



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:16 AM UTC

PDB ID : 7F20 / pdb_00007f20
Title : L-lactate oxidase with L-lactate
Authors : Morimoto, Y.; Inaka, K.
Deposited on : 2021-06-10
Resolution : 1.30 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

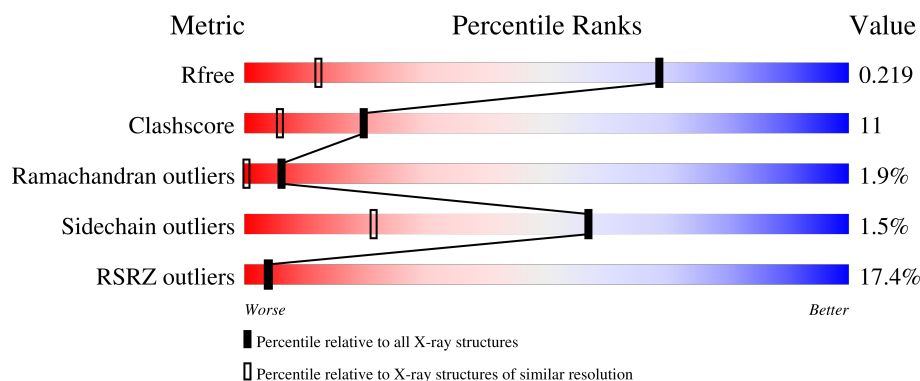
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	7% 47% . 49%
1	B	720	11% 41% 8% 49%

2 Entry composition [i](#)

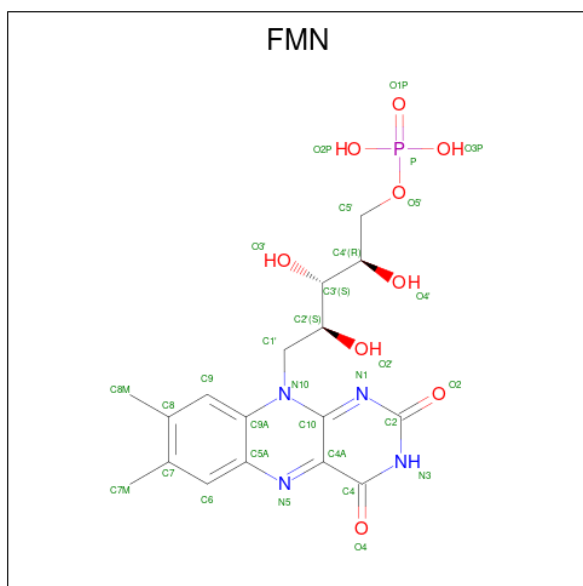
There are 4 unique types of molecules in this entry. The entry contains 6496 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

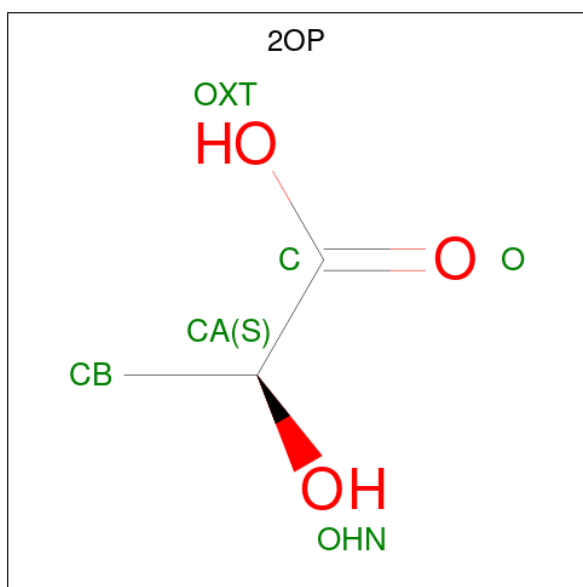
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2841	1795	494	545	7			
1	B	368	Total	C	N	O	S	0	0	0
			2841	1795	494	545	7			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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 (2S)-2-HYDROXYPROPANOIC ACID (CCD ID: 2OP) (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		

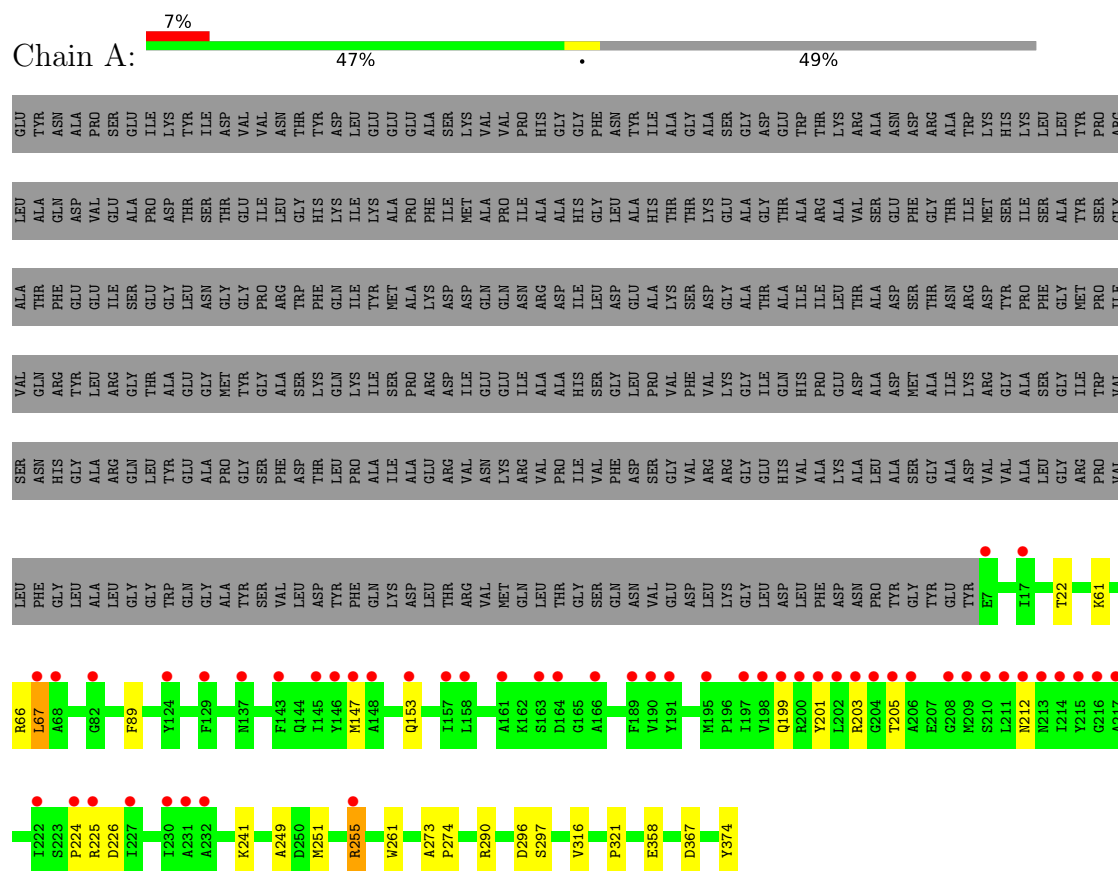
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	360	Total	O	0	0
			360	360		
4	B	380	Total	O	0	0
			380	380		

