



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2023 – 04:13 PM JST

PDB ID : 7F22
Title : L-lactate oxidase with pyruvate
Authors : Morimoto, Y.; Inaka, K.
Deposited on : 2021-06-10
Resolution : 1.41 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

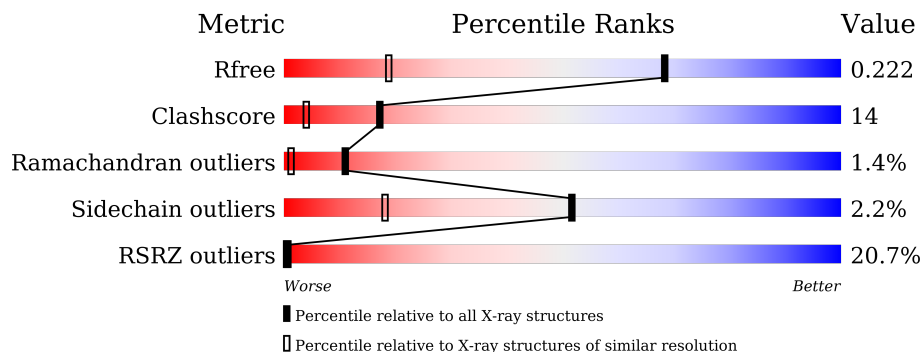
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.41 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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	736	
1	B	736	

2 Entry composition [i](#)

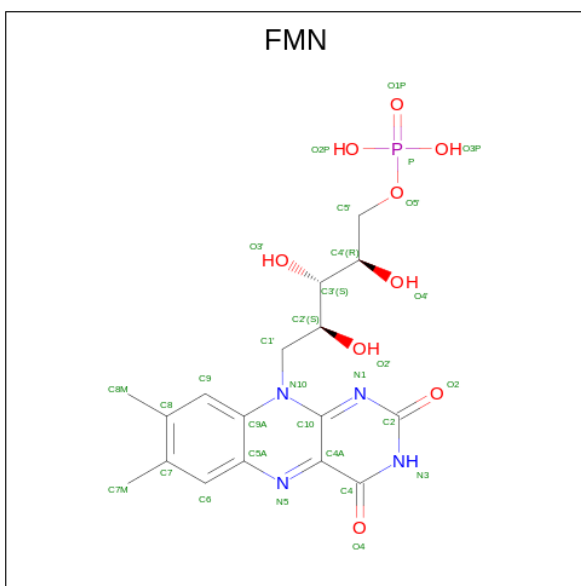
There are 4 unique types of molecules in this entry. The entry contains 6496 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

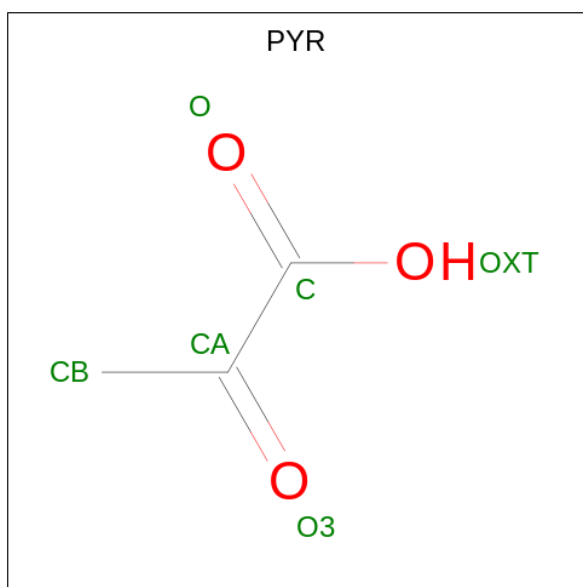
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	368	Total 2841	C 1795	N 494	O 545	S 7	0	0	0
1	B	368	Total 2841	C 1795	N 494	O 545	S 7	0	0	0

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: 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 PYRUVIC ACID (three-letter code: PYR) (formula: C₃H₄O₃) (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	361	Total	O	0	0
			361	361		
4	B	379	Total	O	0	0
			379	379		

