



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2022 – 06:21 PM JST

PDB ID : 7F21  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

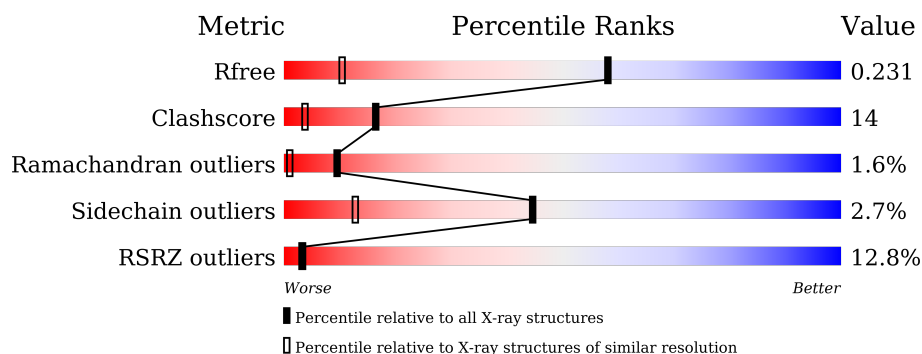
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (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  $\geq 3$ , 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	<div> <div>4%</div> <div>47%</div> <div>.</div> <div>49%</div> </div>
1	B	720	<div> <div>9%</div> <div>40%</div> <div>8%</div> <div>..</div> <div>49%</div> </div>

## 2 Entry composition [i](#)

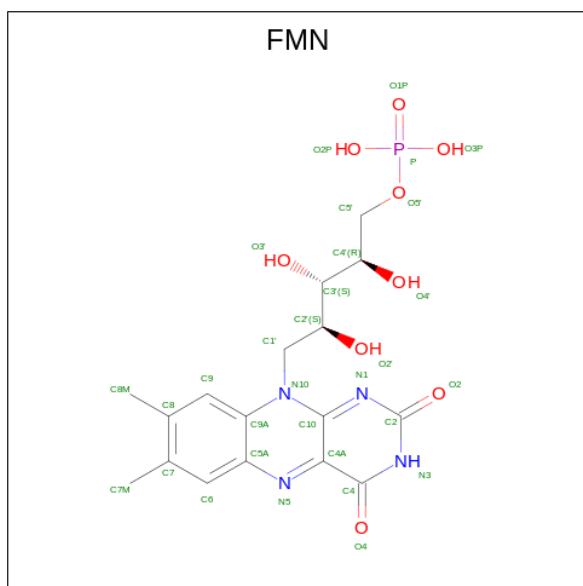
There are 4 unique types of molecules in this entry. The entry contains 6496 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

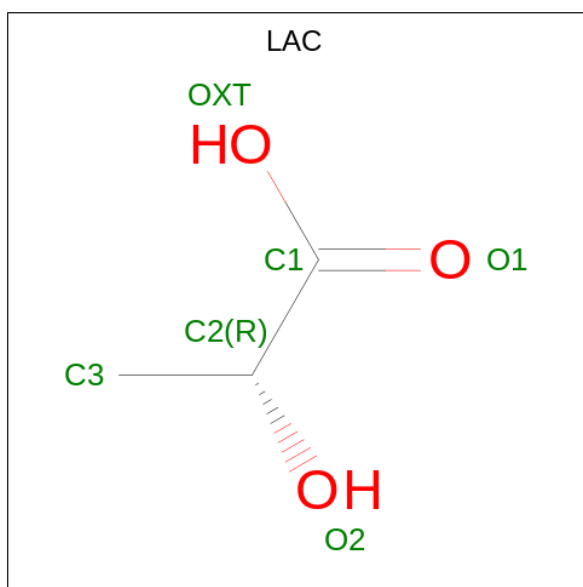
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2841	1795	494	545	7			
1	B	368	Total	C	N	O	S	0	0	0
			2841	1795	494	545	7			

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



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

- Molecule 3 is LACTIC ACID (three-letter code: LAC) (formula:  $C_3H_6O_3$ ) (labeled as "Ligand of Interest" by depositor).