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, α , β , γ	132.97Å 132.97Å 92.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 1.30 47.05 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.05-1.30) 99.9 (47.05-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.194 , 0.211 0.203 , 0.219	Depositor DCC
R_{free} test set	9948 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 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 ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, 2OP

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	1.04	0/2905	1.18	4/3937 (0.1%)
1	B	1.12	6/2905 (0.2%)	1.32	18/3937 (0.5%)
All	All	1.08	6/5810 (0.1%)	1.25	22/7874 (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	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	GLY	C-O	11.90	1.40	1.23
1	B	333	GLY	C-N	7.88	1.44	1.33
1	B	334	ALA	N-CA	7.01	1.55	1.46
1	B	223	SER	CA-CB	-6.15	1.46	1.54
1	B	245	HIS	CE1-NE2	5.56	1.38	1.32
1	B	334	ALA	CA-C	5.43	1.60	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	GLY	CA-C-N	9.59	128.17	121.65
1	B	329	GLY	C-N-CA	9.59	128.17	121.65
1	B	333	GLY	O-C-N	8.08	133.20	122.70
1	B	324	PHE	CB-CA-C	7.88	126.10	110.42
1	B	374	TYR	CA-C-O	-7.01	108.89	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	GLY	CA-C-O	-6.97	108.44	120.57
1	B	334	ALA	N-CA-C	6.90	125.49	110.80
1	B	333	GLY	CA-C-N	6.88	134.67	121.54
1	B	333	GLY	C-N-CA	6.88	134.67	121.54
1	A	374	TYR	CA-C-O	-6.60	109.58	120.80
1	B	327	ALA	CA-C-N	6.58	134.11	121.54
1	B	327	ALA	C-N-CA	6.58	134.11	121.54
1	B	334	ALA	O-C-N	-6.34	114.16	122.59
1	B	29	ALA	CA-C-N	-6.17	112.90	122.16
1	B	29	ALA	C-N-CA	-6.17	112.90	122.16
1	B	334	ALA	N-CA-CB	-6.12	100.15	110.49
1	B	330	GLY	CA-C-O	-5.94	116.31	120.94
1	A	255	ARG	CB-CG-CD	5.92	124.93	111.30
1	A	249	ALA	CA-C-O	-5.71	114.82	120.82
1	B	215	TYR	CA-C-N	5.14	125.69	119.98
1	B	215	TYR	C-N-CA	5.14	125.69	119.98
1	A	249	ALA	O-C-N	5.08	127.31	122.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	32	VAL	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	18	0
1	B	2841	0	2772	113	1
2	A	31	0	19	1	0
2	B	31	0	19	0	0
3	A	6	0	5	1	0
3	B	6	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	360	0	0	3	1
4	B	380	0	0	19	4
All	All	6496	0	5592	130	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 11.