S223	P224	R225	D226	I227	E228	E229	I230	A231	A232	E247	M251	R255	K289	R290	S297	D314	V315	V316	P321	V322	L323	F324	G325	L326	A327	L328	G329	G330	W331	Q332	G333	A334	Q355	E358	D367	Y370	G371	Y372	E373	Y374	GLU	TYR	ASN	ALA	PRO	SER	GLU	ILE																					
LYS	THR	THR	ILE	ASP	VAL	ASN	THR	THR	ASN	GLU	GLU	ALA	VAL	VAL	PRO	HIS	GLY	PHE	ASN	THR	ILE	ALA	GLY	SER	GLY	ASP	GLU	THR	THR	LYS	ARG	ALA	ASN	ASP	ARG	ALA	THR	TPP	LYS	HIS	LYS	LEU	LEU	TYR	PRO	ARG	GLU	TYR	ASN	ALA	PRO	SER	GLU	ILE															
ASP	THR	THR	THR	GLN	ILE	LEU	GLY	HIS	LYS	LYS	PRO	PHE	MET	ALA	ALA	ILE	HIS	GLY	LEU	ALA	HIS	THR	LYS	GLU	ALA	GLY	THR	ALA	ARG	ALA	VAL	SER	GLU	PHE	THR	THR	ILE	MET	SER	ILE	ILE	ASP	ALA	ALA	ALA	ALA	THR	PHE	GLU	ILE	GLU	GLU	GLU	GLU															
GLY	LEU	ASN	GLY	GLY	PRO	ARG	TRP	PHE	GLN	TYR	MET	ALA	LYS	ASP	GLN	ASN	ARG	ASP	ILE	ALA	LYS	SER	ASP	GLY	ALA	THR	THR	ALA	ILE	ILE	LEU	THR	ALA	ASP	SER	THR	VAL	SER	GLY	ASN	ARG	ASP	ASP	ASP	VAL	LYS	ASN	ALA	ALA	THR	PHE	GLU	TYR	PRO	PHE	GLY	GLY												
MET	PRO	ILE	VAL	GLN	ARG	TYR	LEU	ARG	GLY	ALA	GLY	MET	LYS	LEU	ASN	ILE	TYR	GLY	SER	ALA	ILE	LYS	SER	GLN	ALA	ASP	ILE	GLU	GLY	ILE	ALA	ALA	HIS	GLY	GLY	VAL	PHE	VAL	ARG	VAL	ARG	GLY	GLY	ILE	GLN	HIS	VAL	ALA	PRO	GLU	ASP	ALA	ALA	ASP	PRO	ALA	ALA	ASP	ALA	TYR	TYR	ALA	ALA	ASP	LYS				
ARG	GLY	ALA	SER	GLY	ILE	TRP	VAL	SER	ASN	HIS	GLY	ARG	GLN	TYR	ALA	PRO	TYR	SER	PHE	LEU	THR	ASP	THR	LEU	PRO	ALA	ILE	VAL	ARG	VAL	ASN	LYS	ARG	VAL	PHE	ASP	ASP	GLY	VAL	VAL	ARG	ARG	GLY	GLY	GLY	HIS	VAL	ALA	ALA	LYS	ASN	ASN	PRO	PRO	ALA	TYR	GLY	TYR	GLU	ALA	ASP	TYR	TYR	ALA	ASP	ALA	ASP	LYS	
VAL	VAL	ALA	LEU	GLY	PRO	VAL	LEU	LEU	PHE	GLY	LEU	GLY	GLN	TYR	GLY	ALA	TYR	SER	VAL	LEU	ASP	ASP	THR	LEU	PRO	ALA	ILE	VAL	ARG	VAL	ASN	LYS	ARG	VAL	PHE	ASN	VAL	VAL	ASP	ASP	GLY	LEU	LEU	HIS	VAL	PHE	ALA	ALA	LYS	ASN	ASN	PRO	PRO	ALA	TYR	GLY	TYR	GLU	ALA	ASP	ALA	ASP	TYR	TYR	ALA	ASP	ALA	ASP	LYS

