



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:55 PM UTC

PDB ID : 7F21 / pdb_00007f21
Title : L-lactate oxidase with D-lactate
Authors : Morimoto, Y.; Inaka, K.
Deposited on : 2021-06-10
Resolution : 1.38 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

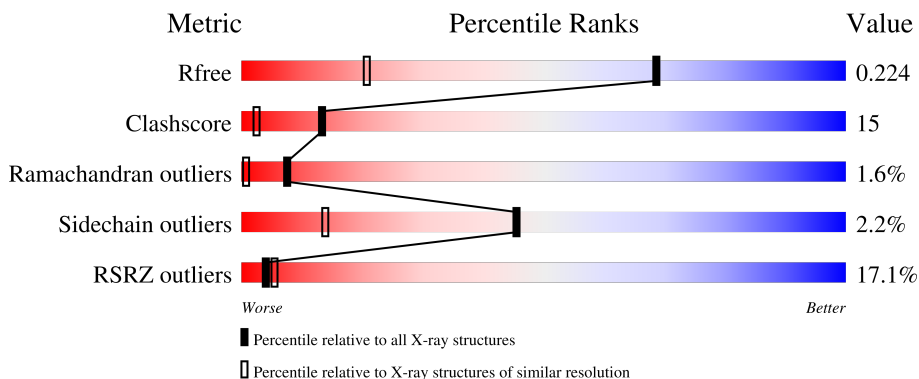
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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	720	
1	B	720	

2 Entry composition [i](#)

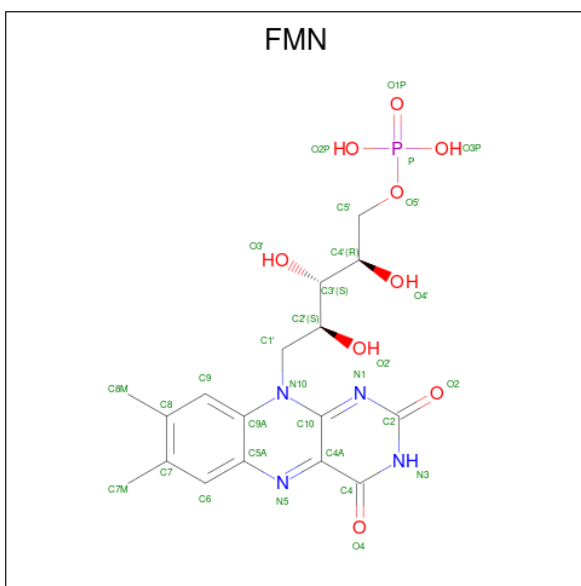
There are 4 unique types of molecules in this entry. The entry contains 6496 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate oxidase.

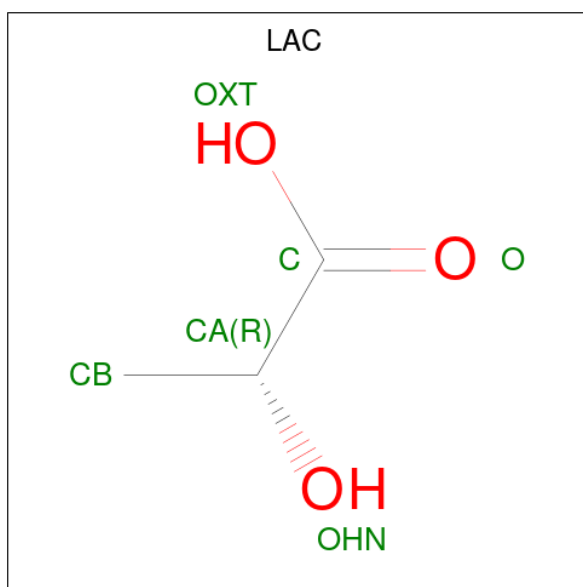
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	368	Total 2841	C 1795	N 494	O 545	S 7	0	0	0
1	B	368	Total 2841	C 1795	N 494	O 545	S 7	0	0	0

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 3 is LACTIC ACID (CCD ID: LAC) (formula: C₃H₆O₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	359	Total O 359 359	0	0
4	B	381	Total O 381 381	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	132.78Å 132.78Å 92.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 1.38 46.99 – 1.38	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.99-1.38) 99.4 (46.99-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.37Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.224 0.196 , 0.224	Depositor DCC
R_{free} test set	8242 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6496	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: LAC, FMN

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	1.14	3/2905 (0.1%)	1.22	4/3937 (0.1%)
1	B	1.20	8/2905 (0.3%)	1.36	17/3937 (0.4%)
All	All	1.17	11/5810 (0.2%)	1.29	21/7874 (0.3%)

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	8

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	GLY	C-O	12.87	1.41	1.23
1	B	333	GLY	C-N	7.55	1.44	1.33
1	B	334	ALA	N-CA	6.93	1.55	1.46
1	A	228	GLU	C-O	6.50	1.31	1.24
1	B	225	ARG	C-O	6.31	1.32	1.24
1	B	67	LEU	C-O	6.07	1.31	1.23
1	A	172	THR	C-O	5.84	1.31	1.24
1	B	223	SER	CA-CB	-5.83	1.46	1.54
1	B	228	GLU	C-O	5.47	1.30	1.24
1	A	145	ILE	C-O	5.35	1.29	1.24
1	B	374	TYR	C-O	5.28	1.34	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	TYR	CA-C-O	-10.78	102.48	120.80
1	B	324	PHE	CB-CA-C	10.02	130.35	110.42
1	A	374	TYR	CA-C-O	-8.67	106.06	120.80
1	B	329	GLY	CA-C-N	8.57	127.48	121.65
1	B	329	GLY	C-N-CA	8.57	127.48	121.65
1	B	333	GLY	O-C-N	8.18	133.34	122.70
1	B	334	ALA	O-C-N	-7.01	113.26	122.59
1	B	334	ALA	N-CA-C	6.98	125.67	110.80
1	B	333	GLY	CA-C-O	-6.67	108.97	120.57
1	A	255	ARG	CB-CG-CD	6.53	126.31	111.30
1	B	333	GLY	CA-C-N	6.47	133.89	121.54
1	B	333	GLY	C-N-CA	6.47	133.89	121.54
1	B	334	ALA	N-CA-CB	-5.75	100.78	110.49
1	B	32	VAL	N-CA-C	-5.74	107.69	113.20
1	B	215	TYR	CA-C-N	5.65	126.21	119.94
1	B	215	TYR	C-N-CA	5.65	126.21	119.94
1	B	296	ASP	CA-C-N	5.62	132.28	121.54
1	B	296	ASP	C-N-CA	5.62	132.28	121.54
1	B	325	GLY	N-CA-C	-5.32	108.35	115.32
1	A	296	ASP	CA-C-N	5.21	131.50	121.54
1	A	296	ASP	C-N-CA	5.21	131.50	121.54

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	28	GLU	Peptide
1	B	30	SER	Peptide
1	B	31	LYS	Peptide
1	B	32	VAL	Peptide
1	B	326	LEU	Peptide
1	B	33	VAL	Peptide
1	B	330	GLY	Peptide
1	B	333	GLY	Peptide