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

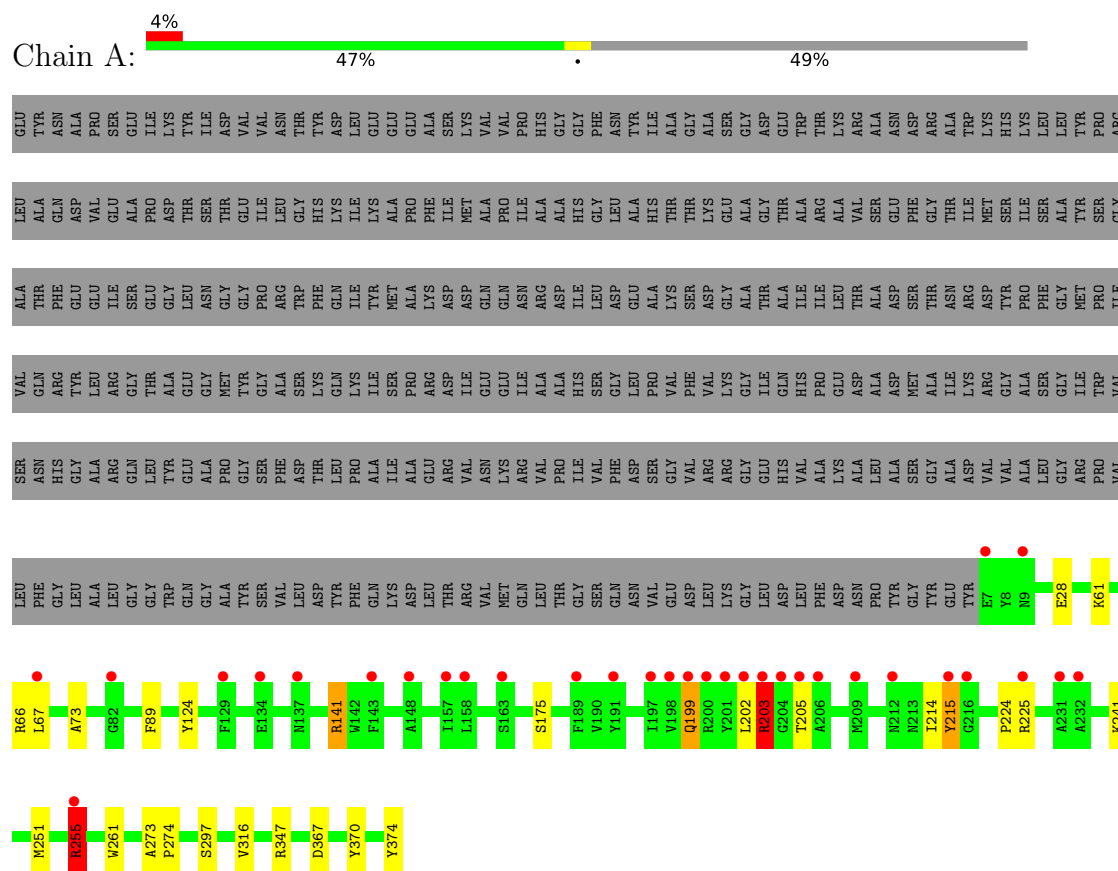
- Molecule 4 is water.

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

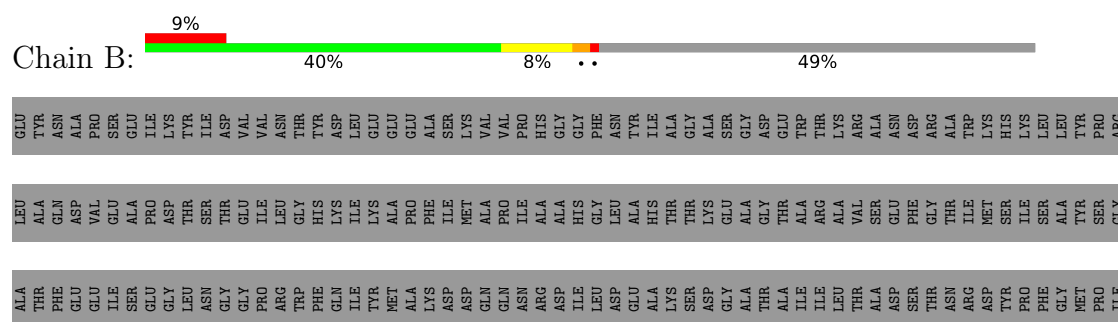
### 3 Residue-property plots

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: L-lactate oxidase



#### • Molecule 1: L-lactate oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.78Å 132.78Å 92.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 1.38 46.95 – 1.38	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.99-1.38) 99.1 (46.95-1.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.37Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.196 , 0.224 0.205 , 0.231	Depositor DCC
$R_{free}$ test set	8242 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.82	0/2905	0.93	8/3937 (0.2%)
1	B	0.86	2/2905 (0.1%)	0.98	9/3937 (0.2%)
All	All	0.84	2/5810 (0.0%)	0.95	17/7874 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	GLY	C-O	11.03	1.41	1.23
1	B	374	TYR	C-O	5.66	1.34	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	PHE	CB-CA-C	9.98	130.35	110.40
1	B	374	TYR	CA-C-O	-8.39	102.48	120.10
1	A	370	TYR	CB-CG-CD1	7.68	125.61	121.00
1	A	370	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	B	370	TYR	CB-CG-CD1	7.44	125.46	121.00
1	A	141	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	A	374	TYR	CA-C-O	-6.68	106.06	120.10
1	B	334	ALA	N-CA-CB	-6.66	100.78	110.10
1	B	333	GLY	O-C-N	6.65	133.34	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	GLY	CA-C-O	-6.46	108.97	120.60
1	B	370	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	A	215	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	B	334	ALA	O-C-N	-5.90	113.26	122.70
1	A	215	TYR	CB-CG-CD1	5.81	124.49	121.00
1	A	255	ARG	CB-CG-CD	5.66	126.31	111.60
1	B	334	ALA	N-CA-C	5.43	125.67	111.00
1	A	347	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	16	0
1	B	2841	0	2771	146	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
3	A	6	0	5	0	0
3	B	6	0	5	1	0
4	A	359	0	0	5	3
4	B	381	0	0	32	2
All	All	6496	0	5591	162	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 14.

