-2.46	121.28	125.64
3	D	402	FMN	C5A-C9A-N10	2.46	120.19	117.97
3	A	402	FMN	C4A-C10-N1	-2.46	118.57	124.59
3	A	402	FMN	O2-C2-N1	-2.30	117.99	121.80
3	B	402	FMN	O2-C2-N1	-2.29	117.99	121.80
3	B	402	FMN	C10-N1-C2	2.29	121.81	116.85
3	D	402	FMN	O2-C2-N1	-2.26	118.05	121.80
3	C	402	FMN	O2-C2-N1	-2.26	118.05	121.80
3	C	402	FMN	C10-N1-C2	2.24	121.70	116.85
3	D	402	FMN	C10-N1-C2	2.23	121.69	116.85
3	A	402	FMN	C10-N1-C2	2.22	121.64	116.85
3	C	402	FMN	N3-C2-N1	2.19	124.16	119.50
3	B	402	FMN	N3-C2-N1	2.18	124.14	119.50
3	D	402	FMN	N3-C2-N1	2.18	124.13	119.50
3	A	402	FMN	N3-C2-N1	2.15	124.07	119.50
3	A	402	FMN	C10-C4A-N5	-2.11	120.50	124.81
3	C	402	FMN	C10-C4A-N5	-2.07	120.58	124.81
3	B	402	FMN	C10-C4A-N5	-2.05	120.61	124.81
3	D	402	FMN	C10-C4A-N5	-2.05	120.63	124.81
3	B	402	FMN	C4A-C10-N10	2.01	119.36	116.48

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	FMN	N10-C1'-C2'-O2'
3	A	402	FMN	N10-C1'-C2'-C3'
3	B	402	FMN	N10-C1'-C2'-O2'

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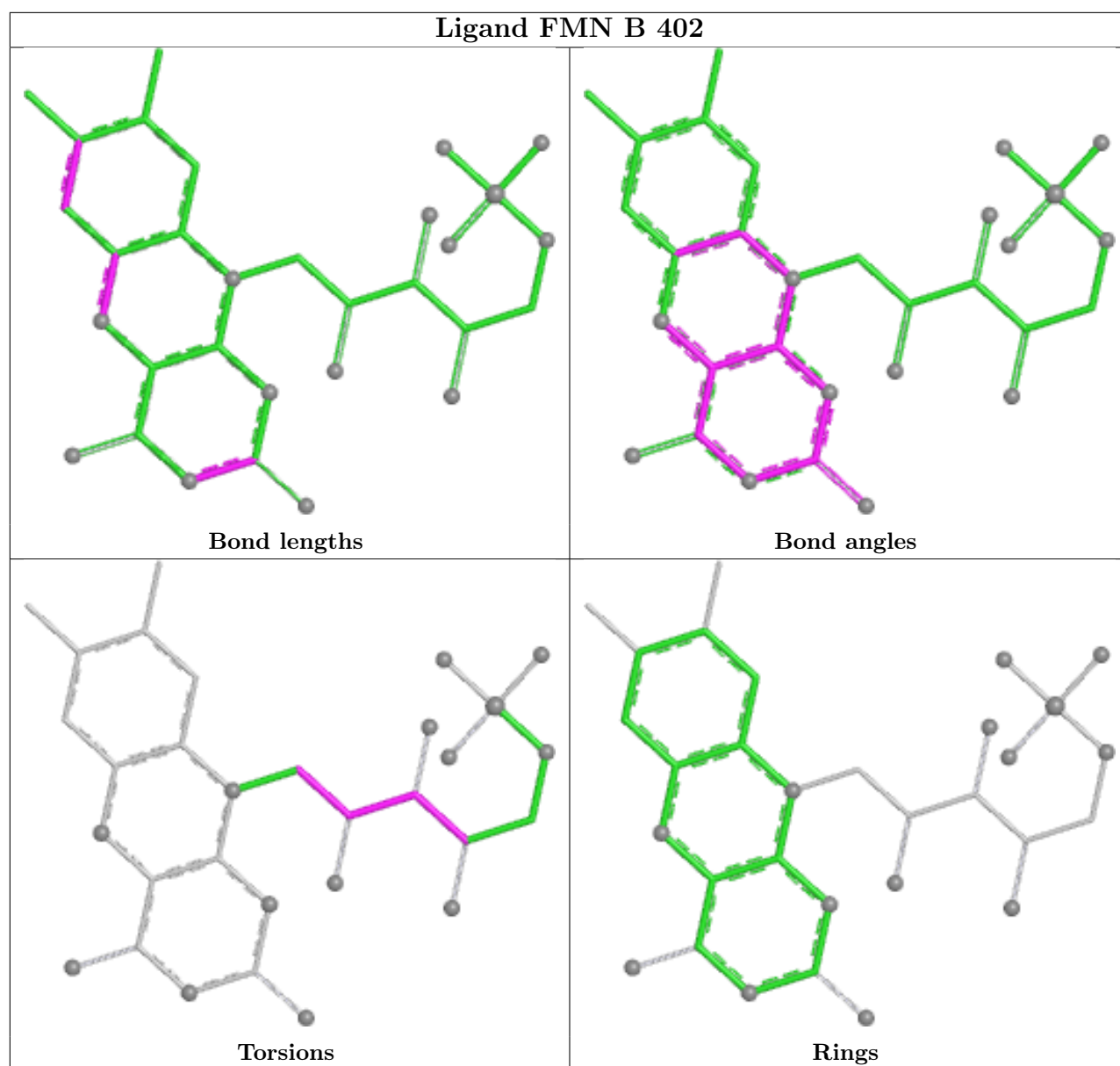
Mol	Chain	Res	Type	Atoms
3	B	402	FMN	N10-C1'-C2'-C3'
3	B	402	FMN	C1'-C2'-C3'-C4'
3	C	402	FMN	N10-C1'-C2'-O2'
3	C	402	FMN	N10-C1'-C2'-C3'
3	D	402	FMN	N10-C1'-C2'-O2'
3	D	402	FMN	N10-C1'-C2'-C3'
3	B	402	FMN	O2'-C2'-C3'-C4'
3	D	402	FMN	O2'-C2'-C3'-C4'
3	B	402	FMN	O2'-C2'-C3'-O3'
3	B	402	FMN	O3'-C3'-C4'-C5'
3	A	402	FMN	O2'-C2'-C3'-C4'
3	C	402	FMN	O2'-C2'-C3'-C4'
3	C	402	FMN	O3'-C3'-C4'-C5'