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	2841	0	2772	17	0
1	B	2841	0	2771	151	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
3	A	6	0	0	0	0
3	B	6	0	0	1	0
4	A	359	0	0	5	3
4	B	381	0	0	34	2
All	All	6496	0	5581	168	5

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 15.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:SER:OG	1:B:328:LEU:HA	1.36	1.23
1:B:33:VAL:HG11	1:B:326:LEU:O	1.39	1.22
1:B:28:GLU:C	1:B:327:ALA:O	1.83	1.21
1:B:325:GLY:O	4:B:501:HOH:O	1.54	1.20
1:B:28:GLU:O	1:B:327:ALA:O	1.63	1.17
1:B:334:ALA:HB3	4:B:557:HOH:O	1.46	1.15
1:B:331:TRP:HE3	4:B:504:HOH:O	1.30	1.11
1:A:224:PRO:HB3	1:A:255:ARG:HG3	1.42	1.00
1:B:29:ALA:N	1:B:327:ALA:O	1.93	0.99
1:B:333:GLY:O	4:B:502:HOH:O	1.81	0.96
1:B:331:TRP:CE3	4:B:504:HOH:O	2.09	0.95
1:B:77:SER:HB2	1:B:84:LYS:HE3	1.49	0.92
1:B:314:ASP:OD2	4:B:503:HOH:O	1.88	0.92
1:B:29:ALA:HB3	1:B:327:ALA:N	1.86	0.91
1:B:30:SER:HA	1:B:33:VAL:HB	1.54	0.90
1:B:325:GLY:O	4:B:504:HOH:O	1.89	0.90
1:B:30:SER:OG	1:B:328:LEU:CA	2.18	0.89
1:B:251:MET:O	1:B:255:ARG:HG2	1.72	0.89
1:B:69:GLN:O	4:B:506:HOH:O	1.90	0.89
1:B:30:SER:CA	1:B:328:LEU:O	2.21	0.89
1:B:143:PHE:HE2	1:B:145:ILE:HG22	1.37	0.89
1:B:33:VAL:CG1	1:B:326:LEU:O	2.19	0.88
1:B:29:ALA:O	4:B:505:HOH:O	1.90	0.88
1:B:30:SER:O	1:B:328:LEU:O	1.93	0.87
1:B:224:PRO:HB3	1:B:255:ARG:HG3	1.55	0.87
1:B:143:PHE:CE2	1:B:145:ILE:HG22	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:SER:N	1:B:328:LEU:O	2.09	0.85
1:B:324:PHE:O	1:B:332:GLN:C	2.20	0.84
1:B:201:TYR:CZ	1:B:217:ALA:O	2.30	0.84
1:B:33:VAL:HG11	1:B:326:LEU:C	2.01	0.83
1:B:331:TRP:HH2	4:B:743:HOH:O	1.62	0.83
1:B:373:GLU:OE2	4:B:507:HOH:O	1.97	0.82
1:B:28:GLU:HB3	1:B:330:GLY:O	1.80	0.81
1:B:333:GLY:N	4:B:508:HOH:O	2.00	0.81
1:B:29:ALA:HA	1:B:330:GLY:C	2.06	0.81
1:B:11:PRO:HG3	1:B:33:VAL:HG22	1.62	0.80
1:B:27:GLU:O	1:B:329:GLY:N	2.14	0.80
1:B:333:GLY:C	4:B:508:HOH:O	2.25	0.79
1:B:202:LEU:O	1:B:204:GLY:N	2.17	0.78
1:B:26:GLU:O	1:B:327:ALA:HB1	1.82	0.77
1:B:150:ASP:OD2	4:B:509:HOH:O	2.03	0.77
1:B:30:SER:CA	1:B:33:VAL:HB	2.16	0.75
1:B:30:SER:HA	1:B:33:VAL:CB	2.17	0.74
1:A:251:MET:O	1:A:255:ARG:HG2	1.87	0.74
1:B:30:SER:HG	1:B:328:LEU:HA	1.53	0.73
1:B:146:TYR:O	4:B:510:HOH:O	2.06	0.73
1:B:33:VAL:CG2	4:B:505:HOH:O	2.36	0.73
1:B:156:ASP:OD2	1:B:200:ARG:NE	2.22	0.72
1:B:333:GLY:O	4:B:508:HOH:O	2.07	0.72
1:B:29:ALA:HB3	1:B:326:LEU:C	2.16	0.71
1:B:29:ALA:HB3	1:B:327:ALA:O	1.91	0.71
1:B:324:PHE:CD1	1:B:327:ALA:HB2	2.25	0.70
1:B:15:LYS:HG2	1:B:331:TRP:CZ2	2.25	0.70
1:B:27:GLU:O	1:B:328:LEU:HB3	1.92	0.70
1:B:33:VAL:HG21	4:B:505:HOH:O	1.92	0.70
1:B:331:TRP:CH2	4:B:743:HOH:O	2.40	0.69
1:B:30:SER:OG	1:B:328:LEU:O	2.11	0.68
1:B:30:SER:C	1:B:328:LEU:O	2.36	0.68
1:B:324:PHE:O	1:B:332:GLN:O	2.11	0.68
1:B:328:LEU:HD22	4:B:801:HOH:O	1.93	0.67
1:B:147:MET:CE	1:B:154:ASN:ND2	2.57	0.67
1:B:17:ILE:HD12	1:B:332:GLN:HB3	1.76	0.66
1:B:27:GLU:O	1:B:328:LEU:CB	2.43	0.66
1:B:41:ILE:HD12	1:B:326:LEU:HD22	1.78	0.64
1:B:33:VAL:HG12	1:B:326:LEU:HD12	1.80	0.64
1:B:226:ASP:O	1:B:230:ILE:HG12	1.97	0.64
1:B:29:ALA:CB	1:B:327:ALA:O	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ALA:HB3	1:B:327:ALA:C	2.22	0.64
1:B:29:ALA:CB	1:B:331:TRP:HA	2.28	0.64
1:B:33:VAL:HG11	1:B:326:LEU:CA	2.29	0.63
1:B:29:ALA:CB	1:B:326:LEU:C	2.73	0.61
1:B:29:ALA:H	1:B:329:GLY:N	1.98	0.61
1:B:325:GLY:C	4:B:504:HOH:O	2.38	0.61
1:B:29:ALA:H	1:B:329:GLY:C	2.08	0.61
1:B:30:SER:HG	1:B:328:LEU:C	2.08	0.61
1:B:29:ALA:CB	1:B:327:ALA:N	2.61	0.61
1:B:201:TYR:OH	1:B:217:ALA:O	2.19	0.61
1:B:29:ALA:CA	1:B:327:ALA:O	2.49	0.60
1:B:147:MET:HG3	1:B:171:LEU:HD11	1.83	0.59
1:B:30:SER:CB	1:B:328:LEU:O	2.51	0.58
1:B:153:GLN:NE2	1:B:200:ARG:HB3	2.19	0.57