All (162) 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: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:28:GLU:C	1:B:327:ALA:O	1.83	1.16
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
1:B:30:SER:N	1:B:328:LEU:O	2.09	0.85
1:B:201:TYR:CZ	1:B:217:ALA:O	2.30	0.84
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:11:PRO:HG3	1:B:33:VAL:HG22	1.62	0.80
1:B:324:PHE:O	1:B:332:GLN:C	2.20	0.80
1:B:27:GLU:O	1:B:329:GLY:N	2.14	0.80
1:B:33:VAL:HG11	1:B:326:LEU:C	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASP:OD2	4:B:509:HOH:O	2.03	0.77
1:B:29:ALA:HA	1:B:330:GLY:C	2.06	0.76
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:333:GLY:C	4:B:508:HOH:O	2.25	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: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: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:29:ALA:HB3	1:B:326:LEU:C	2.16	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
1:B:29:ALA:CB	1:B:331:TRP:HA	2.28	0.64
1:B:30:SER:C	1:B:328:LEU:O	2.36	0.64
1:B:33:VAL:HG11	1:B:326:LEU:CA	2.29	0.63
1:B:29:ALA:H	1:B:329:GLY:N	1.98	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:29:ALA:HB3	1:B:327:ALA:C	2.22	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ALA:CB	1:B:326:LEU:C	2.73	0.57
1:A:202:LEU:O	1:A:203:ARG:O	2.23	0.57
1:B:29:ALA:H	1:B:329:GLY:C	2.08	0.57
1:B:30:SER:HG	1:B:328:LEU:C	2.08	0.56
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:HE2	1:B:154:ASN:ND2	2.20	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:325:GLY:C	4:B:504:HOH:O	2.38	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: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:30:SER:OG	1:B:328:LEU:C	2.50	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: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:A:61:LYS:NZ	1:A:367:ASP:OD1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:66:ARG:C	1:A:67:LEU:HD23	2.38	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:C1	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
1:B:89:PHE:HA	1:B:316:VAL:O	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:29:ALA:HA	1:B:330:GLY:CA	2.49	0.41
1:B:30:SER:N	1:B:328:LEU:C	2.72	0.41
1:B:328:LEU:HA	1:B:328:LEU:HD12	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/720 (51%)	355 (97%)	9 (2%)	2 (0%)	29	9
1	B	366/720 (51%)	341 (93%)	15 (4%)	10 (3%)	5	0
All	All	732/1440 (51%)	696 (95%)	24 (3%)	12 (2%)	9	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

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Mol	Chain	Res	Type
1	B	334	ALA
1	B	211	LEU
1	B	30	SER
1	B	147	MET

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/569 (51%)	287 (98%)	5 (2%)	60	30
1	B	292/569 (51%)	281 (96%)	11 (4%)	33	5
All	All	584/1138 (51%)	568 (97%)	16 (3%)	44	13

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	A	199	GLN
1	A	203	ARG
1	A	205	THR
1	A	255	ARG
1	B	141	ARG
1	B	153	GLN
1	B	160	GLU
1	B	195	MET
1	B	201	TYR
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 monosaccharides 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	-	31,33,33	1.14	2 (6%)	40,50,50	2.11	6 (15%)
2	FMN	B	401	-	31,33,33	1.26	2 (6%)	40,50,50	2.17	6 (15%)
3	LAC	B	402	-	2,5,5	0.18	0	3,6,6	0.44	0
3	LAC	A	402	-	2,5,5	0.27	0	3,6,6	0.59	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	B	401	-	-	1/18/18/18	0/3/3/3
3	LAC	B	402	-	-	0/0/4/4	-
3	LAC	A	402	-	-	0/0/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	C4A-C10	4.39	1.43	1.38
2	B	401	FMN	C4A-C10	4.09	1.42	1.38
2	B	401	FMN	C4-N3	2.97	1.38	1.33
2	A	401	FMN	C4-N3	2.25	1.36	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FMN	C2-N3-C4	8.86	122.62	115.14
2	B	401	FMN	C2-N3-C4	8.63	122.43	115.14
2	B	401	FMN	C10-C4A-C4	-5.94	116.02	119.95
2	A	401	FMN	C10-C4A-C4	-5.14	116.55	119.95
2	B	401	FMN	C10-C4A-N5	4.89	124.64	121.26
2	A	401	FMN	C10-C4A-N5	4.84	124.60	121.26
2	B	401	FMN	C4A-C10-N10	-4.43	115.75	120.30
2	A	401	FMN	C4A-C4-N3	-4.26	117.61	123.43
2	B	401	FMN	C4A-C4-N3	-3.93	118.06	123.43
2	A	401	FMN	C4A-C10-N10	-3.47	116.74	120.30
2	B	401	FMN	C1'-N10-C9A	2.38	120.17	118.29
2	A	401	FMN	O3P-P-O2P	2.11	115.68	107.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