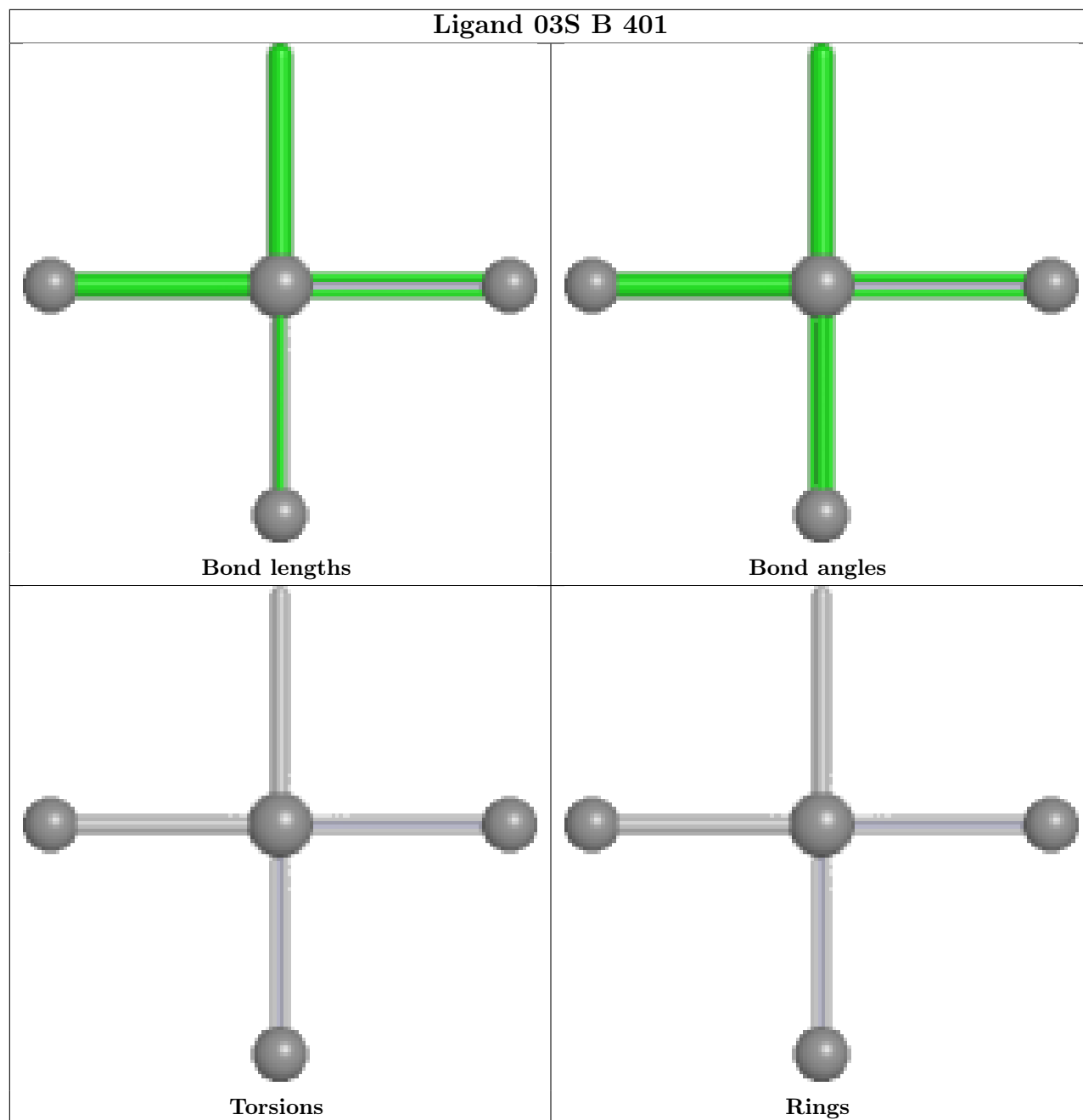
There are no ring outliers.

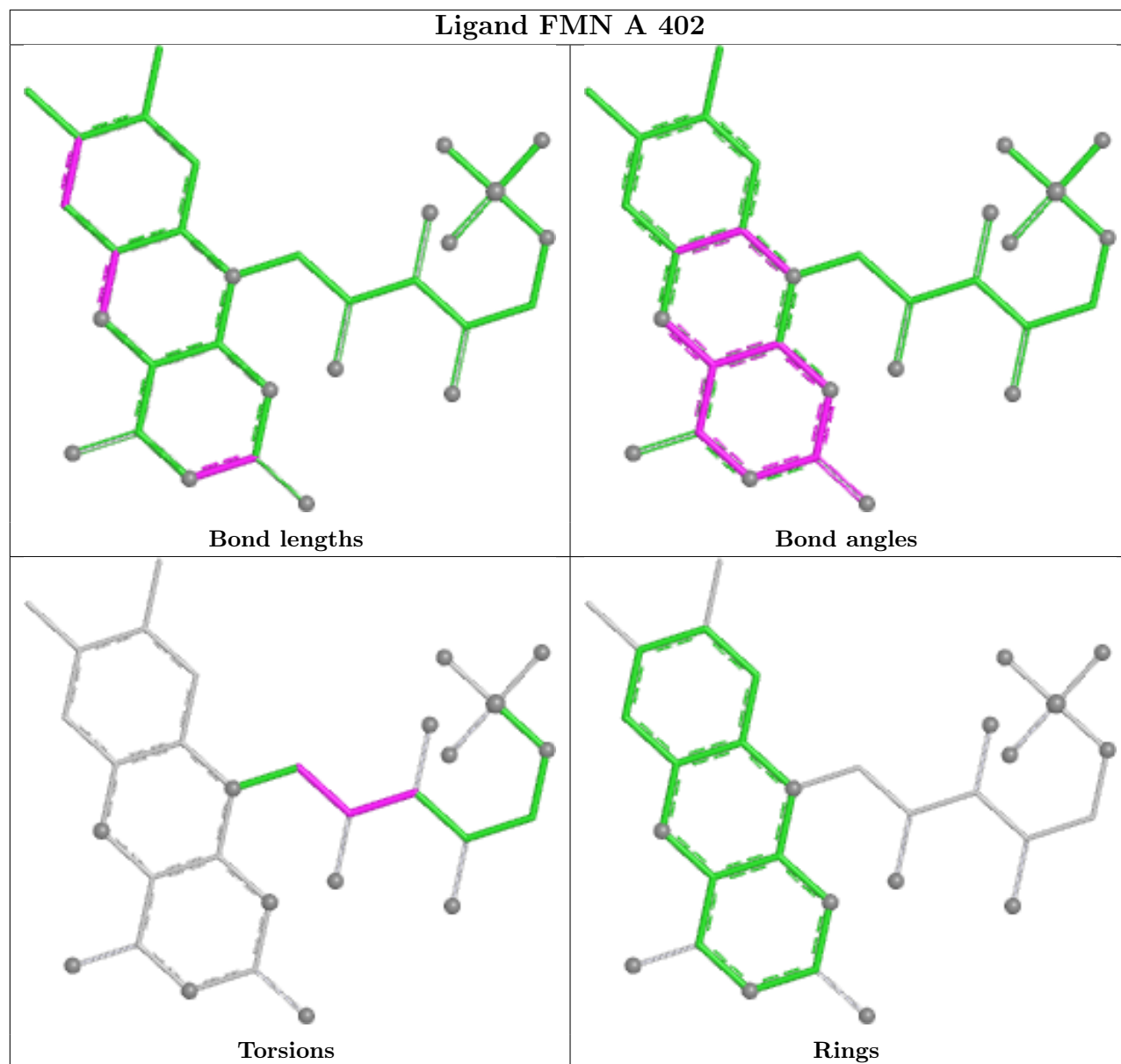
1 monomer is involved in 1 short contact:

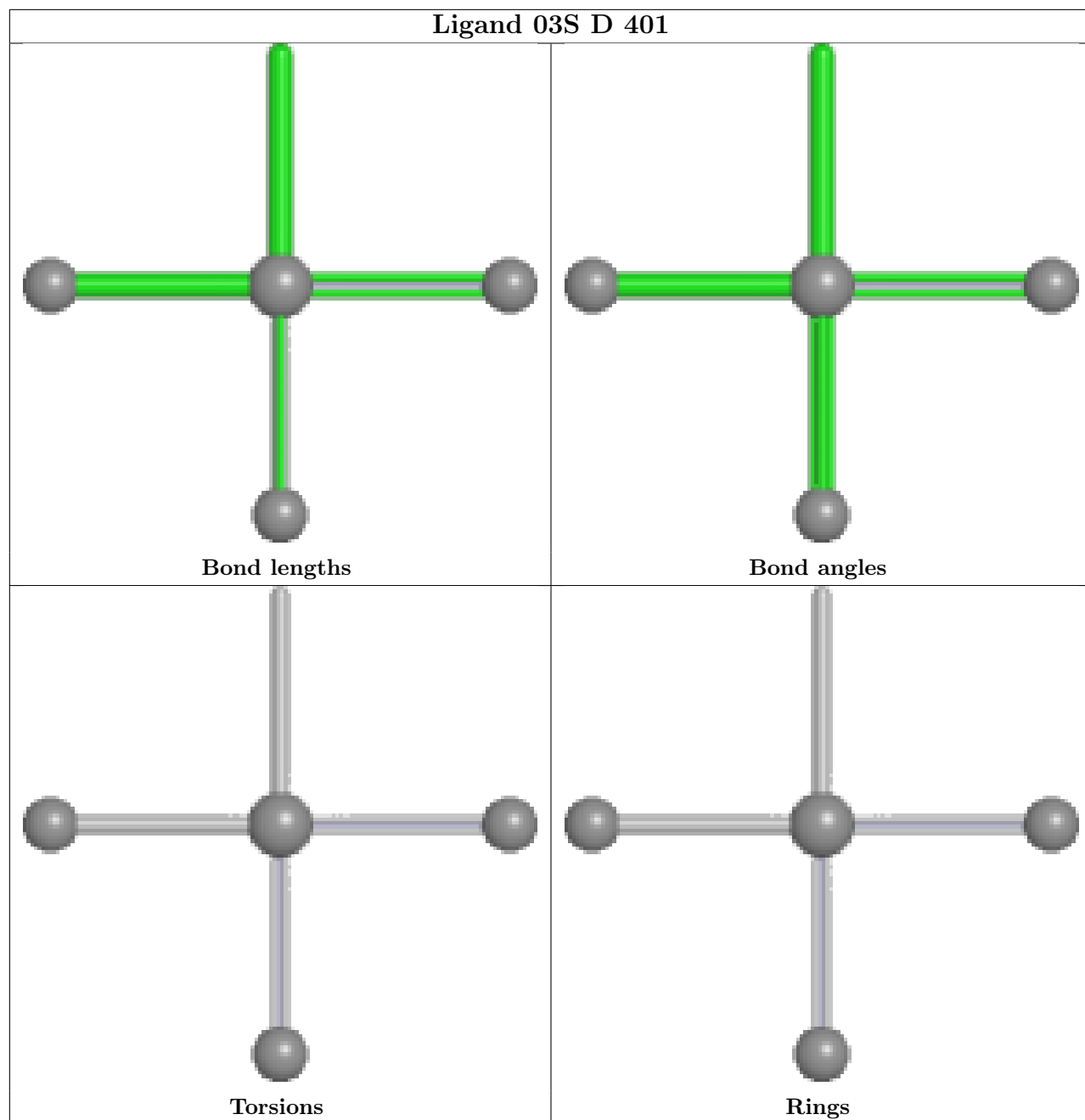
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	FMN	1	0

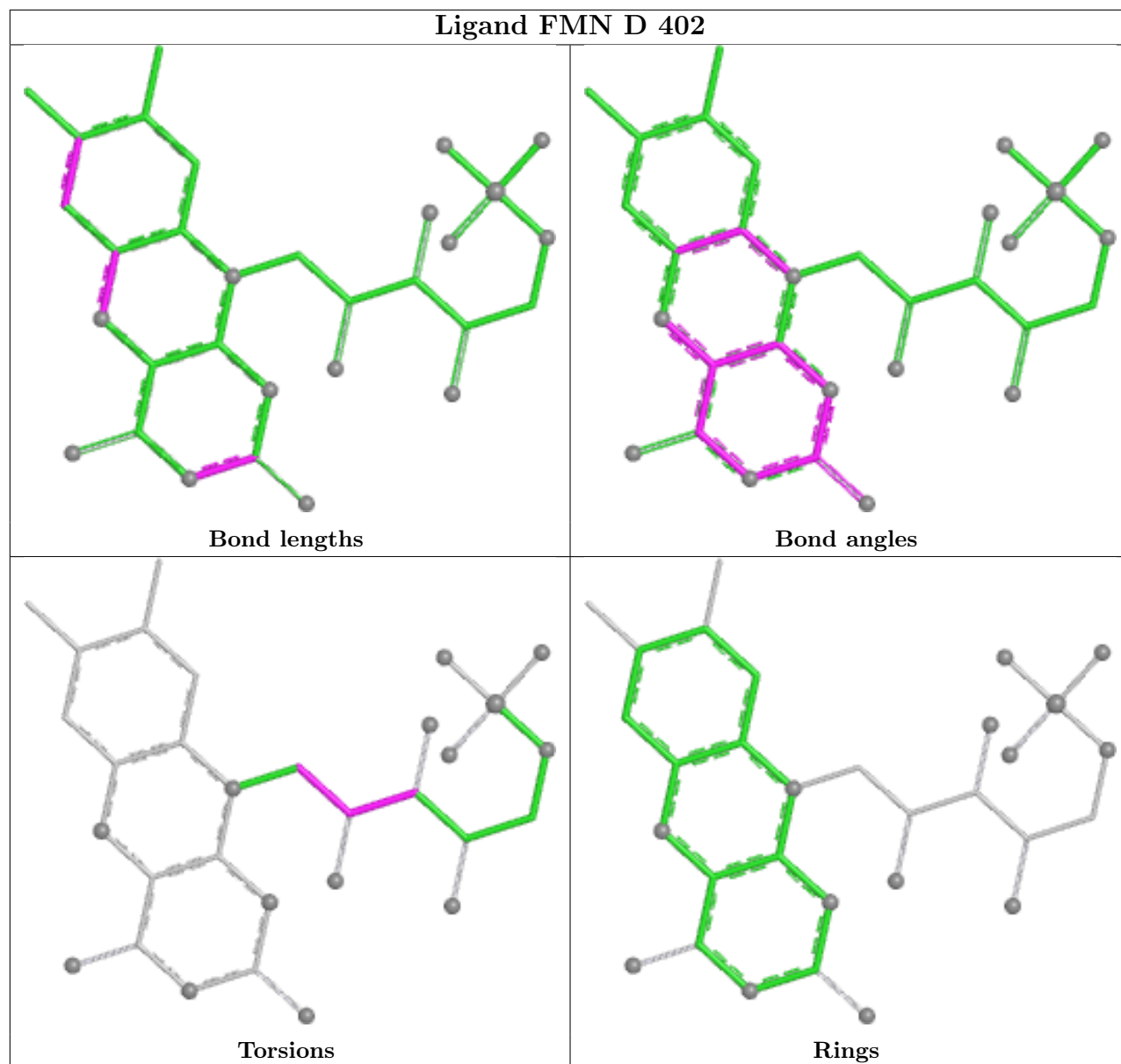
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