1:B:38:PHE:CD1	1:B:327:ALA:HA	2.39	0.57
1:B:29:ALA:HB3	1:B:327:ALA:CA	2.35	0.57
1:A:202:LEU:O	1:A:203:ARG:O	2.23	0.57
1:B:29:ALA:HB2	1:B:331:TRP:HA	1.88	0.56
1:B:129:PHE:CE1	1:B:164:ASP:HB3	2.41	0.56
1:B:147:MET:SD	1:B:226:ASP:HB3	2.46	0.56
1:B:331:TRP:HZ3	4:B:508:HOH:O	1.89	0.56
1:B:147:MET:HE3	1:B:154:ASN:ND2	2.21	0.55
1:B:33:VAL:CG1	1:B:326:LEU:HD12	2.37	0.55
1:B:150:ASP:HB3	4:B:789:HOH:O	2.07	0.55
1:B:30:SER:OG	1:B:328:LEU:C	2.50	0.54
1:A:28:GLU:HG2	4:A:829:HOH:O	2.07	0.54
1:B:203:ARG:HD3	4:B:572:HOH:O	2.08	0.54
1:B:100:ALA:HA	1:B:326:LEU:CB	2.39	0.53
1:B:153:GLN:HE22	1:B:200:ARG:HB3	1.72	0.53
1:B:143:PHE:CE2	1:B:145:ILE:CG2	2.89	0.53
1:B:30:SER:HA	1:B:33:VAL:CG2	2.37	0.53
1:B:331:TRP:HB2	4:B:501:HOH:O	2.08	0.52
1:B:175:SER:HB3	1:B:215:TYR:HE1	1.74	0.52
1:B:41:ILE:CD1	1:B:326:LEU:HD22	2.40	0.51
1:B:331:TRP:O	1:B:332:GLN:HG2	2.11	0.51
1:B:29:ALA:N	1:B:330:GLY:N	2.59	0.51
1:B:94:ILE:HG21	1:B:323:LEU:HD11	1.93	0.50
1:B:100:ALA:HA	1:B:326:LEU:HB3	1.93	0.50
1:B:33:VAL:CB	1:B:326:LEU:O	2.60	0.50
1:B:324:PHE:O	1:B:333:GLY:N	2.45	0.49
1:A:66:ARG:C	1:A:67:LEU:HD23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:SER:HB3	1:B:215:TYR:CE1	2.47	0.48
1:B:331:TRP:O	1:B:332:GLN:CG	2.61	0.48
1:A:175:SER:HB3	1:A:215:TYR:CZ	2.48	0.48
1:B:33:VAL:CG1	1:B:326:LEU:CG	2.92	0.48
1:A:66:ARG:NH2	4:A:512:HOH:O	2.43	0.47
1:B:251:MET:HG2	1:B:255:ARG:HE	1.79	0.47
1:B:176:THR:HB	1:B:220:GLN:HA	1.97	0.47
1:B:149:LYS:N	1:B:201:TYR:OH	2.44	0.47
1:B:29:ALA:H	1:B:330:GLY:N	2.12	0.47
1:B:30:SER:HG	1:B:328:LEU:CA	2.17	0.47
1:B:33:VAL:HG11	1:B:326:LEU:CB	2.44	0.47
1:B:33:VAL:CG1	1:B:326:LEU:HG	2.45	0.46
1:B:38:PHE:CE2	1:B:328:LEU:HD13	2.50	0.46
1:A:225:ARG:NH1	4:A:517:HOH:O	2.48	0.46
1:B:33:VAL:HG12	1:B:326:LEU:CD1	2.44	0.46
1:A:199:GLN:NE2	4:A:513:HOH:O	2.44	0.46
1:B:33:VAL:HG11	1:B:326:LEU:HG	1.96	0.46
1:B:30:SER:N	1:B:328:LEU:C	2.72	0.46
1:B:33:VAL:HA	1:B:34:PRO:HD3	1.71	0.46
1:A:73:ALA:N	4:A:503:HOH:O	2.31	0.46
1:B:38:PHE:HE1	1:B:327:ALA:HB1	1.81	0.46
1:B:29:ALA:H	1:B:329:GLY:CA	2.29	0.45
1:B:147:MET:HG3	1:B:171:LEU:CD1	2.46	0.45
1:B:224:PRO:HB3	1:B:255:ARG:CG	2.38	0.45
1:A:251:MET:HG2	1:A:255:ARG:HE	1.81	0.45
1:B:25:LEU:O	1:B:327:ALA:HB3	2.16	0.45
1:A:124:TYR:CZ	1:A:214:ILE:HG22	2.52	0.45
1:A:89:PHE:HA	1:A:316:VAL:O	2.17	0.45
1:A:273:ALA:HB1	1:A:274:PRO:HD2	1.99	0.44
1:B:29:ALA:HA	1:B:331:TRP:N	2.32	0.44
1:B:29:ALA:N	1:B:329:GLY:N	2.65	0.44
1:B:162:LYS:NZ	4:B:532:HOH:O	2.51	0.44
1:B:331:TRP:C	1:B:332:GLN:CG	2.91	0.44
1:B:17:ILE:HG12	1:B:336:SER:HB2	1.99	0.43
1:B:30:SER:HB3	1:B:33:VAL:O	2.17	0.43
1:B:334:ALA:CA	4:B:557:HOH:O	2.64	0.43
1:B:156:ASP:OD2	1:B:200:ARG:CZ	2.66	0.43
1:B:325:GLY:CA	4:B:502:HOH:O	2.66	0.43
1:B:181:ARG:HH22	3:B:402:LAC:C	2.31	0.42
1:B:201:TYR:CE1	1:B:217:ALA:O	2.73	0.42
1:B:31:LYS:HA	1:B:31:LYS:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:PHE:HA	1:B:316:VAL:O	2.20	0.42
1:B:124:TYR:O	1:B:195:MET:HE2	2.20	0.42
1:B:325:GLY:HA2	4:B:502:HOH:O	2.19	0.42
1:B:41:ILE:HD12	1:B:326:LEU:CD2	2.47	0.42
1:B:328:LEU:HA	1:B:328:LEU:HD12	1.91	0.41
1:B:29:ALA:HA	1:B:330:GLY:CA	2.49	0.41
1:A:296:ASP:OD1	1:A:296:ASP:C	2.64	0.41
1:B:296:ASP:OD1	1:B:296:ASP:C	2.64	0.41
1:A:202:LEU:O	1:A:203:ARG:C	2.64	0.41
1:B:178:SER:HB2	1:B:215:TYR:CD2	2.56	0.41
1:A:241:LYS:HA	1:A:261:TRP:HB3	2.03	0.41
1:B:33:VAL:HG11	1:B:326:LEU:CG	2.51	0.41
1:B:201:TYR:CD1	4:B:789:HOH:O	2.73	0.41
1:B:22:THR:HB	1:B:321:PRO:HB3	2.03	0.40
1:B:289:LYS:NZ	4:B:523:HOH:O	2.42	0.40
1:B:363:LEU:HD22	4:B:613:HOH:O	2.21	0.40
1:B:334:ALA:CB	4:B:557:HOH:O	2.29	0.40
1:B:334:ALA:CB	4:B:756:HOH:O	2.69	0.40
1:B:195:MET:HB3	1:B:198:VAL:HG22	2.03	0.40