All (130) 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:331:TRP:CE3	4:B:771:HOH:O	1.83	1.25
1:B:27:GLU:O	1:B:329:GLY:N	1.76	1.17
1:B:29:ALA:CB	1:B:326:LEU:O	1.91	1.17
1:B:29:ALA:HB3	1:B:326:LEU:O	1.44	1.16
1:B:334:ALA:HB3	4:B:553:HOH:O	1.47	1.13
1:B:33:VAL:HG11	1:B:326:LEU:CA	1.80	1.12
1:B:33:VAL:HG11	1:B:326:LEU:HA	1.09	1.07
1:B:38:PHE:HA	1:B:326:LEU:HD21	1.12	1.04
1:B:69:GLN:O	4:B:501:HOH:O	1.75	1.04
1:B:224:PRO:HB3	1:B:255:ARG:HG3	1.42	1.01
1:B:325:GLY:HA2	4:B:771:HOH:O	1.57	1.01
1:B:143:PHE:CE2	1:B:145:ILE:HG22	1.97	0.98
1:B:331:TRP:HE3	4:B:771:HOH:O	1.28	0.98
1:B:41:ILE:HD12	1:B:326:LEU:HD22	1.46	0.98
1:B:29:ALA:HB3	1:B:326:LEU:C	1.90	0.97
1:A:251:MET:O	1:A:255:ARG:HG2	1.64	0.96
1:B:251:MET:O	1:B:255:ARG:HG2	1.68	0.92
1:B:33:VAL:CG1	1:B:326:LEU:HA	1.98	0.92
1:B:38:PHE:HA	1:B:326:LEU:CD2	1.98	0.92
1:B:323:LEU:O	1:B:325:GLY:N	2.02	0.91
1:B:30:SER:HB3	1:B:328:LEU:N	1.87	0.90
1:B:30:SER:HB2	4:B:667:HOH:O	1.74	0.87
1:B:38:PHE:CE2	1:B:327:ALA:HB1	2.10	0.86
1:B:155:ARG:NH2	4:B:503:HOH:O	1.97	0.86
1:B:33:VAL:CG2	4:B:523:HOH:O	2.22	0.86
1:B:314:ASP:OD2	4:B:502:HOH:O	1.95	0.85
1:B:143:PHE:HE2	1:B:145:ILE:HG22	1.36	0.84
1:A:224:PRO:HB3	1:A:255:ARG:HG3	1.59	0.84
1:B:324:PHE:O	1:B:332:GLN:C	2.21	0.84
1:B:201:TYR:CZ	1:B:217:ALA:O	2.33	0.82
1:B:17:ILE:HD12	1:B:332:GLN:HB3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:PHE:CD2	1:B:327:ALA:CB	2.64	0.81
1:B:29:ALA:CB	1:B:326:LEU:C	2.51	0.79
1:B:29:ALA:H	1:B:330:GLY:N	1.80	0.79
1:B:77:SER:HB2	1:B:84:LYS:HE3	1.65	0.78
1:B:29:ALA:HB1	1:B:326:LEU:O	1.83	0.77
1:B:333:GLY:C	4:B:504:HOH:O	2.28	0.76
1:B:333:GLY:N	4:B:504:HOH:O	2.05	0.75
1:B:226:ASP:O	1:B:230:ILE:HG12	1.87	0.74
1:B:333:GLY:O	4:B:504:HOH:O	2.06	0.72
1:B:38:PHE:CA	1:B:326:LEU:HD21	2.07	0.72
1:B:143:PHE:CE2	1:B:145:ILE:CG2	2.72	0.71
1:B:29:ALA:HB2	1:B:331:TRP:HA	1.70	0.71
1:B:29:ALA:H	1:B:329:GLY:C	1.98	0.70
1:B:200:ARG:NH1	4:B:507:HOH:O	2.23	0.70
1:B:33:VAL:HG23	4:B:523:HOH:O	1.86	0.69
1:B:331:TRP:O	1:B:332:GLN:CG	2.40	0.69
1:B:27:GLU:HA	1:B:328:LEU:CB	2.23	0.69
1:B:30:SER:H	1:B:328:LEU:C	2.01	0.68
1:B:30:SER:H	1:B:329:GLY:N	1.91	0.68
1:B:38:PHE:CE2	1:B:327:ALA:CB	2.75	0.68
1:B:28:GLU:HB3	1:B:330:GLY:O	1.94	0.67
1:B:373:GLU:OE2	4:B:505:HOH:O	2.12	0.67
1:B:195:MET:HB3	1:B:198:VAL:HG22	1.77	0.67
1:B:367:ASP:OD2	4:B:506:HOH:O	2.13	0.67
1:B:11:PRO:HG3	1:B:33:VAL:HG22	1.76	0.66
1:B:27:GLU:HA	1:B:328:LEU:HB2	1.78	0.66
1:B:41:ILE:HD12	1:B:326:LEU:CD2	2.24	0.66
1:B:41:ILE:CD1	1:B:326:LEU:HD22	2.22	0.66
1:A:61:LYS:NZ	1:A:367:ASP:OD1	2.21	0.64
1:B:331:TRP:O	1:B:332:GLN:HG3	1.96	0.64
1:B:38:PHE:CD2	1:B:327:ALA:HB2	2.31	0.64
1:A:225:ARG:NH1	4:A:503:HOH:O	2.32	0.61
1:B:324:PHE:O	1:B:332:GLN:O	2.17	0.61
1:B:201:TYR:CE1	1:B:217:ALA:O	2.53	0.61
1:B:26:GLU:O	1:B:327:ALA:HB3	2.00	0.60
1:B:33:VAL:HG11	1:B:326:LEU:C	2.27	0.59
1:B:326:LEU:O	1:B:327:ALA:O	2.21	0.59
1:B:38:PHE:CD2	1:B:327:ALA:HA	2.38	0.59
1:B:30:SER:HB3	1:B:328:LEU:CA	2.33	0.58
1:B:181:ARG:NH1	1:B:215:TYR:OH	2.37	0.57
1:B:38:PHE:CZ	1:B:328:LEU:HD13	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:VAL:HG21	4:B:523:HOH:O	1.95	0.56
1:B:30:SER:OG	1:B:30:SER:O	2.23	0.56
1:B:147:MET:HG2	1:B:171:LEU:HD11	1.88	0.55
1:B:323:LEU:O	1:B:324:PHE:C	2.50	0.55
1:B:38:PHE:CG	1:B:327:ALA:HA	2.42	0.54
1:B:331:TRP:O	1:B:332:GLN:HG2	2.09	0.53
1:B:27:GLU:HA	1:B:328:LEU:HB3	1.91	0.52
1:B:29:ALA:HB1	1:B:326:LEU:C	2.34	0.51
1:B:29:ALA:O	1:B:33:VAL:CG2	2.59	0.51
1:B:38:PHE:CD2	1:B:327:ALA:CA	2.93	0.51
1:B:29:ALA:HB3	1:B:327:ALA:O	2.10	0.50
1:B:124:TYR:O	1:B:195:MET:HE2	2.11	0.50
1:B:29:ALA:C	1:B:326:LEU:O	2.55	0.50
1:B:324:PHE:O	1:B:333:GLY:N	2.44	0.50
1:A:147:MET:HE1	1:A:226:ASP:OD1	2.12	0.49
2:A:401:FMN:N5	3:A:402:2OP:HA	2.28	0.48
1:B:143:PHE:CD2	1:B:145:ILE:CG2	2.97	0.47
1:A:251:MET:HG2	1:A:255:ARG:HE	1.79	0.47
1:B:31:LYS:HB3	4:B:832:HOH:O	2.15	0.47
1:B:33:VAL:CG1	1:B:326:LEU:HD12	2.45	0.47
1:B:201:TYR:CE2	1:B:218:SER:HA	2.50	0.47
1:A:66:ARG:C	1:A:67:LEU:HD23	2.40	0.46
1:B:28:GLU:O	1:B:29:ALA:CB	2.65	0.45
1:B:77:SER:HB2	1:B:84:LYS:CE	2.42	0.45
1:A:199:GLN:NE2	4:A:519:HOH:O	2.49	0.45
1:B:38:PHE:HB2	1:B:326:LEU:HG	1.98	0.45
1:A:212:ASN:ND2	4:A:523:HOH:O	2.49	0.45
1:B:224:PRO:HB3	1:B:255:ARG:CG	2.30	0.45
1:A:273:ALA:HB1	1:A:274:PRO:HD2	1.99	0.44
1:B:215:TYR:OH	3:B:402:2OP:HB3	2.18	0.44
1:B:29:ALA:CA	1:B:326:LEU:O	2.63	0.43
1:B:38:PHE:CD2	1:B:38:PHE:C	2.96	0.43
1:B:331:TRP:C	1:B:332:GLN:CG	2.92	0.43
1:B:38:PHE:HD2	1:B:327:ALA:HB2	1.82	0.43
1:A:358:GLU:O	1:B:290:ARG:HD3	2.18	0.43
1:B:178:SER:HB2	1:B:215:TYR:CD2	2.54	0.43
1:B:334:ALA:CA	4:B:553:HOH:O	2.65	0.42
1:B:331:TRP:C	1:B:332:GLN:HG3	2.43	0.42
1:B:296:ASP:OD1	1:B:296:ASP:C	2.63	0.42
1:B:241:LYS:HA	1:B:261:TRP:HB3	2.02	0.42
1:A:89:PHE:HA	1:A:316:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ALA:O	1:B:33:VAL:HG23	2.19	0.42
1:A:22:THR:HB	1:A:321:PRO:HB3	2.02	0.42
1:B:29:ALA:N	1:B:330:GLY:C	2.77	0.42
1:B:30:SER:N	1:B:328:LEU:C	2.74	0.42
1:B:89:PHE:HA	1:B:316:VAL:O	2.20	0.42
1:A:296:ASP:OD1	1:A:296:ASP:C	2.63	0.41
1:B:15:LYS:HG2	1:B:331:TRP:CZ2	2.55	0.41
1:B:77:SER:CB	1:B:84:LYS:HE3	2.43	0.41
1:B:309:LEU:HD23	1:B:357:VAL:HG13	2.03	0.41
1:A:199:GLN:HE21	1:A:199:GLN:HB3	1.69	0.41
1:B:33:VAL:O	1:B:33:VAL:HG12	2.19	0.41
1:B:320:ARG:N	1:B:321:PRO:HD2	2.36	0.41
1:B:25:LEU:HD22	1:B:332:GLN:CB	2.51	0.40
1:A:153:GLN:OE1	1:A:201:TYR:HB3	2.21	0.40
1:B:30:SER:HB3	1:B:327:ALA:C	2.44	0.40
1:A:290:ARG:HD3	1:B:358:GLU:O	2.21	0.40
1:A:241:LYS:HA	1:A:261:TRP:HB3	2.04	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:B:836:HOH:O	4:B:836:HOH:O[3_655]	1.91	0.29
4:A:814:HOH:O	4:A:814:HOH:O[3_655]	2.00	0.20
4:B:601:HOH:O	4:B:601:HOH:O[3_655]	2.03	0.17
4:B:505:HOH:O	4:B:733:HOH:O[4_565]	2.14	0.06
1:B:373:GLU:OE1	4:B:505:HOH:O[3_655]	2.17	0.03