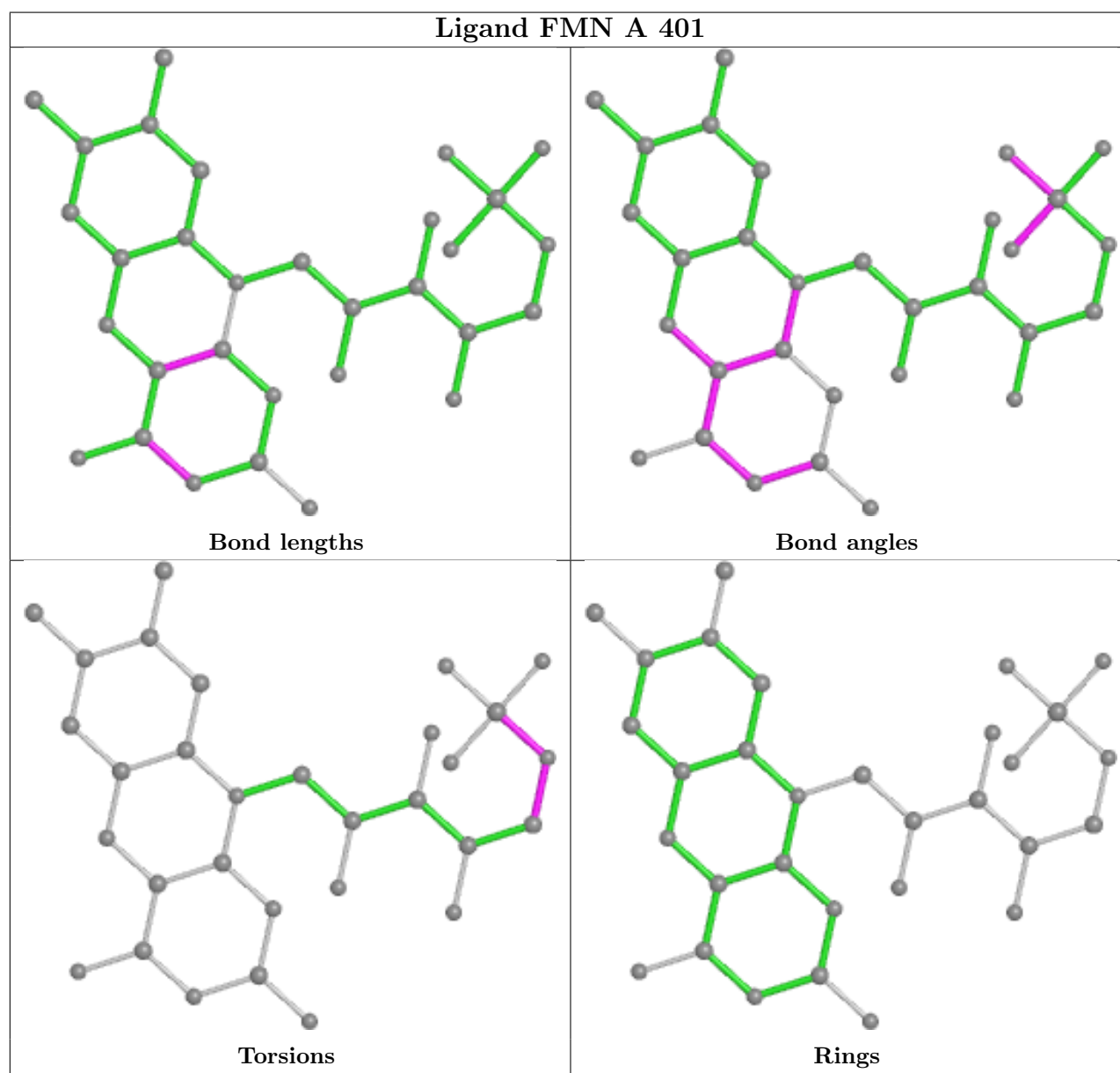
Mol	Chain	Res	Type	Atoms
2	A	401	FMN	C4'-C5'-O5'-P
2	B	401	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C5'-O5'-P-O1P

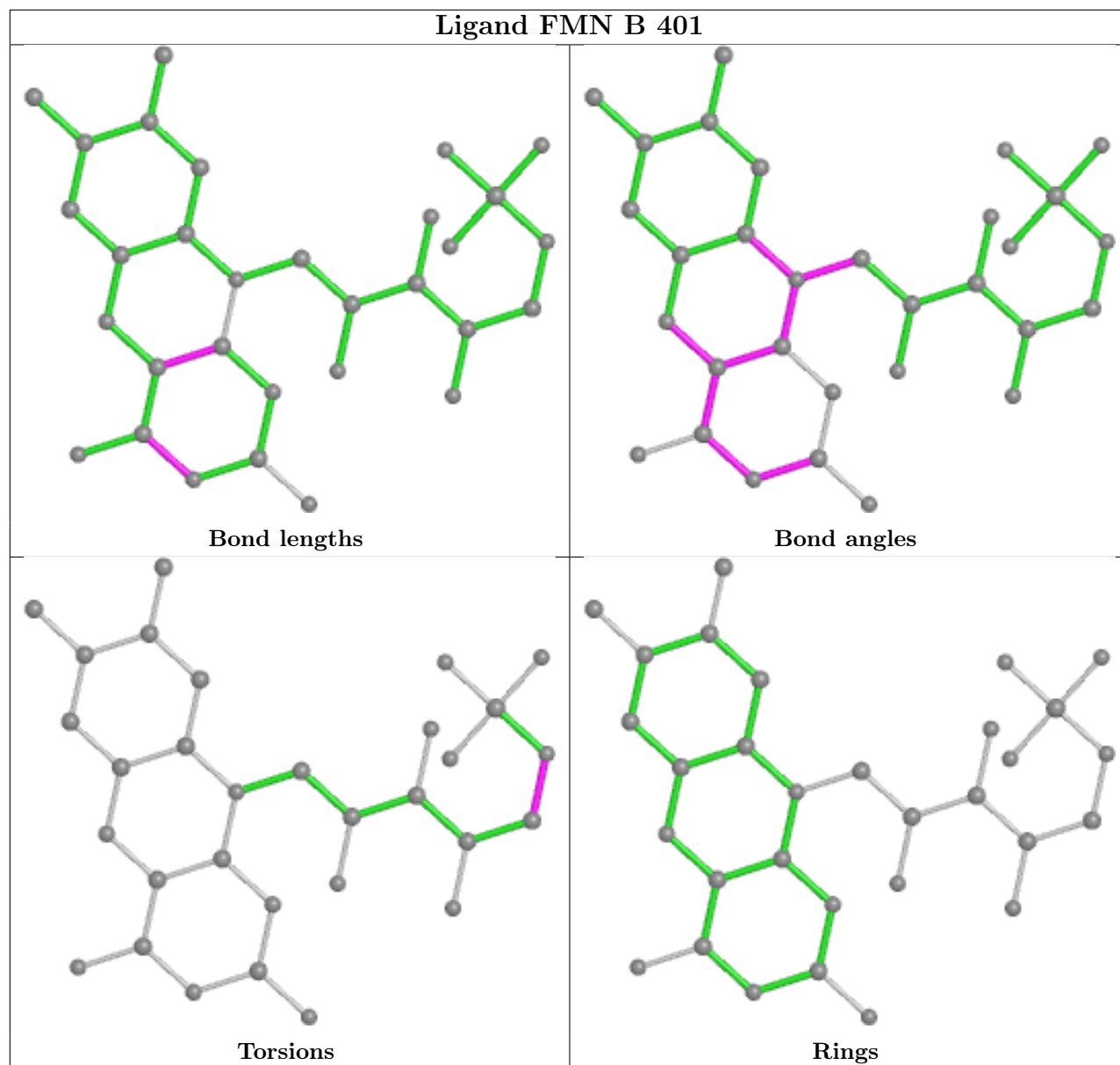
There are no ring outliers.