All (5) 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)
4:A:840:HOH:O	4:A:840:HOH:O[3_655]	1.62	0.58
4:B:833:HOH:O	4:B:833:HOH:O[3_655]	1.91	0.29
4:A:687:HOH:O	4:A:687:HOH:O[3_655]	1.95	0.25
4:A:760:HOH:O	4:A:760:HOH:O[3_655]	1.99	0.21
4:B:633:HOH:O	4:B:633:HOH:O[3_655]	2.04	0.16

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	366/720 (51%)	355 (97%)	9 (2%)	2 (0%)	24 7
1	B	366/720 (51%)	341 (93%)	15 (4%)	10 (3%)	4 0
All	All	732/1440 (51%)	696 (95%)	24 (3%)	12 (2%)	7 1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ARG
1	A	297	SER
1	B	29	ALA
1	B	200	ARG
1	B	203	ARG
1	B	297	SER
1	B	324	PHE
1	B	328	LEU
1	B	334	ALA
1	B	211	LEU
1	B	30	SER
1	B	147	MET

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	292/569 (51%)	288 (99%)	4 (1%)	59 27
1	B	292/569 (51%)	283 (97%)	9 (3%)	35 7
All	All	584/1138 (51%)	571 (98%)	13 (2%)	45 14

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

Mol	Chain	Res	Type
1	A	67	LEU
1	A	203	ARG
1	A	205	THR
1	A	255	ARG

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Mol	Chain	Res	Type
1	B	153	GLN
1	B	160	GLU
1	B	188	LYS
1	B	213	ASN
1	B	224	PRO
1	B	225	ARG
1	B	326	LEU
1	B	328	LEU
1	B	331	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	HIS
1	B	153	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	A	401	-	33,33,33	0.78	0	48,50,50	0.76	1 (2%)
3	LAC	A	402	-	4,5,5	1.27	0	2,6,6	0.51	0
3	LAC	B	402	-	4,5,5	0.87	0	2,6,6	0.43	0
2	FMN	B	401	-	33,33,33	0.98	2 (6%)	48,50,50	0.74	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
2	FMN	A	401	-	-	2/18/18/18	0/3/3/3
3	LAC	A	402	-	-	2/4/4/4	-
3	LAC	B	402	-	-	0/4/4/4	-
2	FMN	B	401	-	-	1/18/18/18	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FMN	C1'-C2'	2.56	1.56	1.52
2	B	401	FMN	C4A-N5	2.13	1.35	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FMN	O3P-P-O2P	2.10	115.68	107.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

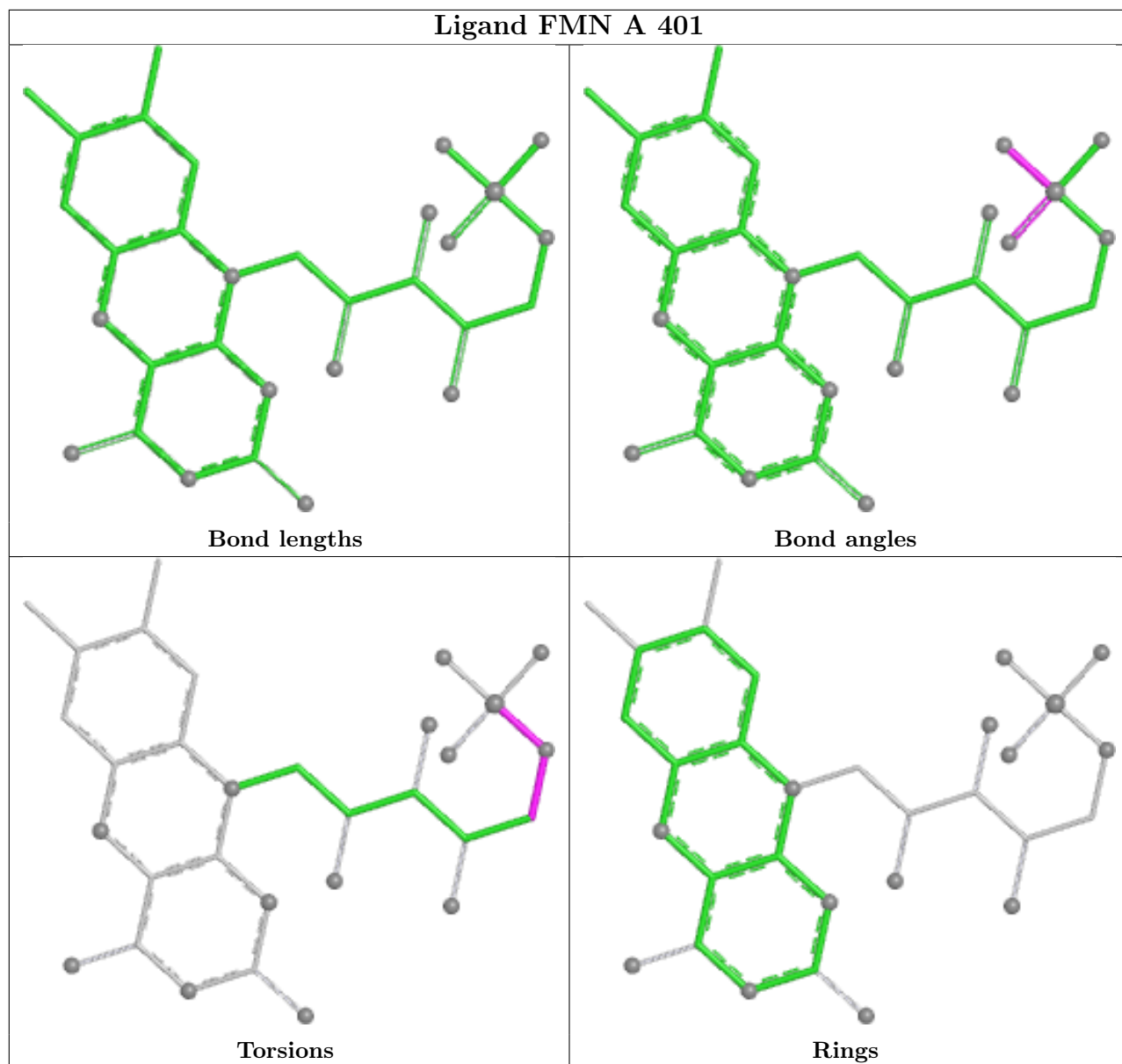
Mol	Chain	Res	Type	Atoms
3	A	402	LAC	OXT-C-CA-CB
2	A	401	FMN	C4'-C5'-O5'-P
2	B	401	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C5'-O5'-P-O1P
3	A	402	LAC	O-C-CA-CB