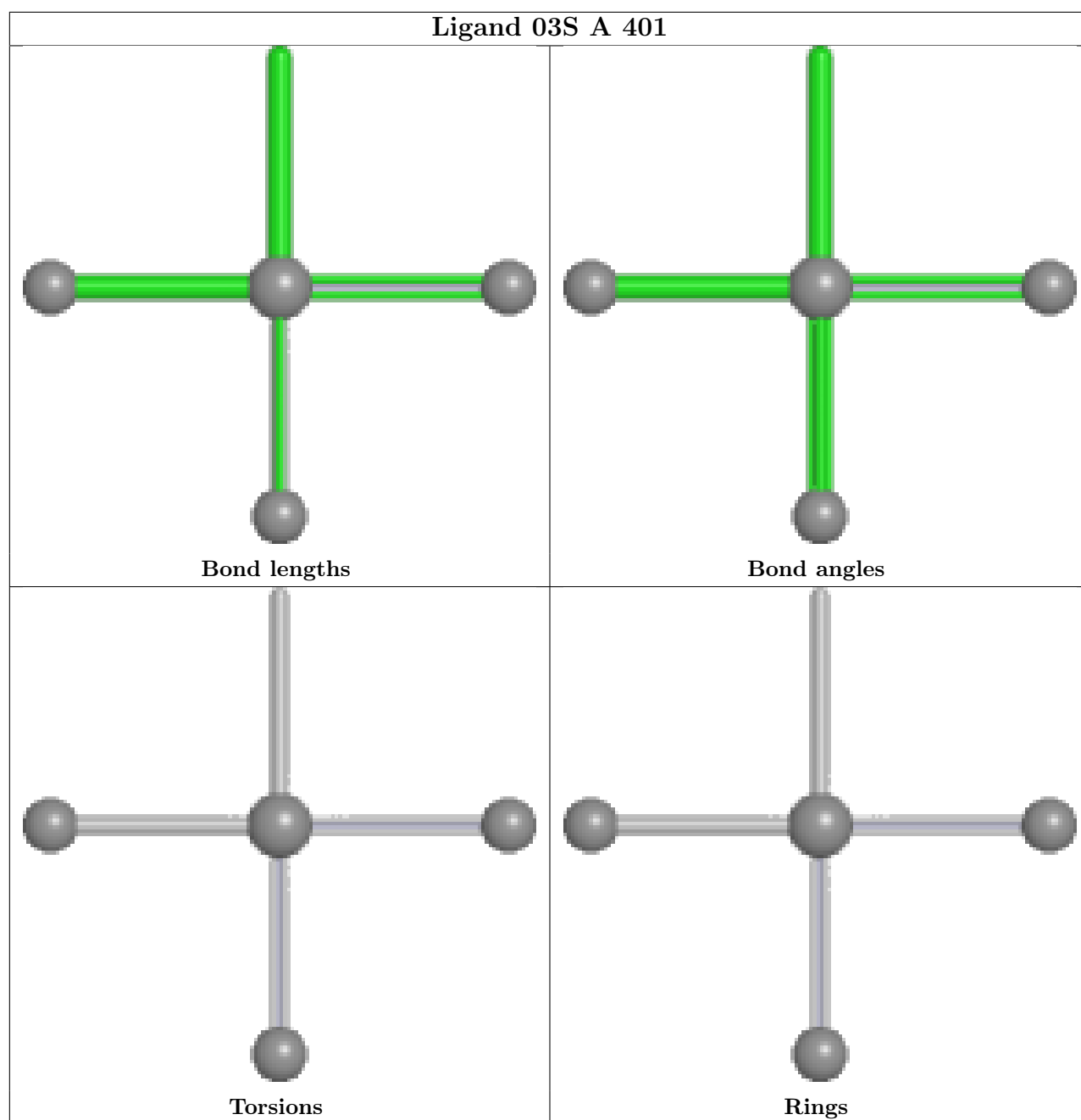


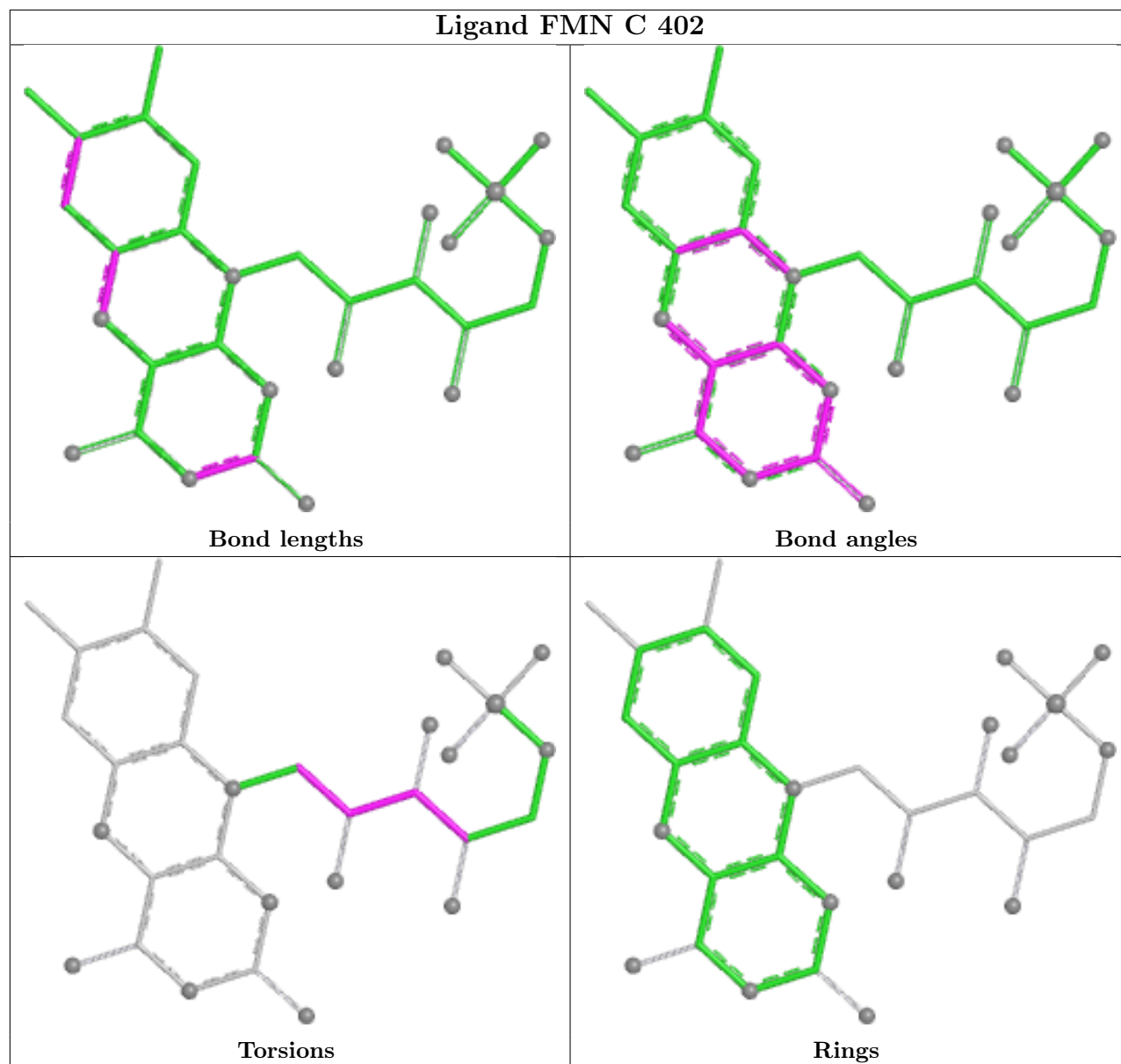


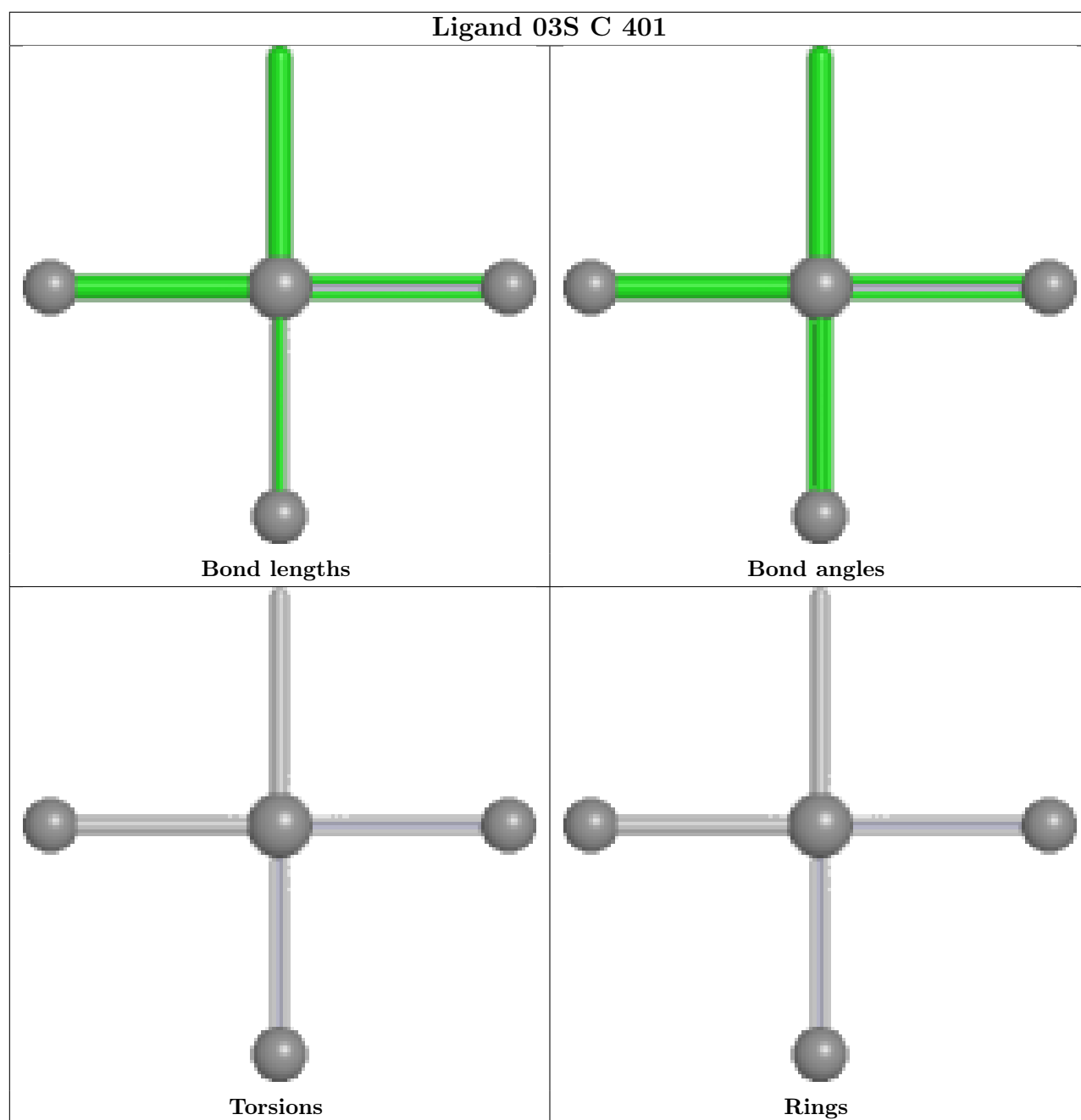












5.7 Other polymers [i](#)

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	378/404 (93%)	0.31	22 (5%)	29 25	32, 52, 89, 103	1 (0%)
1	B	378/404 (93%)	0.36	20 (5%)	32 28	34, 54, 90, 104	1 (0%)
1	C	378/404 (93%)	0.34	20 (5%)	32 28	37, 54, 90, 107	0
1	D	378/404 (93%)	0.29	21 (5%)	30 26	30, 51, 95, 113	2 (0%)
All	All	1512/1616 (93%)	0.33	83 (5%)	30 27	30, 52, 91, 113	4 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	366	PHE	4.3
1	D	359	VAL	4.2
1	C	375	LEU	4.0
1	B	377	ALA	3.8
1	B	375	LEU	3.7
1	D	377	ALA	3.7
1	A	375	LEU	3.6
1	A	377	ALA	3.6
1	C	377	ALA	3.5
1	D	358	GLY	3.4
1	B	366	PHE	3.3
1	D	371	ALA	3.2
1	C	359	VAL	3.2
1	A	366	PHE	3.2
1	A	359	VAL	3.2
1	B	248	ILE	3.2
1	D	356	GLY	3.1
1	A	374	VAL	3.1
1	B	374	VAL	3.1
1	D	374	VAL	3.1