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%)	354 (97%)	9 (2%)	3 (1%)	16	2
1	B	366/720 (51%)	338 (92%)	17 (5%)	11 (3%)	3	0
All	All	732/1440 (51%)	692 (94%)	26 (4%)	14 (2%)	6	0

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	THR
1	A	297	SER
1	B	200	ARG
1	B	297	SER
1	B	324	PHE
1	B	327	ALA
1	B	328	LEU
1	B	334	ALA
1	B	29	ALA
1	B	326	LEU
1	A	203	ARG
1	B	203	ARG
1	B	204	GLY
1	B	332	GLN

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%)	291 (100%)	1 (0%)	86	67
1	B	292/569 (51%)	284 (97%)	8 (3%)	39	7
All	All	584/1138 (51%)	575 (98%)	9 (2%)	57	21

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	B	30	SER

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Mol	Chain	Res	Type
1	B	32	VAL
1	B	38	PHE
1	B	67	LEU
1	B	188	LYS
1	B	199	GLN
1	B	326	LEU
1	B	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	199	GLN
1	B	35	HIS
1	B	332	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	1 (3%)	48,50,50	0.77	0
3	2OP	A	402	-	4,5,5	1.34	1 (25%)	2,6,6	0.41	0
2	FMN	B	401	-	33,33,33	0.83	0	48,50,50	0.81	1 (2%)
3	2OP	B	402	-	4,5,5	1.06	0	2,6,6	0.63	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	2OP	A	402	-	-	2/4/4/4	-
2	FMN	B	401	-	-	1/18/18/18	0/3/3/3
3	2OP	B	402	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	2OP	OXT-C	-2.55	1.22	1.30
2	A	401	FMN	C9-C8	-2.01	1.36	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FMN	C4A-C4-N3	2.15	118.71	113.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

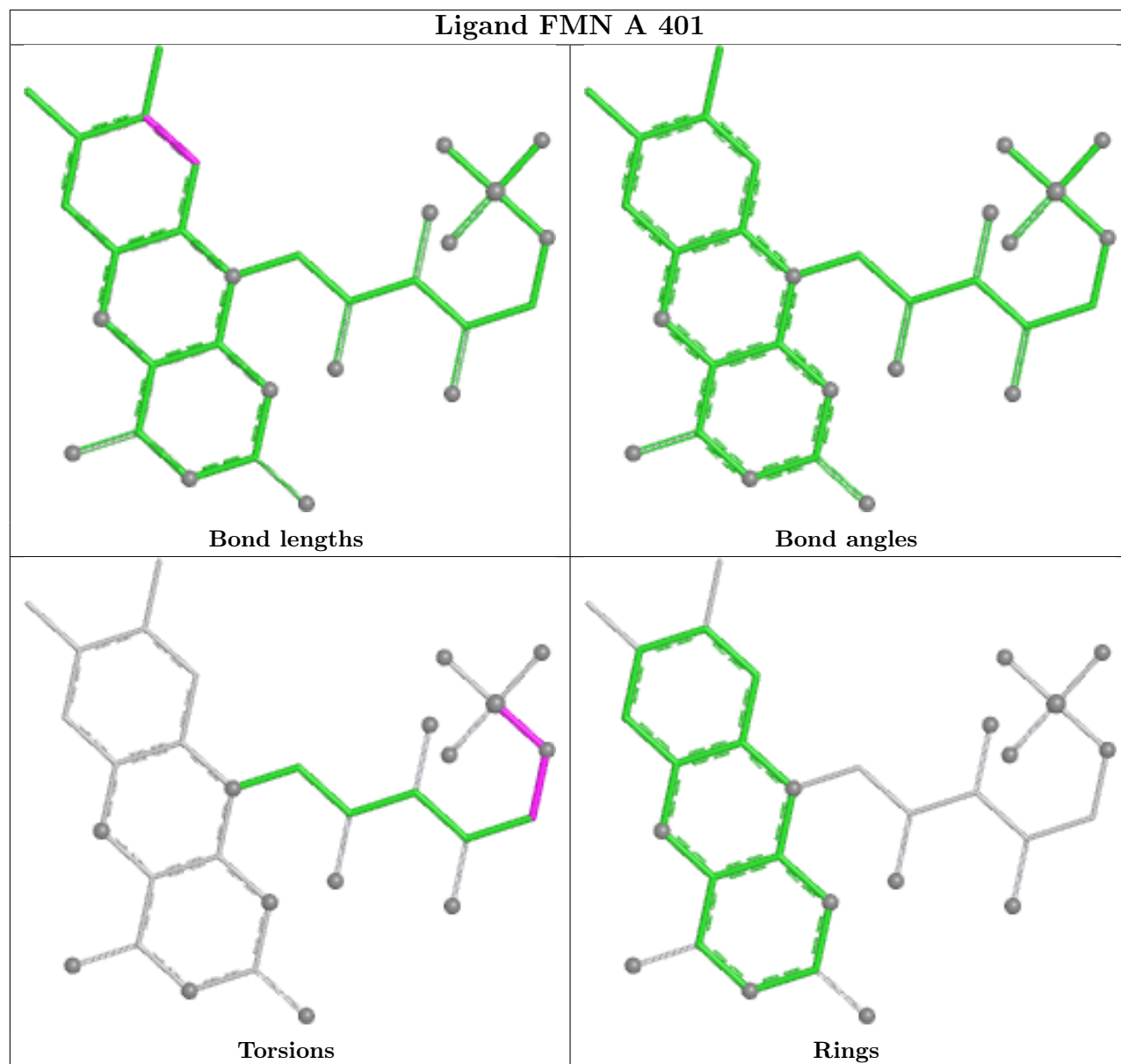
Mol	Chain	Res	Type	Atoms
3	A	402	2OP	OXT-C-CA-CB
2	B	401	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C5'-O5'-P-O1P
3	A	402	2OP	O-C-CA-CB