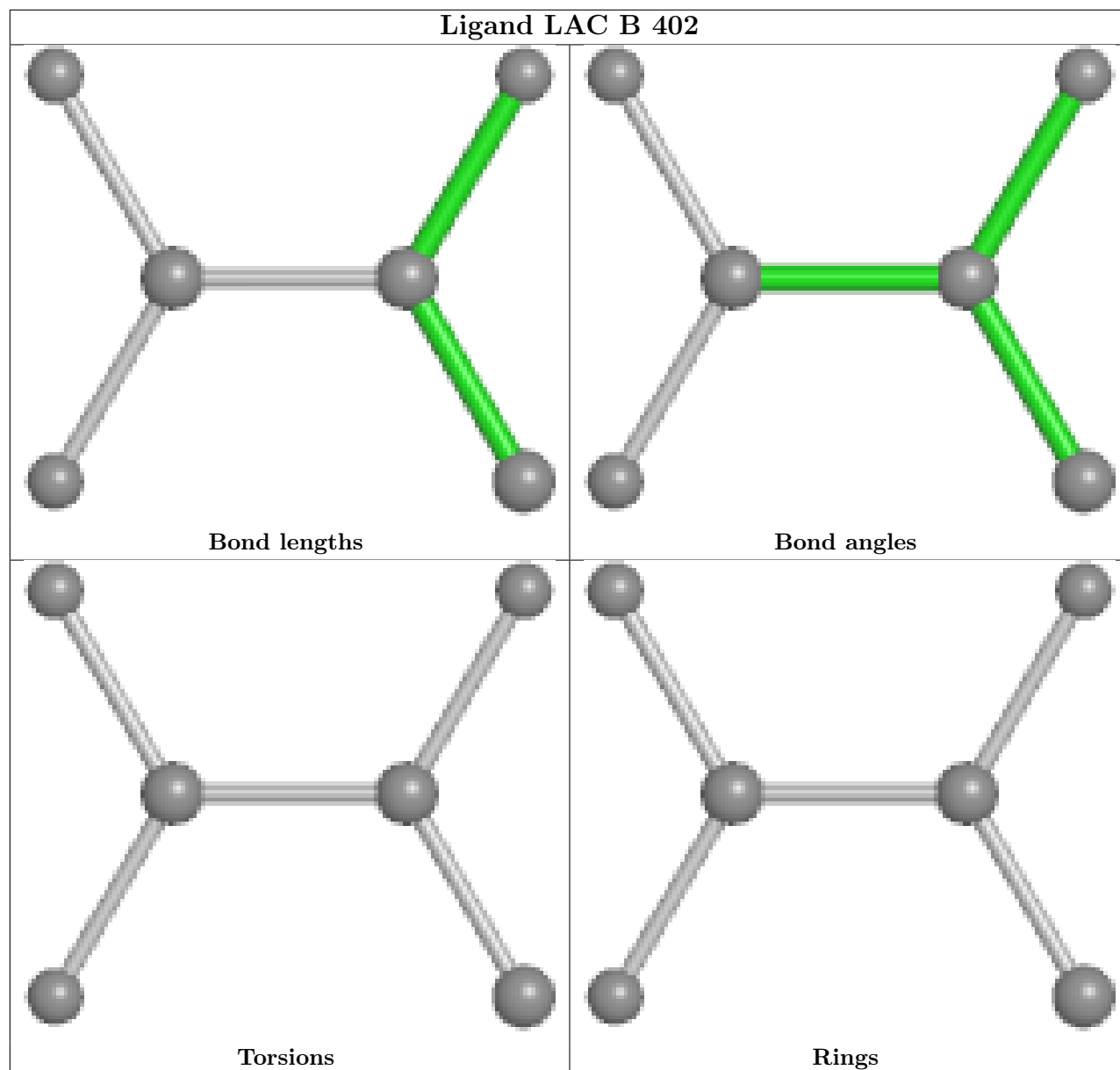
1 monomer is involved in 1 short contact:

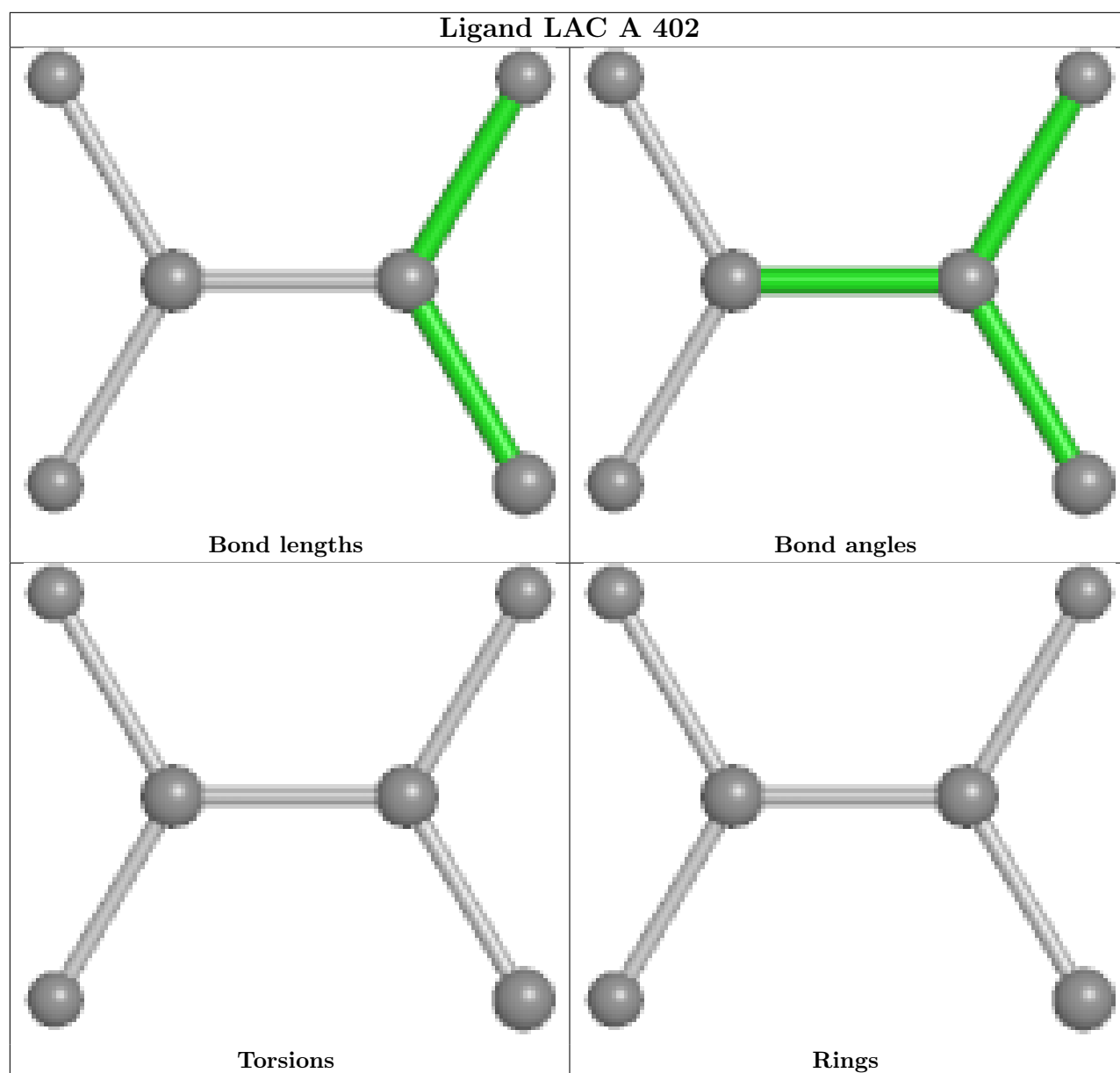
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	LAC	1	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	368/720 (51%)	0.49	32 (8%)	10 10	11, 18, 34, 85	0
1	B	368/720 (51%)	1.74	62 (16%)	1 1	11, 19, 84, 170	0
All	All	736/1440 (51%)	1.11	94 (12%)	3 3	11, 19, 48, 170	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	VAL	34.3
1	B	326	LEU	32.4
1	B	331	TRP	29.2
1	B	211	LEU	28.9
1	B	330	GLY	26.0
1	B	201	TYR	25.5
1	B	203	ARG	22.3
1	B	205	THR	22.2
1	B	210	SER	21.2
1	B	332	GLN	19.4
1	B	29	ALA	19.3
1	B	329	GLY	19.1
1	B	202	LEU	14.0
1	B	327	ALA	13.9
1	A	203	ARG	13.3
1	B	206	ALA	11.1
1	B	209	MET	11.0
1	B	212	ASN	10.1
1	B	328	LEU	10.0
1	B	31	LYS	9.4
1	B	207	GLU	9.2
1	A	205	THR	8.9
1	B	200	ARG	8.6
1	B	204	GLY	8.6

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Mol	Chain	Res	Type	RSRZ
1	B	208	GLY	8.6
1	B	33	VAL	8.2
1	B	215	TYR	8.1
1	B	216	GLY	8.0
1	B	30	SER	7.1
1	B	333	GLY	6.6
1	B	214	ILE	6.3
1	B	199	GLN	6.0
1	B	325	GLY	5.7
1	B	334	ALA	5.5
1	A	201	TYR	4.6
1	A	215	TYR	4.4
1	A	157	ILE	4.0
1	B	185	VAL	4.0
1	B	129	PHE	3.9
1	A	7	GLU	3.9
1	B	232	ALA	3.8
1	A	199	GLN	3.7
1	B	67	LEU	3.7
1	B	198	VAL	3.6
1	B	191	TYR	3.6
1	B	255	ARG	3.6
1	B	73	ALA	3.5
1	B	213	ASN	3.5
1	A	163	SER	3.5
1	A	204	GLY	3.2
1	A	129	PHE	3.2
1	B	220	GLN	3.2
1	A	189	PHE	3.2
1	B	188	LYS	3.1
1	B	197	ILE	3.0
1	A	212	ASN	3.0
1	A	200	ARG	2.9
1	B	190	VAL	2.9
1	B	7	GLU	2.9
1	B	189	PHE	2.8
1	A	197	ILE	2.7
1	A	82	GLY	2.7
1	B	18	ASP	2.7
1	A	202	LEU	2.6
1	A	216	GLY	2.6
1	A	148	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	217	ALA	2.6
1	B	225	ARG	2.6
1	B	177	VAL	2.6
1	A	158	LEU	2.5
1	B	153	GLN	2.5
1	A	137	ASN	2.4
1	A	255	ARG	2.4
1	B	148	ALA	2.3
1	B	218	SER	2.3
1	A	67	LEU	2.3
1	A	143	PHE	2.3
1	A	9	ASN	2.3
1	A	225	ARG	2.2
1	A	231	ALA	2.2
1	A	232	ALA	2.2
1	B	224	PRO	2.2
1	B	230	ILE	2.2
1	B	147	MET	2.1
1	A	134	GLU	2.1
1	B	164	ASP	2.1
1	A	198	VAL	2.1
1	B	17	ILE	2.1
1	B	157	ILE	2.1
1	B	222	ILE	2.1
1	A	206	ALA	2.1
1	A	191	TYR	2.0
1	A	209	MET	2.0
1	B	143	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