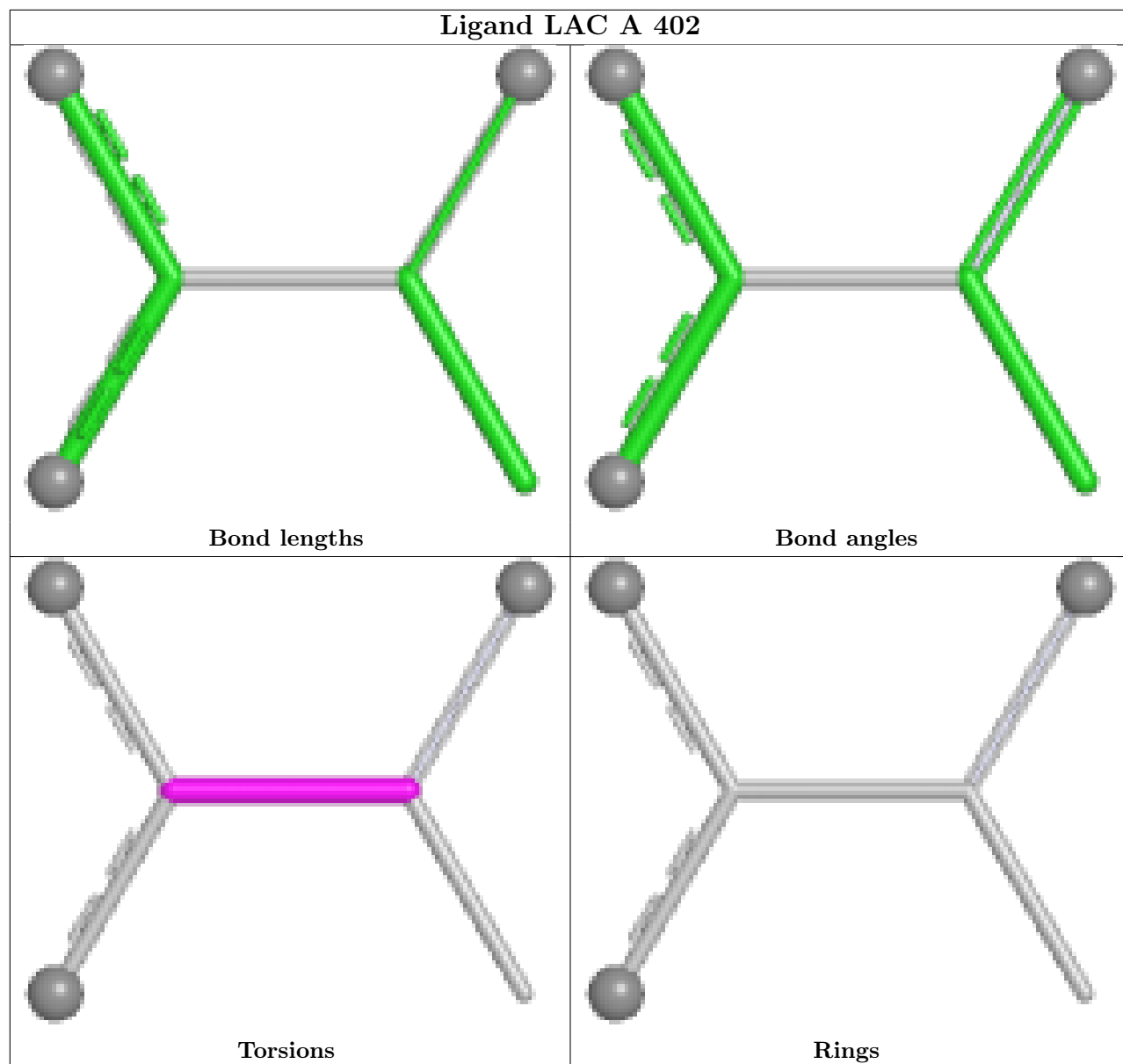
There are no ring outliers.

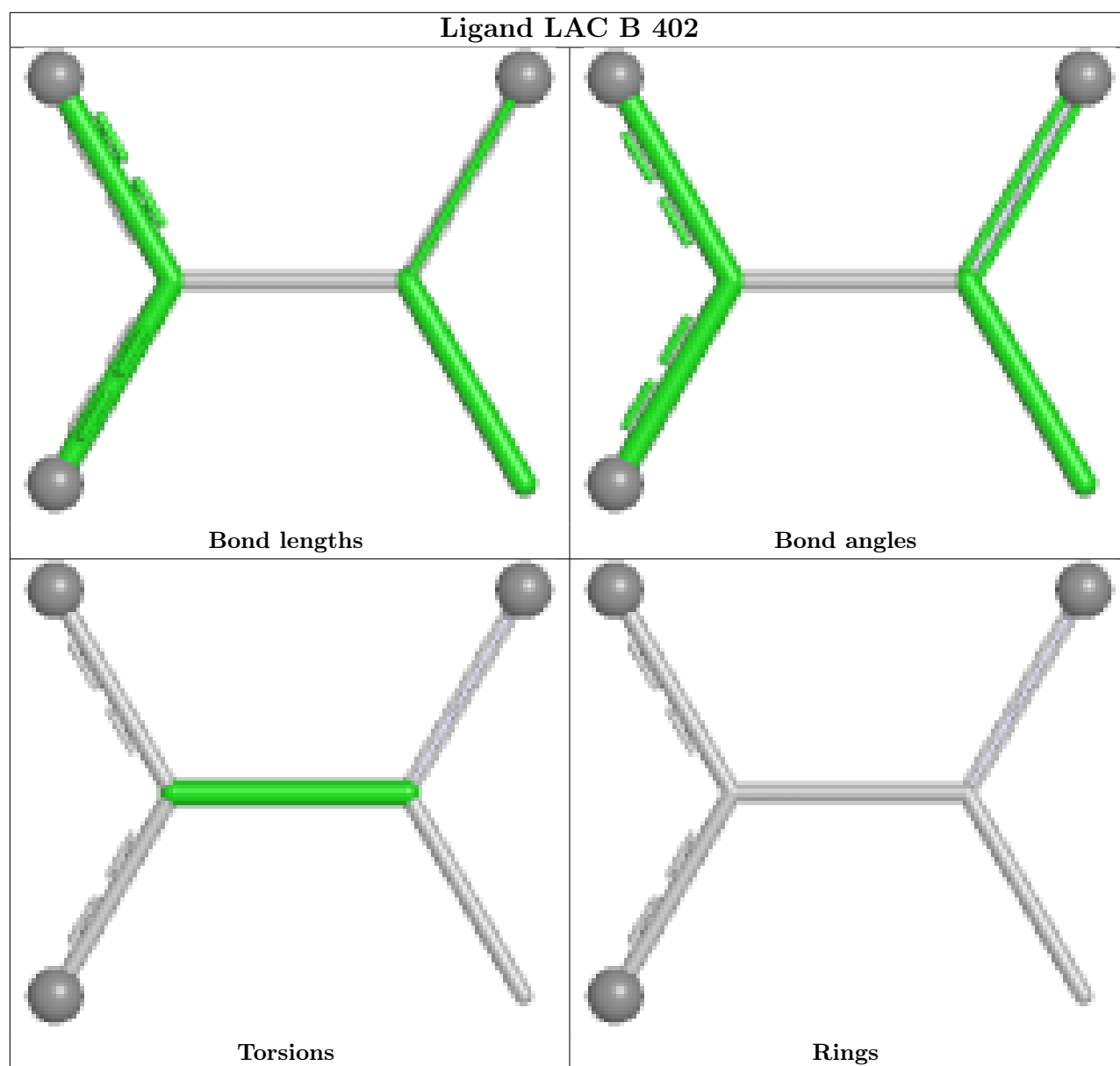
1 monomer is involved in 1 short contact:

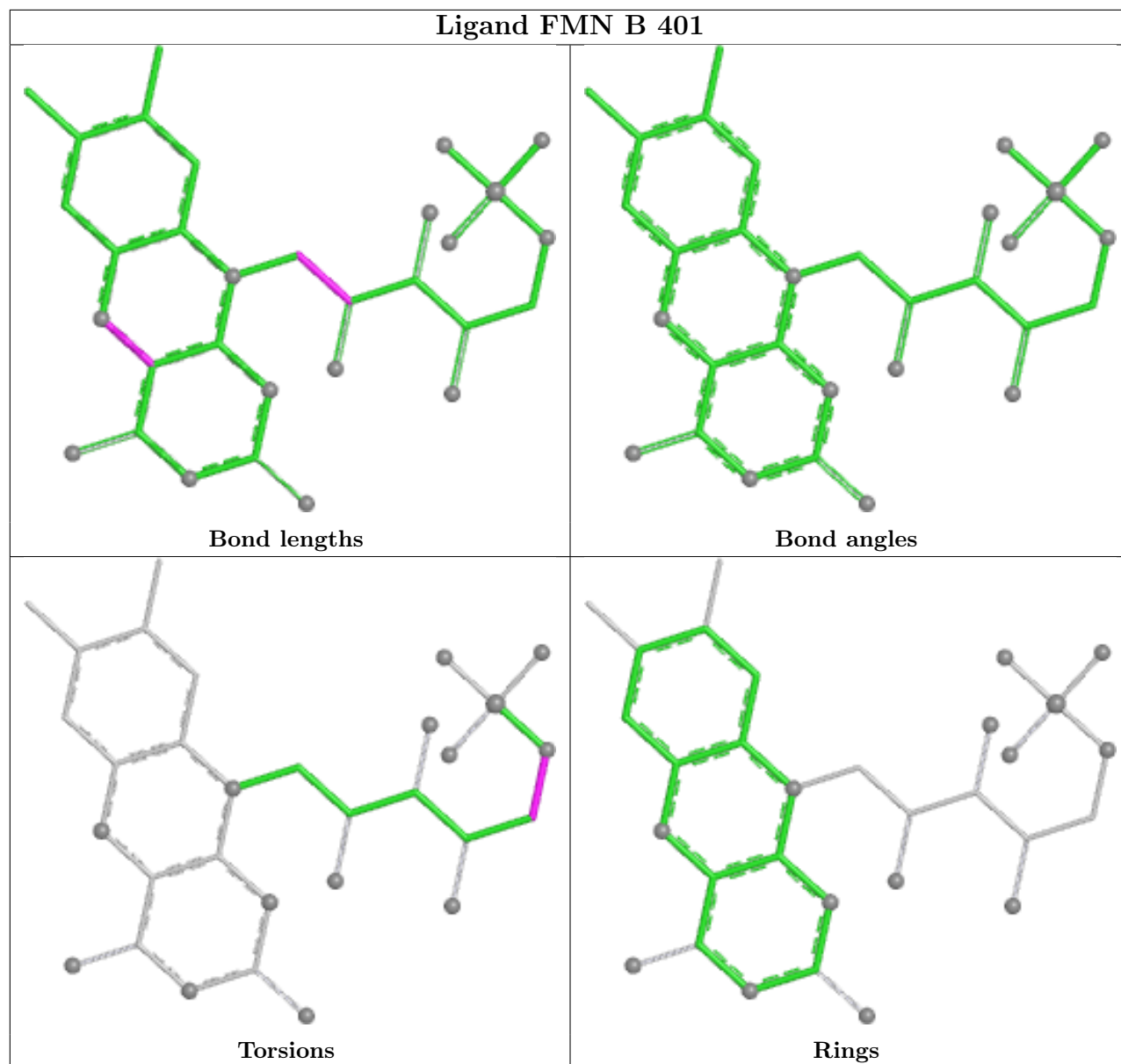
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	LAC	1	0

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	368/720 (51%)	0.62	40 (10%) 10 13	11, 18, 34, 85	0
1	B	368/720 (51%)	1.63	86 (23%) 2 2	11, 19, 84, 170	0
All	All	736/1440 (51%)	1.13	126 (17%) 4 5	11, 19, 48, 170	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	LEU	24.8
1	B	331	TRP	19.8
1	B	211	LEU	16.8
1	B	29	ALA	16.3
1	B	32	VAL	16.1
1	B	327	ALA	15.4
1	B	201	TYR	14.5
1	B	330	GLY	14.0
1	B	202	LEU	13.4
1	B	329	GLY	13.3
1	B	332	GLN	11.7
1	B	33	VAL	11.2
1	B	214	ILE	10.4
1	B	328	LEU	10.0
1	B	206	ALA	9.1
1	B	215	TYR	8.8
1	B	333	GLY	8.1
1	B	30	SER	8.0
1	B	210	SER	7.9
1	B	31	LYS	7.8
1	B	205	THR	7.5
1	B	216	GLY	7.2
1	B	209	MET	7.1
1	B	334	ALA	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	325	GLY	6.7
1	B	200	ARG	6.4
1	B	232	ALA	5.9
1	B	129	PHE	5.8
1	A	203	ARG	5.7
1	B	208	GLY	5.7
1	B	199	GLN	5.6
1	B	198	VAL	5.5
1	B	217	ALA	5.5
1	B	204	GLY	5.3
1	A	205	THR	5.1
1	B	67	LEU	4.9
1	B	203	ARG	4.8
1	B	212	ASN	4.7
1	A	204	GLY	4.6
1	B	197	ILE	4.4
1	B	148	ALA	4.2
1	B	207	GLU	4.1
1	B	255	ARG	4.0
1	A	215	TYR	4.0
1	A	232	ALA	3.9
1	B	224	PRO	3.9
1	B	213	ASN	3.9
1	B	231	ALA	3.9
1	A	82	GLY	3.9
1	B	230	ILE	3.8
1	B	185	VAL	3.8
1	B	218	SER	3.7
1	A	67	LEU	3.6
1	B	18	ASP	3.6
1	A	201	TYR	3.5
1	B	82	GLY	3.4
1	B	7	GLU	3.4
1	B	191	TYR	3.4
1	A	216	GLY	3.3
1	B	157	ILE	3.3
1	B	222	ILE	3.3
1	A	199	GLN	3.3
1	B	153	GLN	3.3
1	A	255	ARG	3.2
1	A	158	LEU	3.1
1	B	190	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	164	ASP	3.1
1	B	225	ARG	3.0
1	B	220	GLN	3.0
1	B	227	ILE	2.9
1	B	195	MET	2.9
1	B	73	ALA	2.9
1	B	228	GLU	2.8
1	A	230	ILE	2.8
1	A	163	SER	2.8
1	B	189	PHE	2.8
1	B	147	MET	2.7
1	A	189	PHE	2.7
1	A	212	ASN	2.7
1	A	157	ILE	2.7
1	B	193	PHE	2.7
1	B	68	ALA	2.7
1	A	222	ILE	2.7
1	A	137	ASN	2.6
1	A	129	PHE	2.6
1	A	148	ALA	2.6
1	A	7	GLU	2.6
1	B	143	PHE	2.5
1	B	81	LEU	2.5
1	B	176	THR	2.4
1	A	198	VAL	2.4
1	B	234	SER	2.4
1	B	146	TYR	2.3
1	B	156	ASP	2.3
1	A	202	LEU	2.3
1	B	323	LEU	2.3
1	B	188	LYS	2.3
1	A	73	ALA	2.3
1	A	231	ALA	2.3
1	B	71	VAL	2.3
1	A	225	ARG	2.2
1	B	158	LEU	2.2
1	A	214	ILE	2.2
1	B	17	ILE	2.2
1	A	213	ASN	2.2
1	A	147	MET	2.2
1	A	143	PHE	2.2
1	A	227	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	177	VAL	2.2
1	B	226	ASP	2.2
1	B	72	GLU	2.2
1	B	235	GLY	2.1
1	B	163	SER	2.1
1	A	9	ASN	2.1
1	A	166	ALA	2.1
1	A	191	TYR	2.1
1	A	224	PRO	2.1
1	B	223	SER	2.1
1	B	161	ALA	2.1
1	B	251	MET	2.1
1	A	20	VAL	2.1
1	B	134	GLU	2.0
1	A	18	ASP	2.0
1	A	83	HIS	2.0
1	B	160	GLU	2.0
1	A	208	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