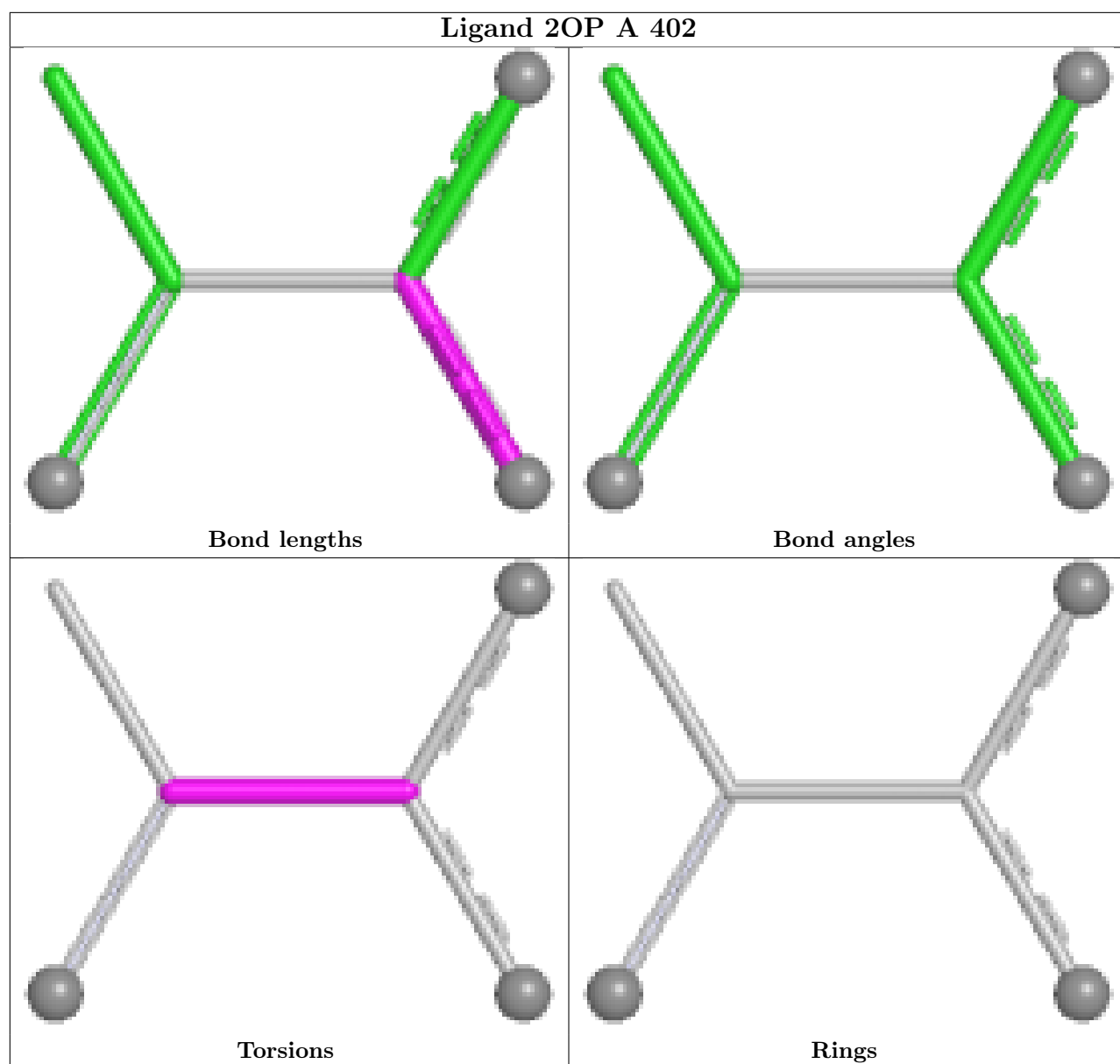
There are no ring outliers.

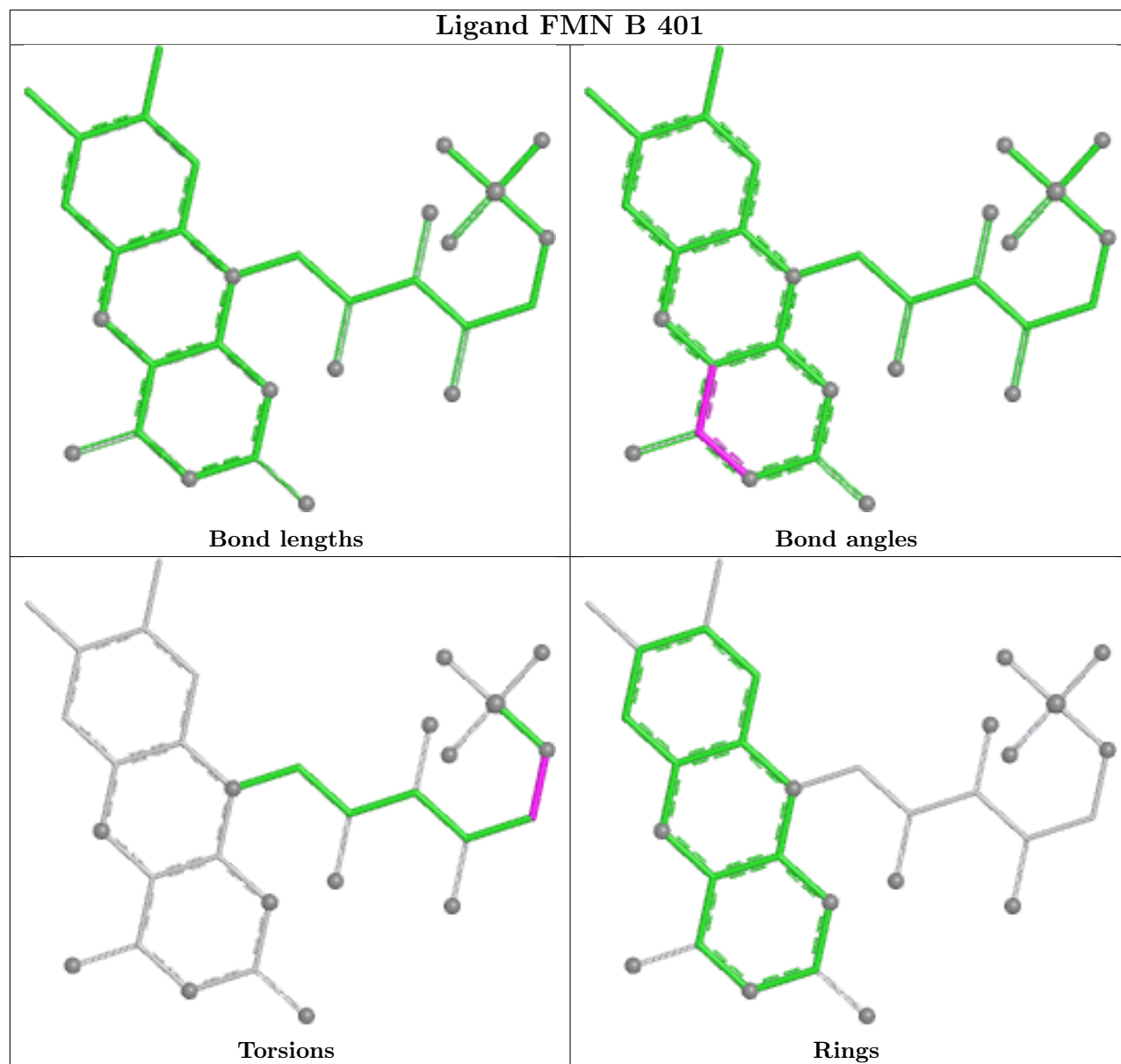
3 monomers are involved in 2 short contacts:

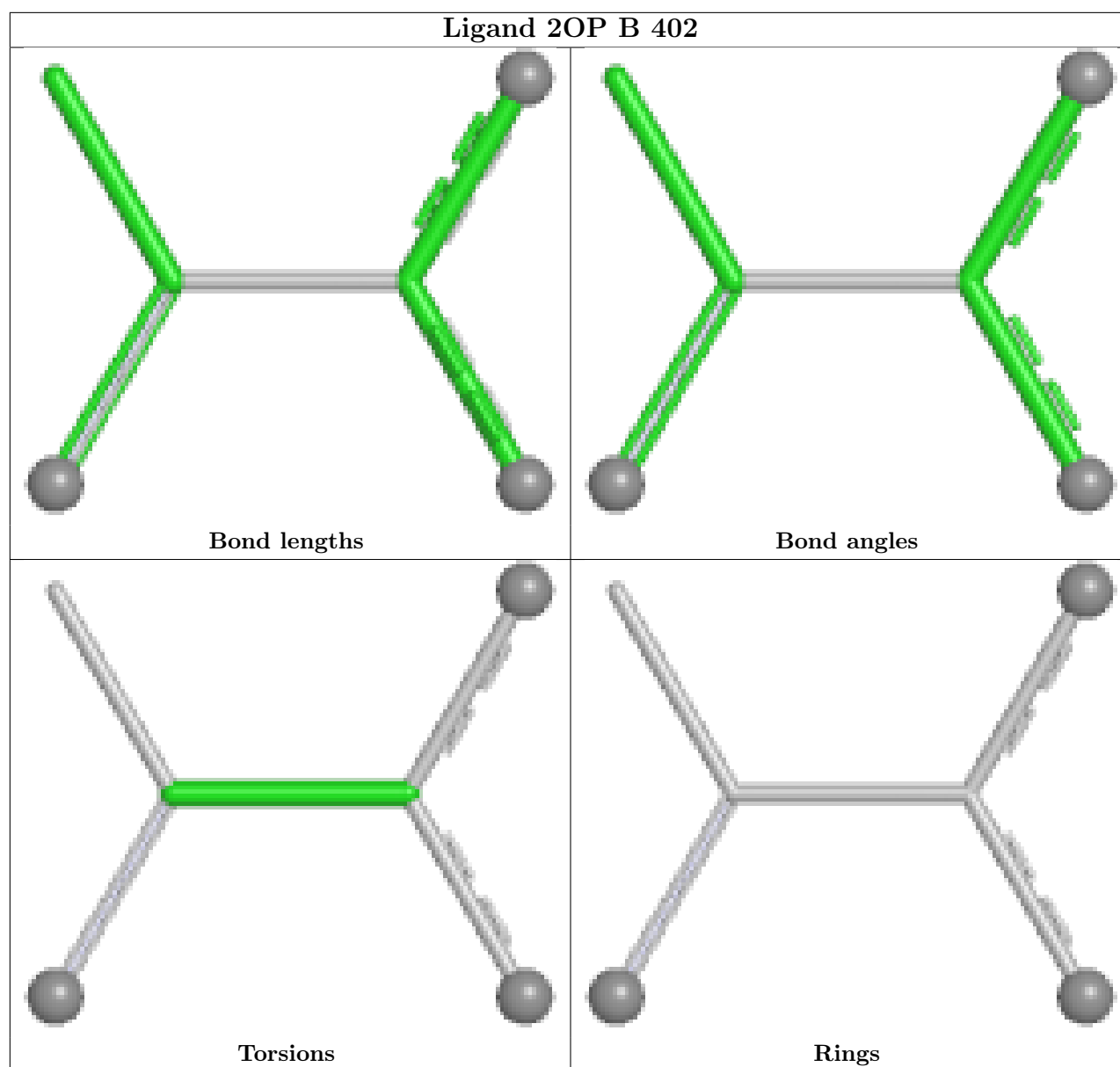
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FMN	1	0
3	A	402	2OP	1	0
3	B	402	2OP	1	0

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%)	0.83	52 (14%) 6 7	12, 18, 39, 97	0
1	B	368/720 (51%)	1.69	76 (20%) 2 2	12, 20, 73, 187	0
All	All	736/1440 (51%)	1.26	128 (17%) 4 4	12, 19, 52, 187	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	LEU	27.0
1	B	331	TRP	20.6
1	B	32	VAL	17.0
1	B	211	LEU	16.2
1	B	328	LEU	14.7
1	B	325	GLY	14.5
1	B	327	ALA	14.4
1	B	330	GLY	13.3
1	B	202	LEU	12.3
1	B	332	GLN	11.7
1	B	201	TYR	11.5
1	B	206	ALA	11.3
1	B	214	ILE	11.0
1	B	29	ALA	10.9
1	B	33	VAL	10.3
1	B	329	GLY	9.6
1	B	191	TYR	9.2
1	B	198	VAL	9.1
1	B	333	GLY	8.8
1	B	30	SER	8.4
1	B	31	LYS	7.9
1	B	205	THR	7.5
1	B	38	PHE	7.2
1	B	209	MET	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	210	SER	6.9
1	B	143	PHE	6.7
1	A	215	TYR	6.7
1	B	215	TYR	6.6
1	A	198	VAL	6.3
1	B	208	GLY	6.3
1	A	202	LEU	6.2
1	B	197	ILE	6.2
1	B	334	ALA	6.1
1	B	199	GLN	6.1
1	A	214	ILE	5.9
1	B	216	GLY	5.9
1	B	200	ARG	5.7
1	B	124	TYR	5.7
1	A	205	THR	5.5
1	A	211	LEU	5.4
1	B	204	GLY	5.4
1	B	212	ASN	5.3
1	B	232	ALA	5.2
1	A	201	TYR	5.1
1	A	206	ALA	5.1
1	A	208	GLY	5.0
1	B	207	GLU	5.0
1	B	203	ARG	4.7
1	A	204	GLY	4.7
1	A	230	ILE	4.5
1	A	232	ALA	4.4
1	B	193	PHE	4.4
1	A	203	ARG	4.4
1	A	216	GLY	4.3
1	B	217	ALA	4.3
1	A	129	PHE	4.3
1	A	157	ILE	4.1
1	A	143	PHE	4.0
1	B	147	MET	4.0
1	A	212	ASN	3.9
1	A	213	ASN	3.8
1	B	213	ASN	3.8
1	B	255	ARG	3.8
1	A	199	GLN	3.8
1	B	129	PHE	3.7
1	B	196	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	218	SER	3.6
1	A	231	ALA	3.5
1	A	210	SER	3.5
1	A	209	MET	3.5
1	A	163	SER	3.5
1	B	185	VAL	3.4
1	B	190	VAL	3.4
1	A	197	ILE	3.4
1	A	67	LEU	3.4
1	B	18	ASP	3.4
1	B	82	GLY	3.3
1	B	231	ALA	3.3
1	A	158	LEU	3.3
1	B	189	PHE	3.3
1	B	195	MET	3.3
1	B	134	GLU	3.2
1	B	128	THR	3.2
1	A	200	ARG	3.2
1	B	67	LEU	3.2
1	B	123	ALA	3.1
1	A	227	ILE	3.0
1	A	124	TYR	3.0
1	A	147	MET	3.0
1	B	17	ILE	3.0
1	B	230	ILE	2.9
1	A	146	TYR	2.9
1	A	255	ARG	2.9
1	B	73	ALA	2.9
1	A	222	ILE	2.9
1	A	148	ALA	2.9
1	A	217	ALA	2.9
1	A	82	GLY	2.8
1	A	189	PHE	2.8
1	A	7	GLU	2.8
1	B	235	GLY	2.8
1	A	195	MET	2.8
1	A	161	ALA	2.7
1	B	225	ARG	2.6
1	B	222	ILE	2.6
1	B	227	ILE	2.6
1	B	7	GLU	2.6
1	B	228	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	191	TYR	2.5
1	B	132	ILE	2.5
1	A	17	ILE	2.4
1	B	188	LYS	2.4
1	A	68	ALA	2.4
1	B	83	HIS	2.3
1	A	190	VAL	2.3
1	A	224	PRO	2.3
1	B	224	PRO	2.3
1	A	166	ALA	2.3
1	B	9	ASN	2.2
1	A	145	ILE	2.2
1	B	10	ALA	2.2
1	B	220	GLN	2.1
1	B	157	ILE	2.1
1	A	225	ARG	2.1
1	B	324	PHE	2.1
1	A	164	ASP	2.0
1	A	137	ASN	2.0
1	A	153	GLN	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	2OP	A	402	6/6	0.92	0.10	26,28,30,32	0
3	2OP	B	402	6/6	0.94	0.09	27,32,33,37	0
2	FMN	A	401	31/31	0.98	0.05	13,14,18,20	0