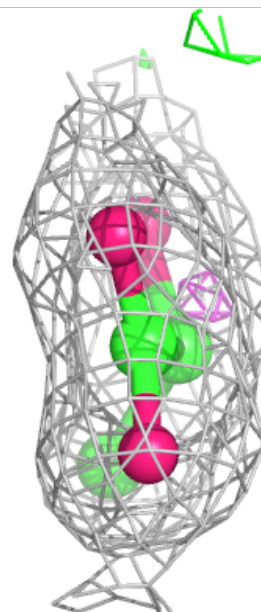
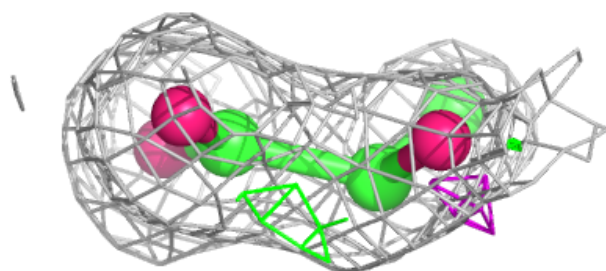
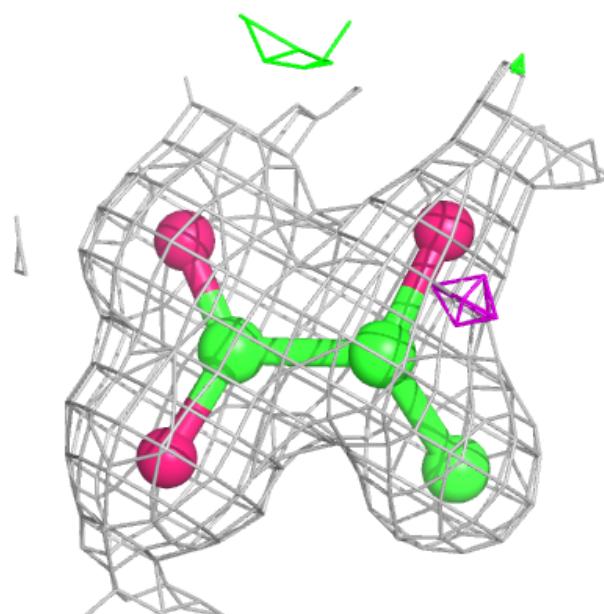
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	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	B	401	31/31	0.97	0.07	12,14,17,18	0
2	FMN	A	401	31/31	0.98	0.06	12,14,16,16	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.

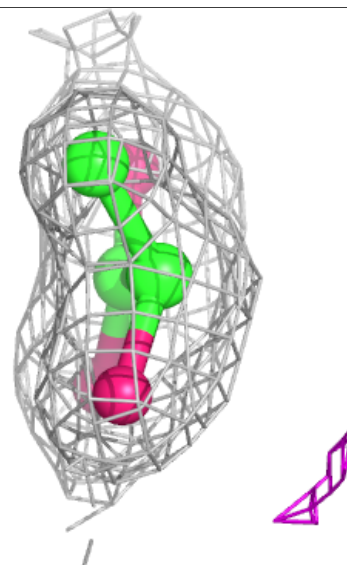
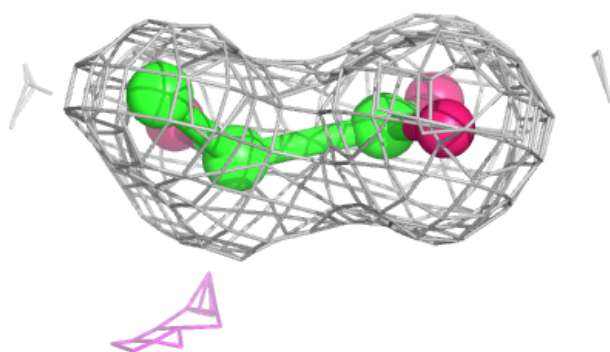
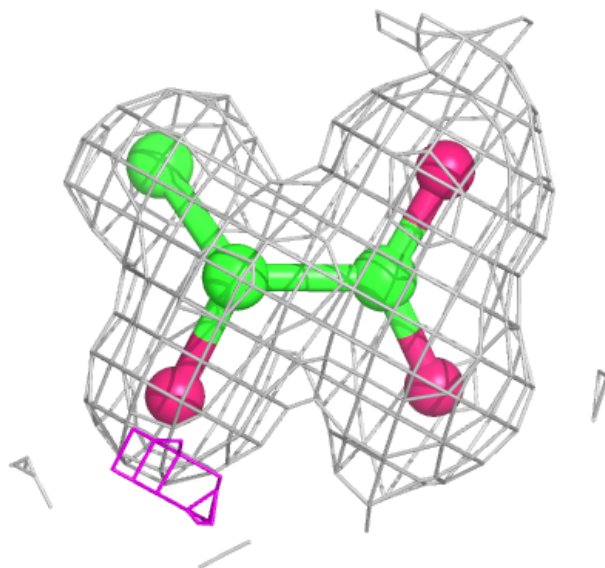
**Electron density around LAC B 402:**