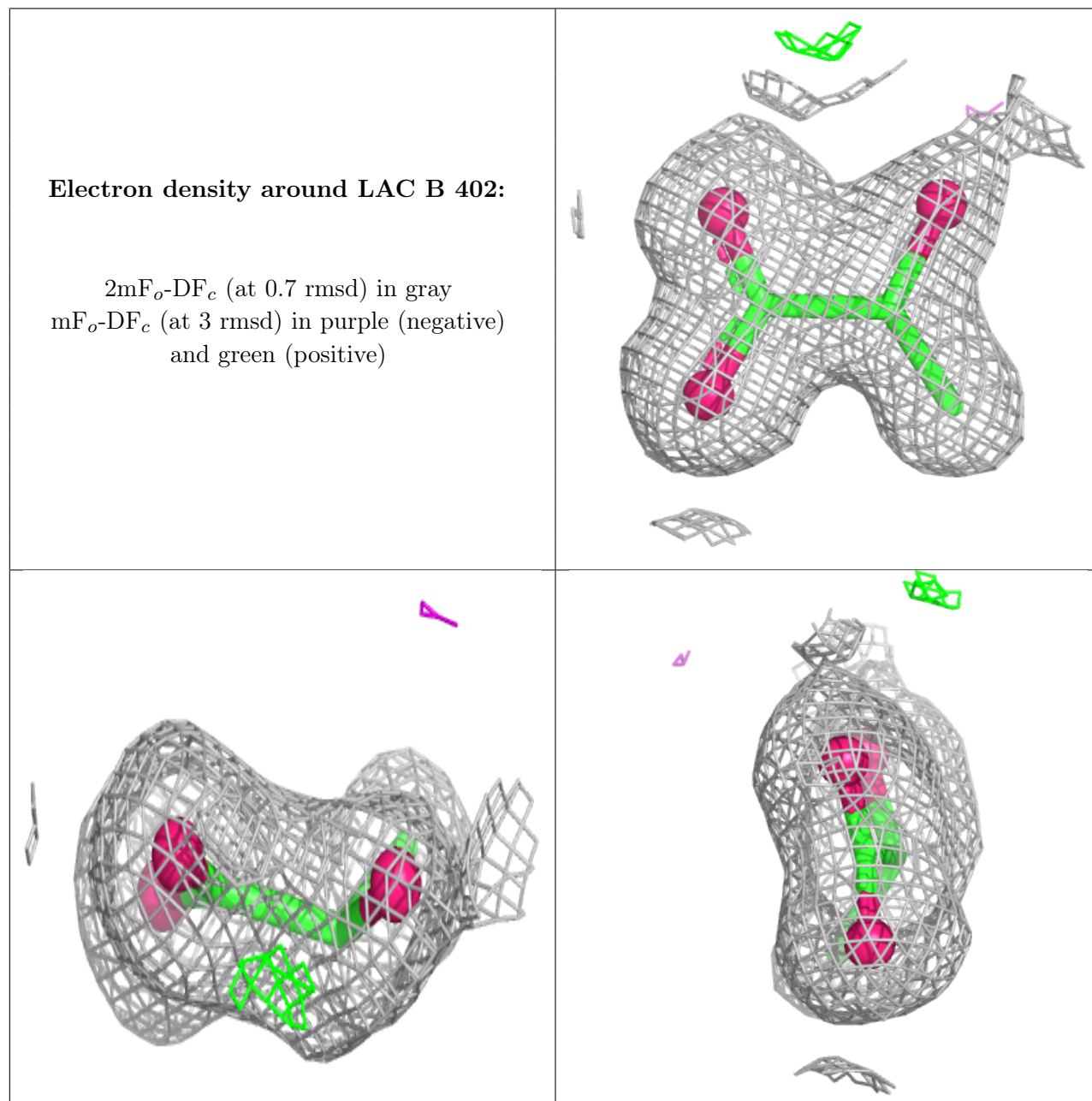
There are no oligosaccharides in this entry.

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.

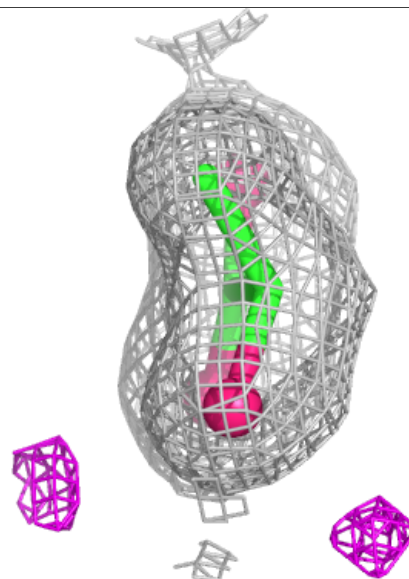
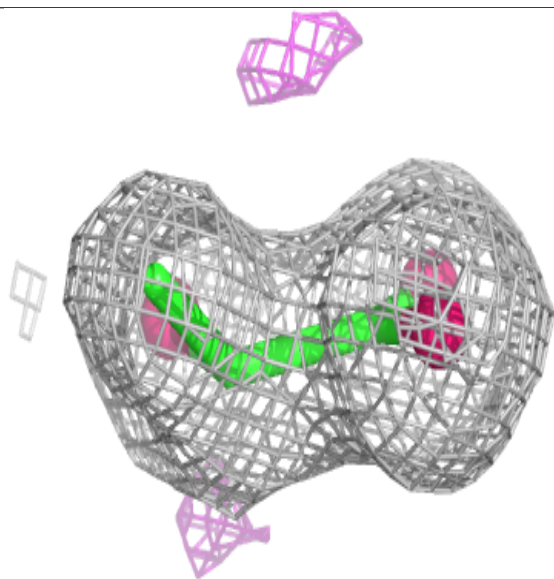
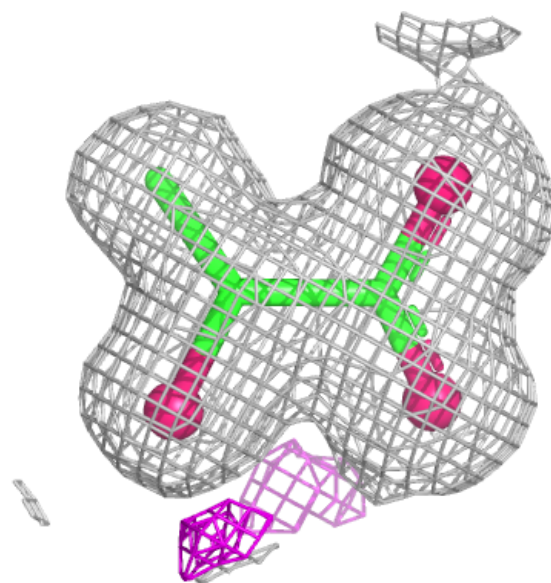
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LAC	B	402	6/6	0.95	0.08	24,27,29,36	0
3	LAC	A	402	6/6	0.97	0.06	21,22,23,24	0
2	FMN	A	401	31/31	0.98	0.04	12,14,16,16	0
2	FMN	B	401	31/31	0.98	0.06	12,14,17,18	0