4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	132.60Å 132.60Å 91.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.93 – 1.41 46.88 – 1.41	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.93-1.41) 99.8 (46.88-1.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.42Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.193 , 0.216 0.198 , 0.222	Depositor DCC
R_{free} test set	7774 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 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)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: FMN, PYR

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	0.76	0/2905	0.93	5/3937 (0.1%)
1	B	0.79	2/2905 (0.1%)	0.97	10/3937 (0.3%)
All	All	0.78	2/5810 (0.0%)	0.95	15/7874 (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	A	0	1
1	B	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	GLY	C-O	10.45	1.40	1.23
1	B	67	LEU	C-O	5.01	1.32	1.23

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	TYR	CB-CG-CD2	-9.64	115.22	121.00
1	B	324	PHE	CB-CA-C	8.39	127.18	110.40
1	A	370	TYR	CB-CG-CD1	8.18	125.91	121.00
1	B	370	TYR	CB-CG-CD2	-7.08	116.75	121.00
1	A	374	TYR	CA-C-O	-6.67	106.10	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ILE	Peptide
1	B	33	VAL	Peptide
1	B	330	GLY	Peptide
1	B	333	GLY	Peptide

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	2841	0	2772	29	0
1	B	2841	0	2772	130	0
2	A	31	0	19	1	0
2	B	31	0	19	0	0
3	A	6	0	0	1	0
3	B	6	0	0	0	0
4	A	361	0	0	9	3
4	B	379	0	0	26	2
All	All	6496	0	5582	158	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.

The worst 5 of 158 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:325:GLY:HA3	4:B:932:HOH:O	1.26	1.31
1:B:41:ILE:HD12	1:B:326:LEU:HD22	1.29	1.13
1:B:156:ASP:OD2	1:B:200:ARG:NE	1.83	1.12
1:B:38:PHE:HA	1:B:326:LEU:HD21	1.27	1.11
1:B:33:VAL:HG11	1:B:326:LEU:HA	1.09	1.07

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:1216:HOH:O	4:A:1216:HOH:O[3_655]	1.88	0.32
4:A:1150:HOH:O	4:A:1150:HOH:O[3_655]	1.92	0.28
4:B:1235:HOH:O	4:B:1235:HOH:O[3_655]	1.95	0.25
4:B:1043:HOH:O	4:B:1043:HOH:O[3_655]	1.99	0.21
4:A:1019:HOH:O	4:A:1019:HOH:O[3_655]	2.03	0.17

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	366/736 (50%)	355 (97%)	9 (2%)	2 (0%)	29	8
1	B	366/736 (50%)	343 (94%)	15 (4%)	8 (2%)	6	0
All	All	732/1472 (50%)	698 (95%)	24 (3%)	10 (1%)	11	1

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ARG
1	A	297	SER
1	B	200	ARG
1	B	297	SER
1	B	324	PHE

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	292/584 (50%)	288 (99%)	4 (1%)	67	38
1	B	292/584 (50%)	283 (97%)	9 (3%)	40	9
All	All	584/1168 (50%)	571 (98%)	13 (2%)	52	18

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	195	MET
1	B	199	GLN
1	B	328	LEU
1	B	224	PRO
1	B	225	ARG

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	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
3	PYR	B	802	-	5,5,5	3.01	2 (40%)	3,6,6	2.04	1 (33%)
3	PYR	A	802	-	5,5,5	3.06	2 (40%)	3,6,6	1.44	0
2	FMN	A	801	-	33,33,33	0.74	0	48,50,50	0.81	1 (2%)
2	FMN	B	801	-	33,33,33	0.91	0	48,50,50	0.87	1 (2%)

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	PYR	B	802	-	-	0/4/4/4	-
3	PYR	A	802	-	-	0/4/4/4	-
2	FMN	A	801	-	-	2/18/18/18	0/3/3/3
2	FMN	B	801	-	-	1/18/18/18	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	PYR	CA-C	-6.41	1.31	1.54
3	A	802	PYR	CA-C	-5.74	1.33	1.54
3	A	802	PYR	OXT-C	-3.32	1.20	1.30
3	B	802	PYR	OXT-C	-2.00	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	PYR	OXT-C-CA	2.95	122.03	113.97
2	A	801	FMN	O5'-C5'-C4'	2.24	115.34	109.36
2	B	801	FMN	C4-N3-C2	-2.18	121.62	125.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