1	C	356	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	238	TRP	3.0
1	B	252	THR	2.9
1	B	367	GLY	2.9
1	D	360	THR	2.9
1	A	372	ASN	2.9
1	C	366	PHE	2.9
1	A	25	VAL	2.9
1	C	374	VAL	2.9
1	D	363	THR	2.9
1	D	253	ILE	2.7
1	C	238	TRP	2.7
1	A	373	ASP	2.7
1	D	375	LEU	2.7
1	A	365	PRO	2.6
1	D	17	GLY	2.6
1	B	370	ILE	2.6
1	A	371	ALA	2.6
1	A	16	LEU	2.5
1	B	359	VAL	2.5
1	A	368	GLU	2.5
1	A	358	GLY	2.5
1	D	367	GLY	2.5
1	B	358	GLY	2.5
1	C	248	ILE	2.5
1	C	365	PRO	2.4
1	C	363	THR	2.4
1	A	370	ILE	2.4
1	C	358	GLY	2.4
1	A	263	PHE	2.4
1	D	370	ILE	2.4
1	D	376	PRO	2.4
1	C	17	GLY	2.3
1	C	360	THR	2.3
1	B	356	GLY	2.3
1	C	259	SER	2.3
1	A	247	HIS	2.3
1	B	372	ASN	2.3
1	A	252	THR	2.3
1	B	245	ILE	2.3
1	A	376	PRO	2.2
1	A	367	GLY	2.2
1	A	18	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	354	LEU	2.1
1	D	0	SER	2.1
1	D	281	ASN	2.1
1	D	252	THR	2.1
1	C	295	VAL	2.1
1	D	18	THR	2.1
1	C	253	ILE	2.1
1	D	365	PRO	2.1