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



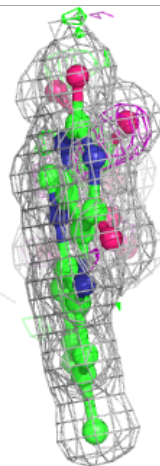
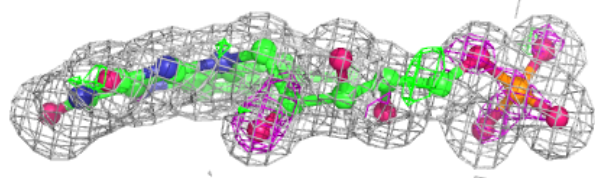
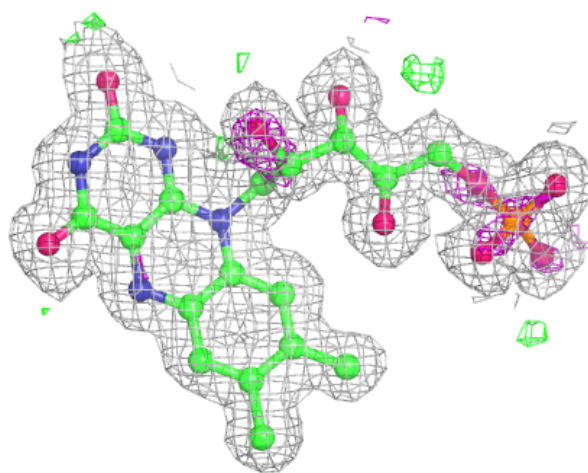
**Electron density around LAC A 402:**

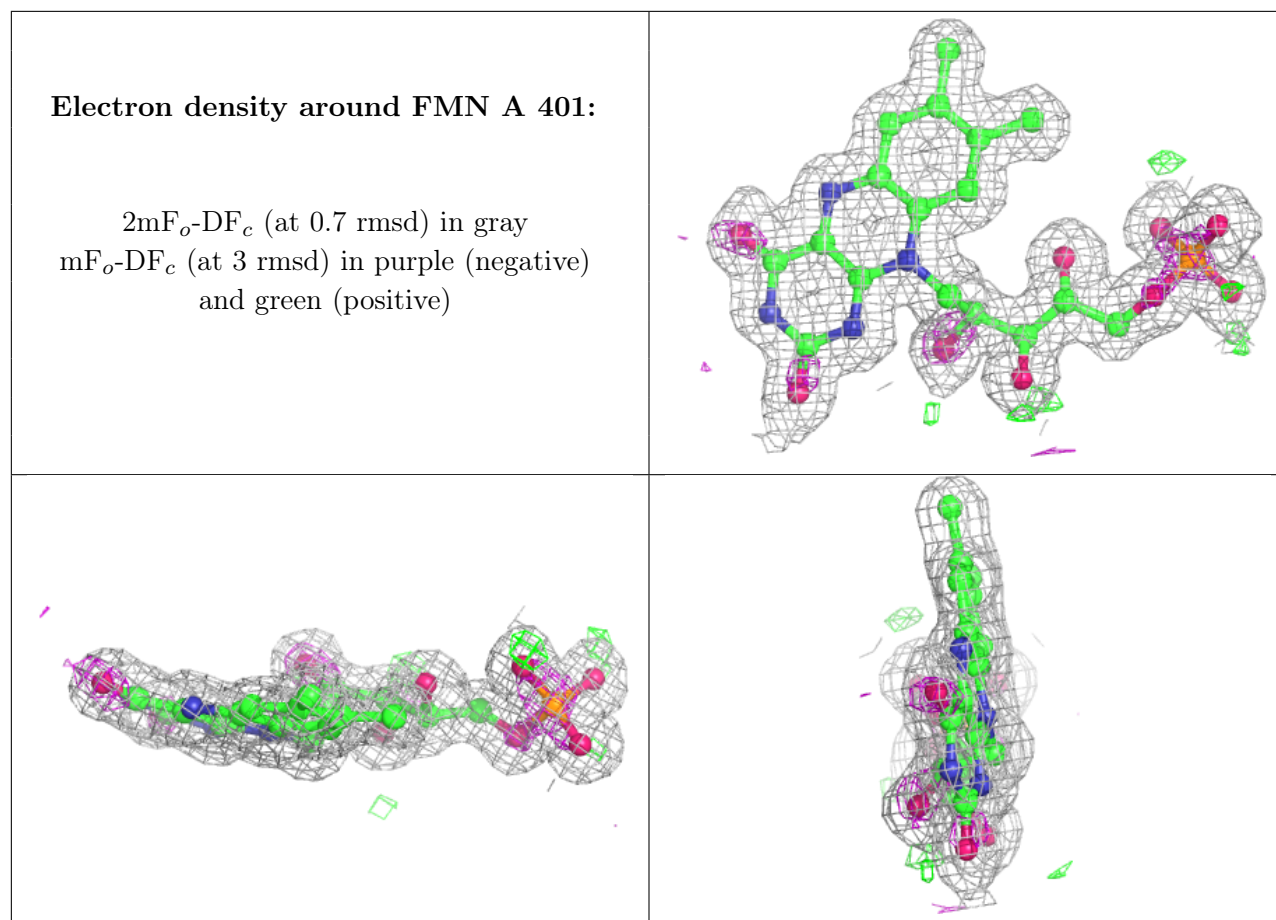
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN 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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.