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.



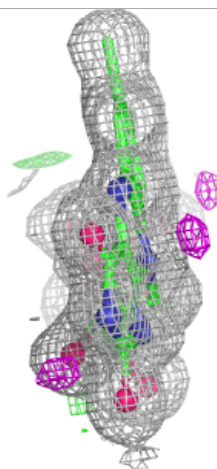
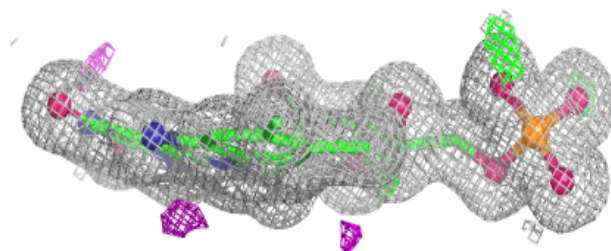
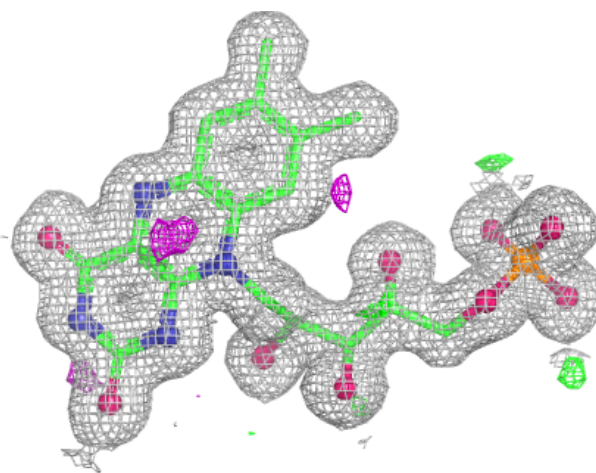
Electron density around LAC A 402:

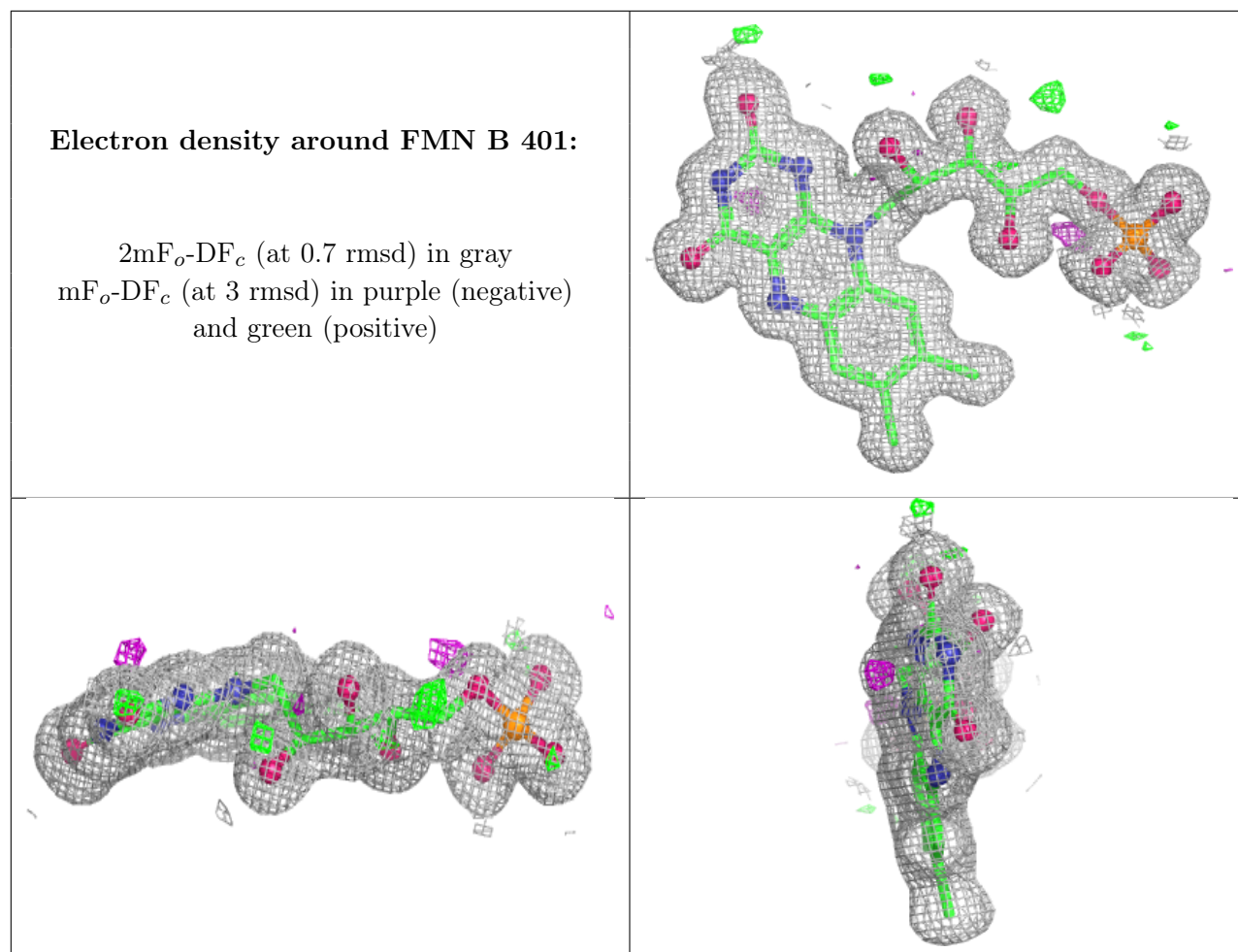
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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.