1	C	263	PHE	2.1
1	A	238	TRP	2.1
1	A	0	SER	2.0
1	B	0	SER	2.0
1	B	280	ASP	2.0
1	B	373	ASP	2.0
1	C	370	ILE	2.0
1	C	18	THR	2.0
1	B	234	ALA	2.0
1	D	355	ALA	2.0
1	B	276	ASP	2.0
1	B	294	LEU	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(Å ²)	Q<0.9
4	NA	A	403	1/1	0.89	0.15	68,68,68,68	0
3	FMN	B	402	31/31	0.92	0.09	49,61,66,69	0
3	FMN	D	402	31/31	0.94	0.09	46,57,65,67	0

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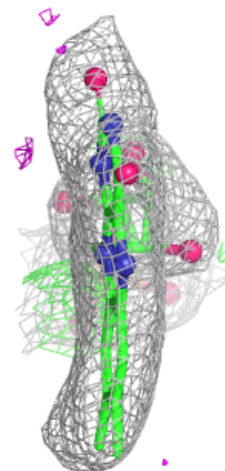
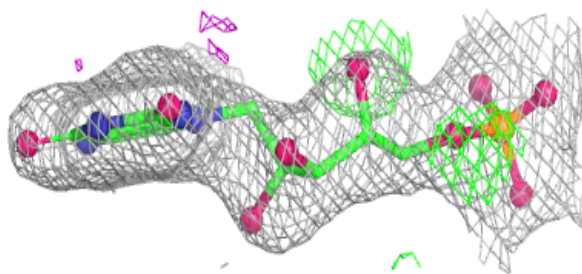
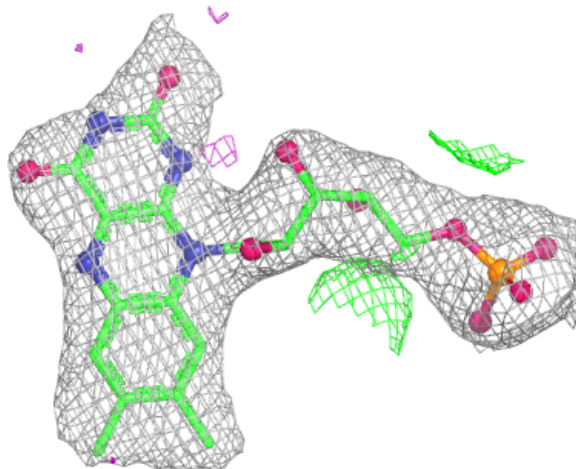
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMN	A	402	31/31	0.94	0.08	43,51,57,59	0
3	FMN	C	402	31/31	0.95	0.07	42,50,58,60	0
2	03S	B	401	5/5	0.96	0.09	44,56,62,67	0
2	03S	D	401	5/5	0.97	0.10	59,59,62,62	0
2	03S	A	401	5/5	0.99	0.05	36,47,54,57	0
2	03S	C	401	5/5	0.99	0.05	38,45,51,52	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.