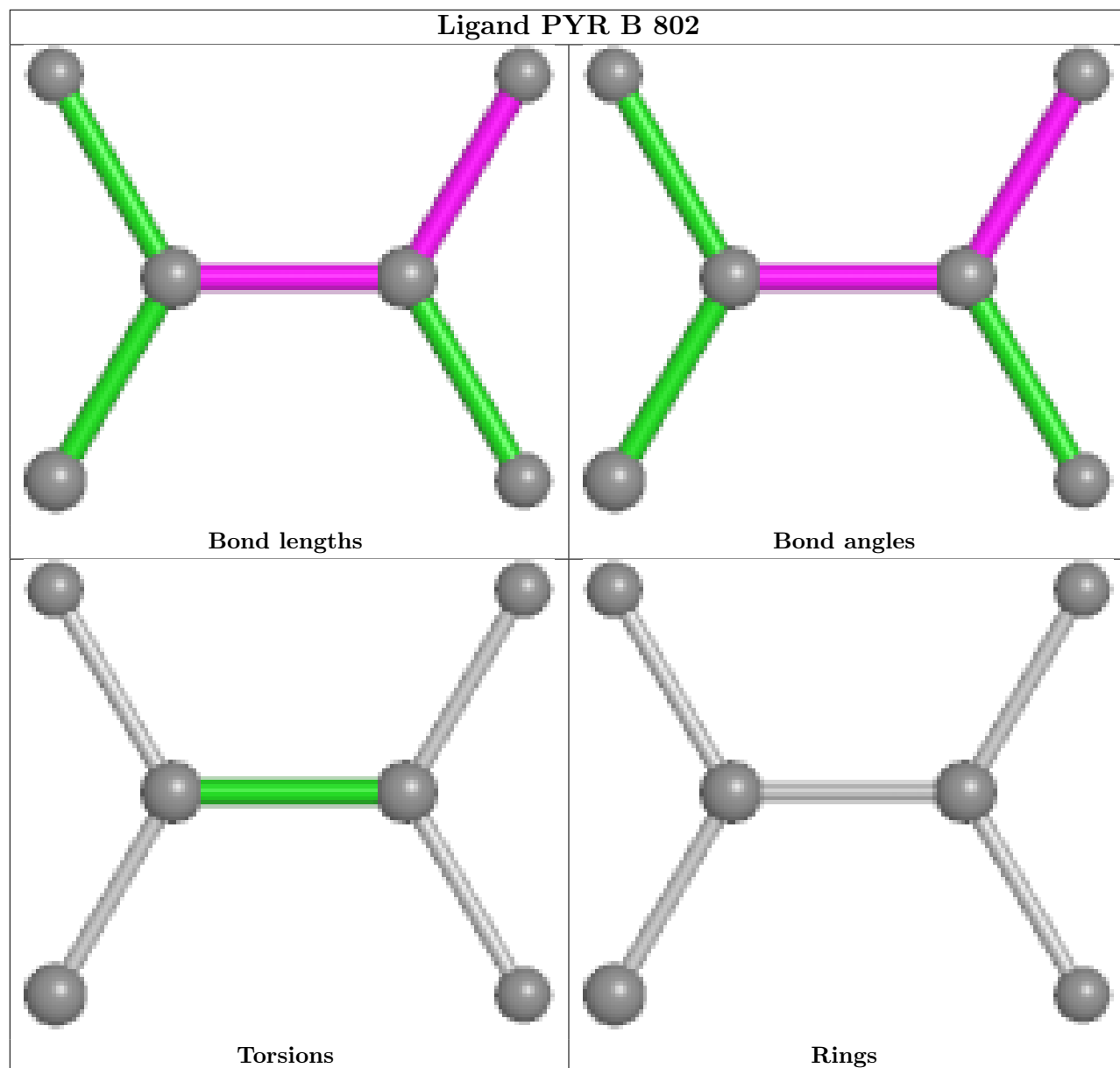
Mol	Chain	Res	Type	Atoms
2	A	801	FMN	C5'-O5'-P-O1P
2	A	801	FMN	C4'-C5'-O5'-P
2	B	801	FMN	C4'-C5'-O5'-P