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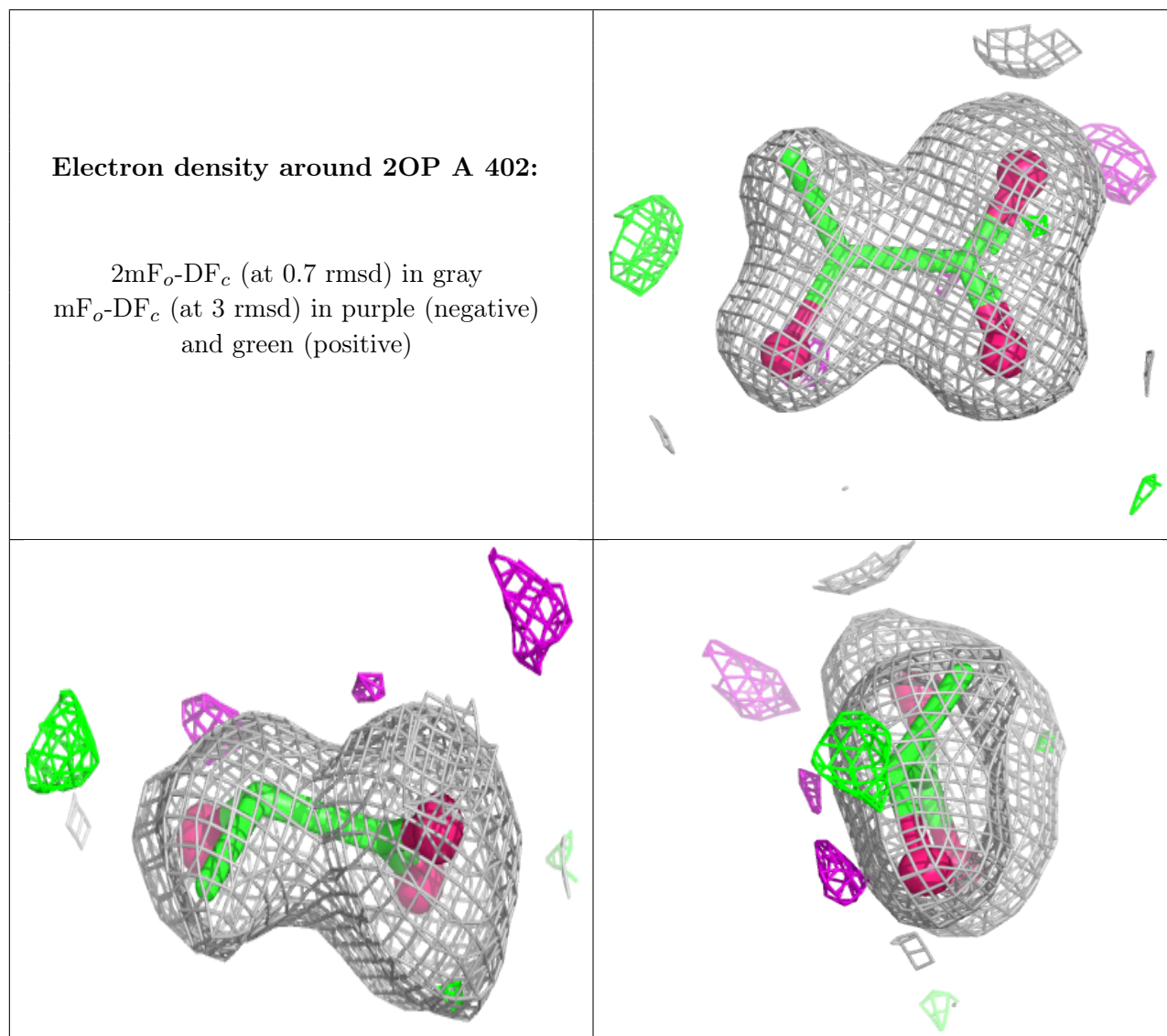
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	B	401	31/31	0.98	0.05	13,14,19,20	0

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.