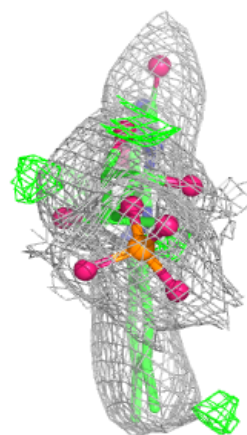
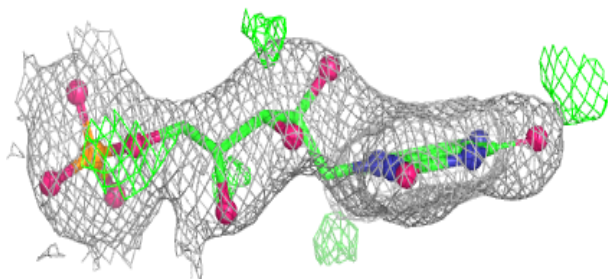
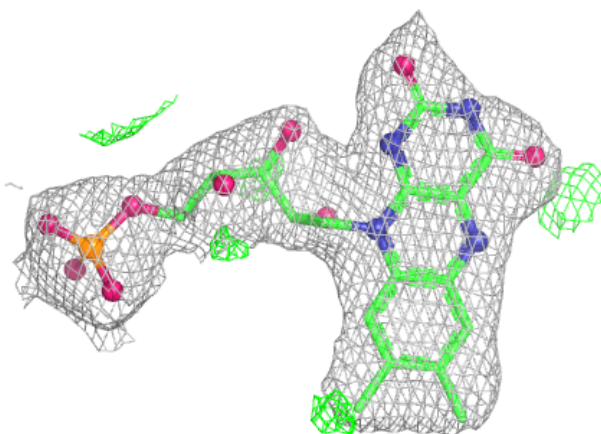
Electron density around FMN B 402:

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



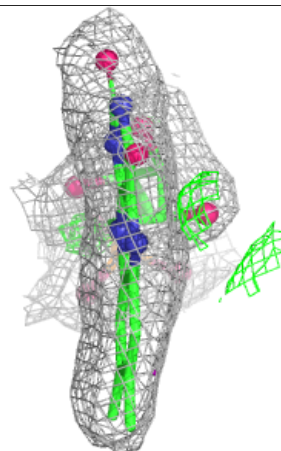
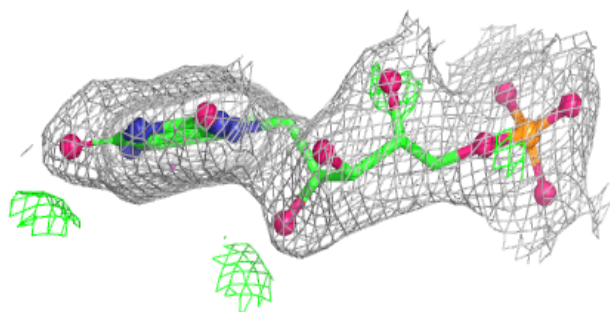
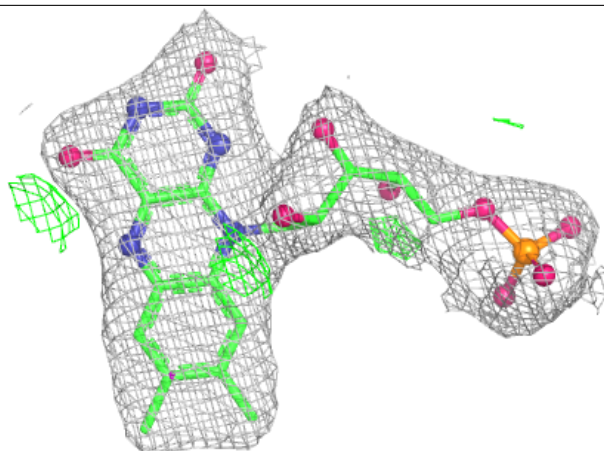
Electron density around FMN D 402:

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



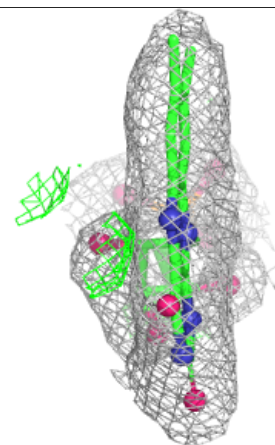
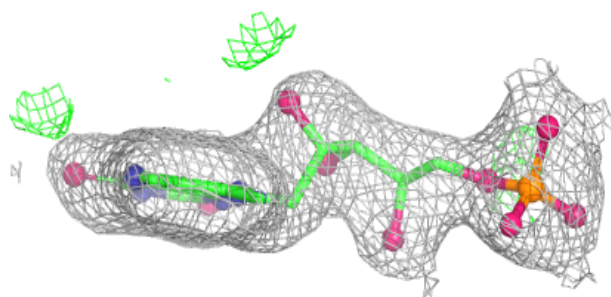
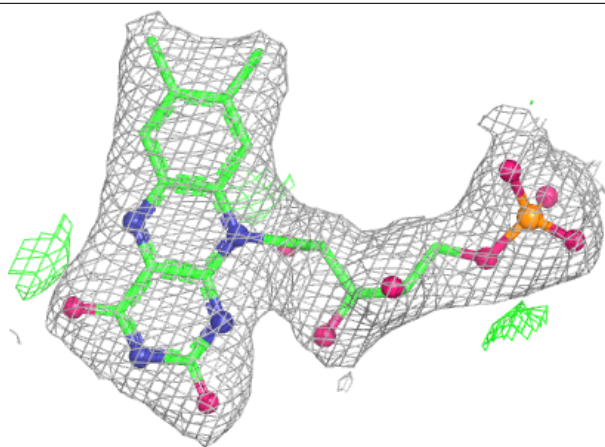
Electron density around FMN A 402:

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



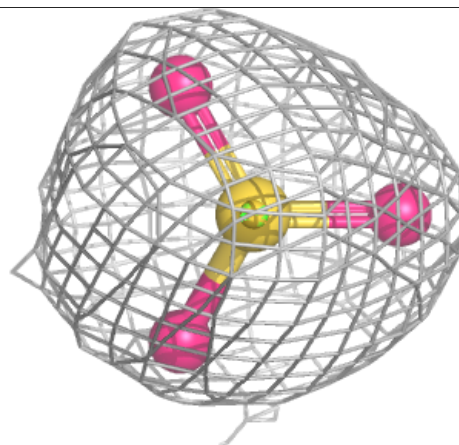
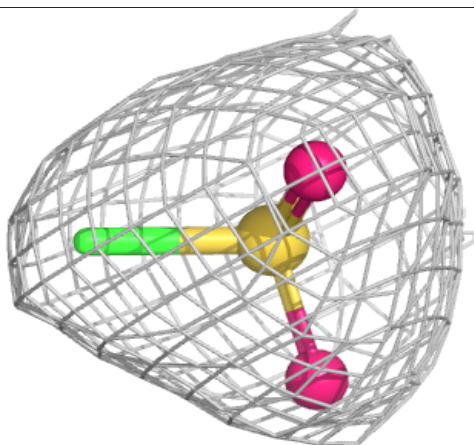
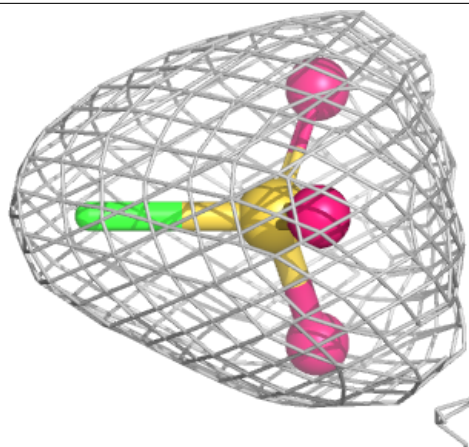
Electron density around FMN C 402:

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



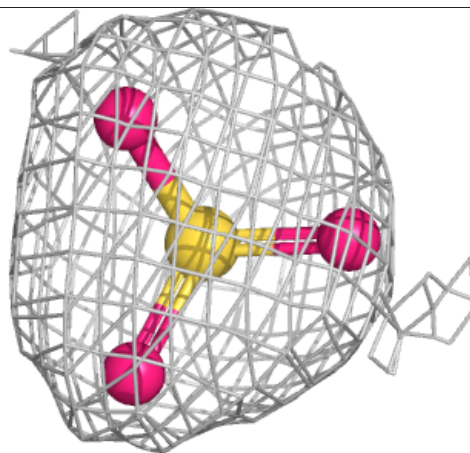
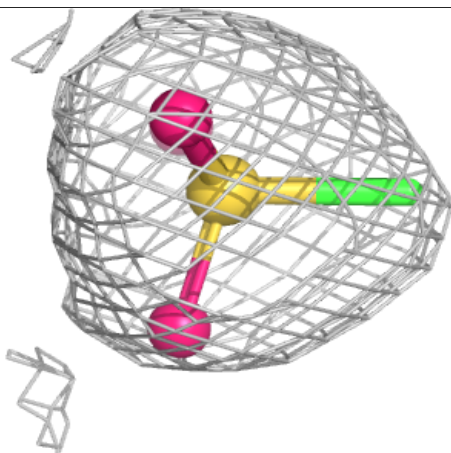
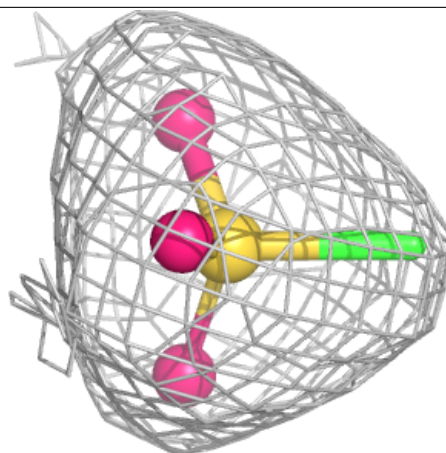
Electron density around 03S B 401:

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



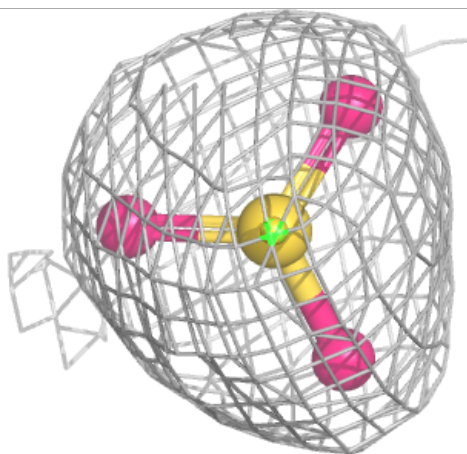
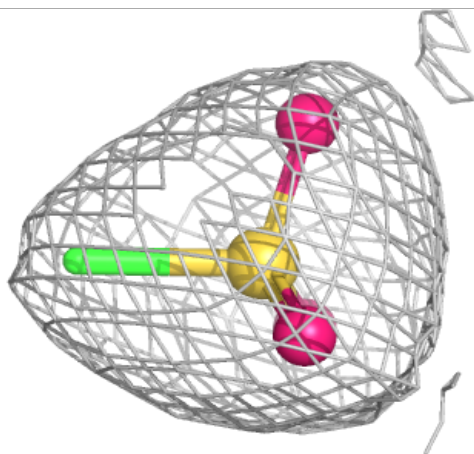
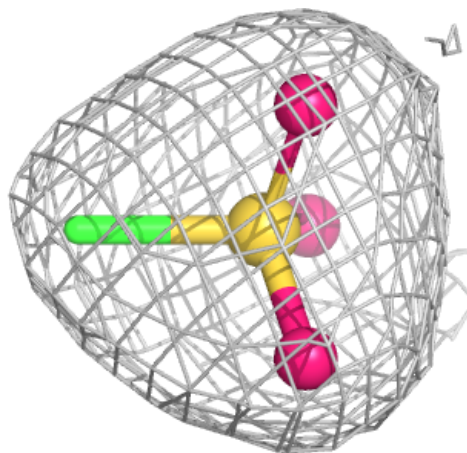
Electron density around 03S D 401:

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



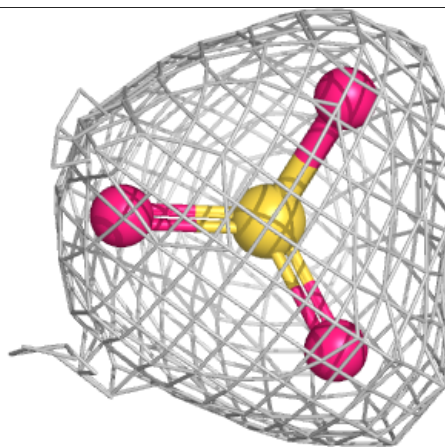
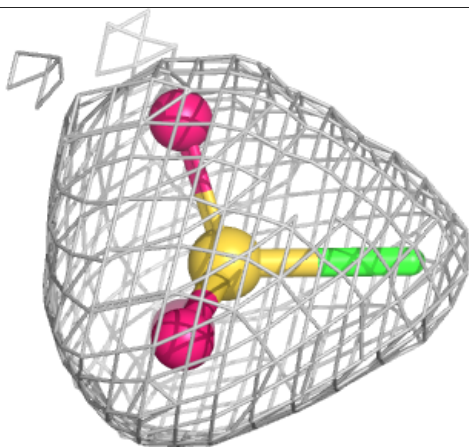
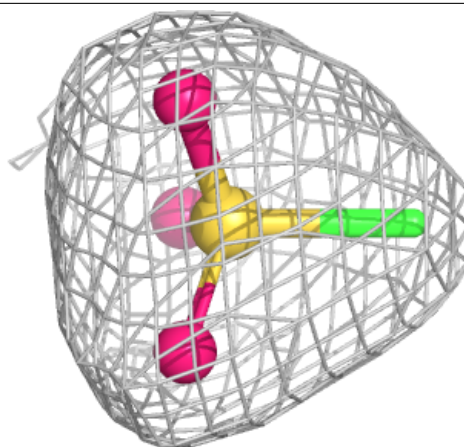
Electron density around 03S A 401:

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



Electron density around 03S 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.