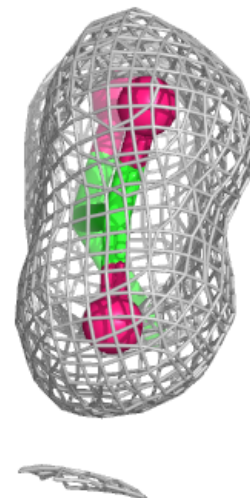
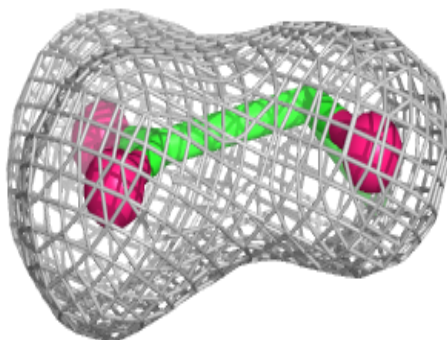
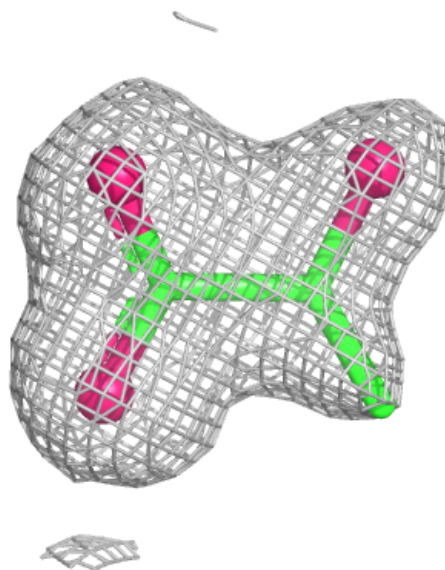
Electron density around 2OP A 402:

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



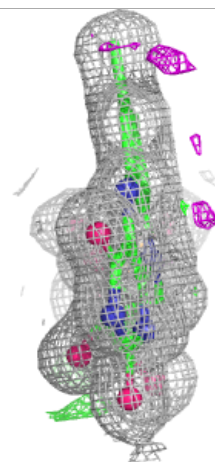
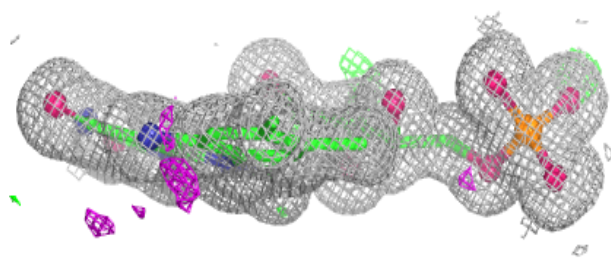
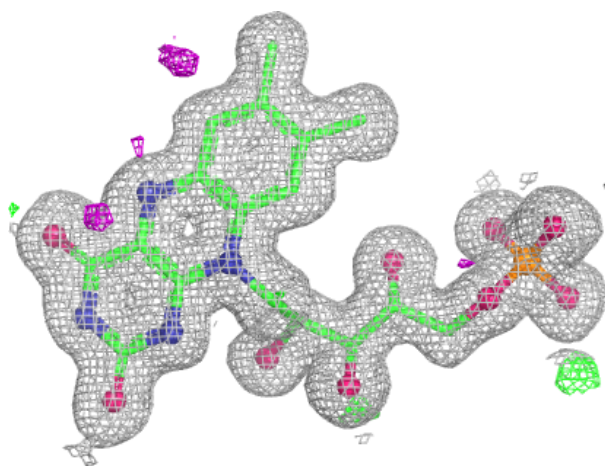
Electron density around 2OP B 402:

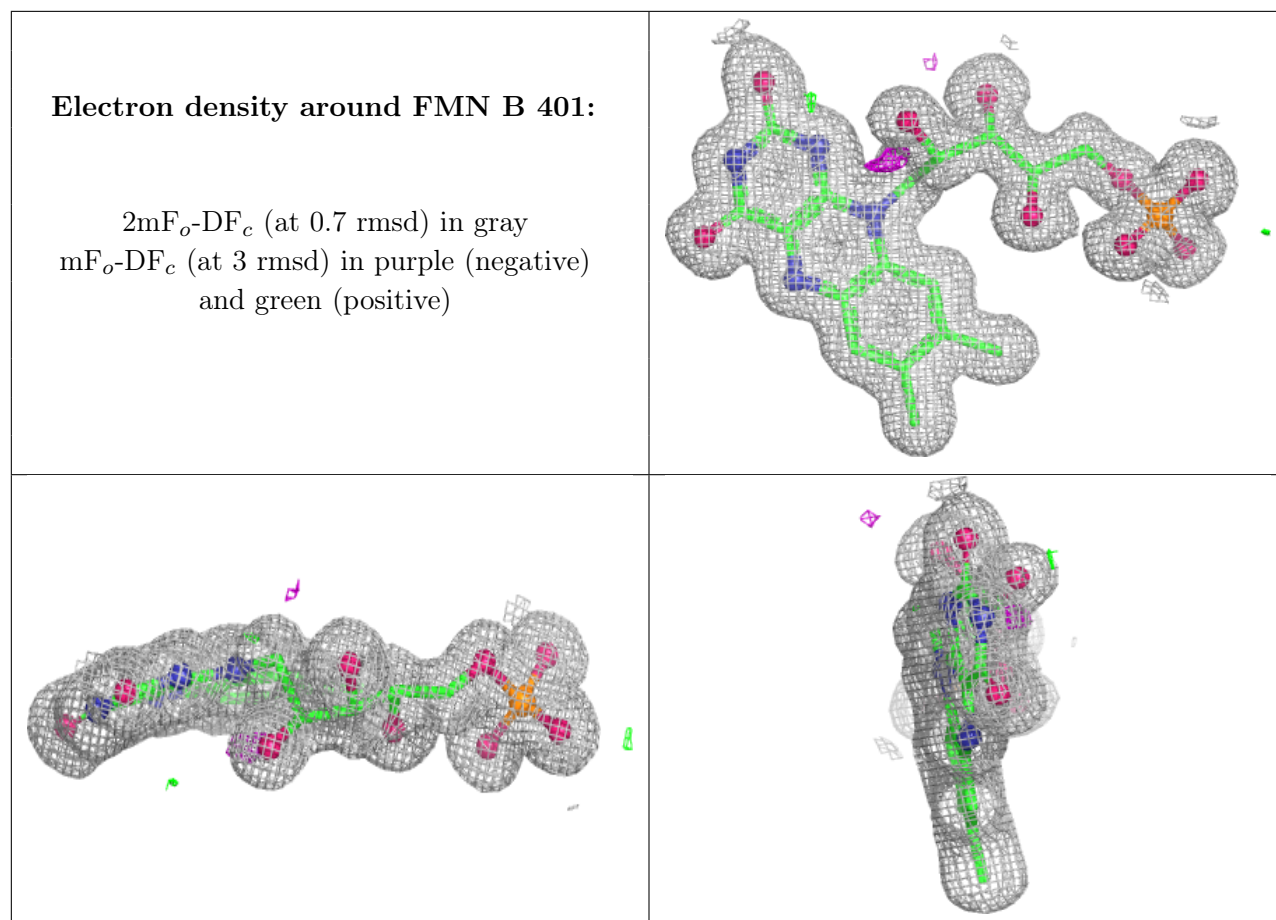
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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 ⓘ

There are no such residues in this entry.