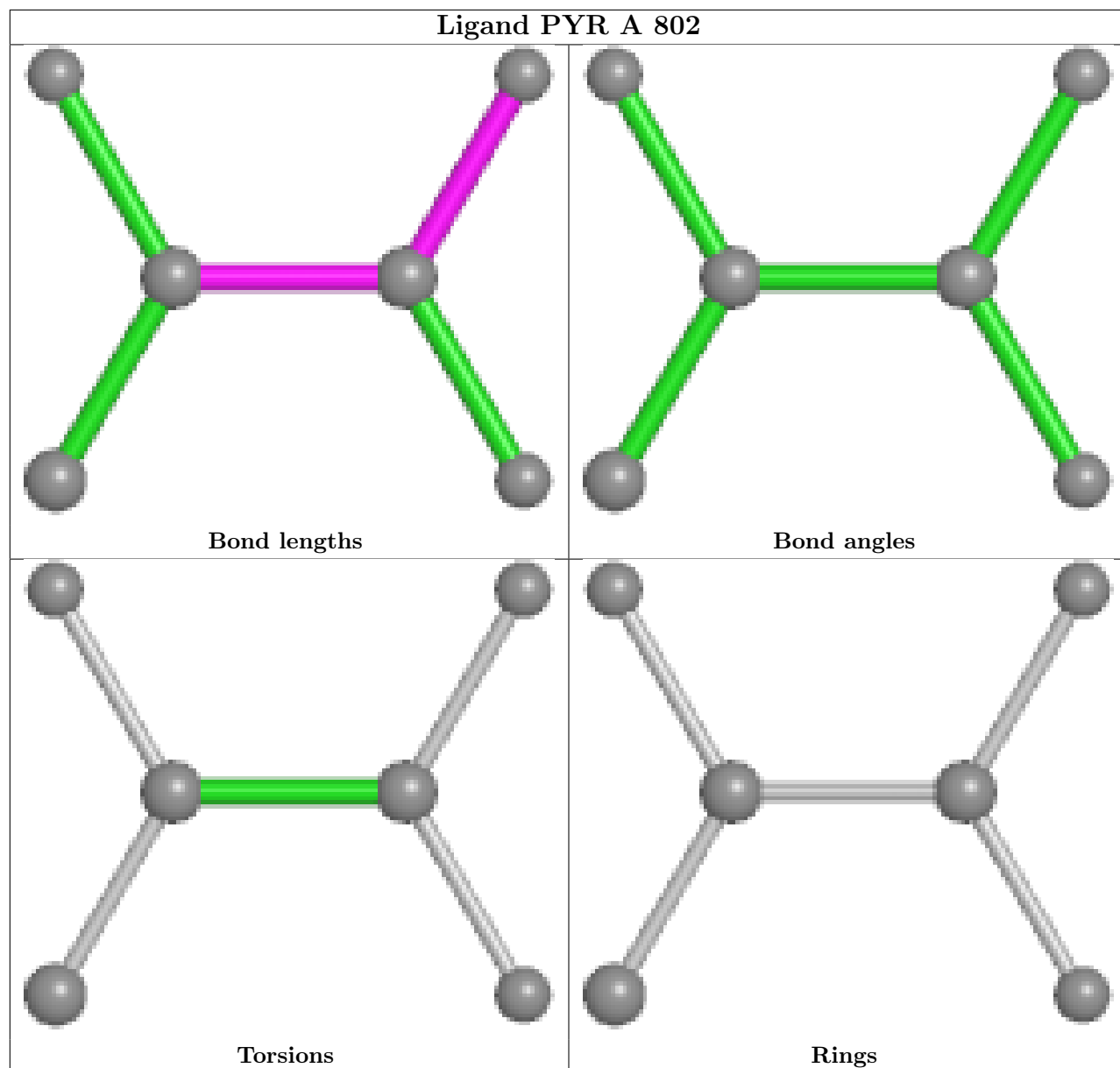
There are no ring outliers.

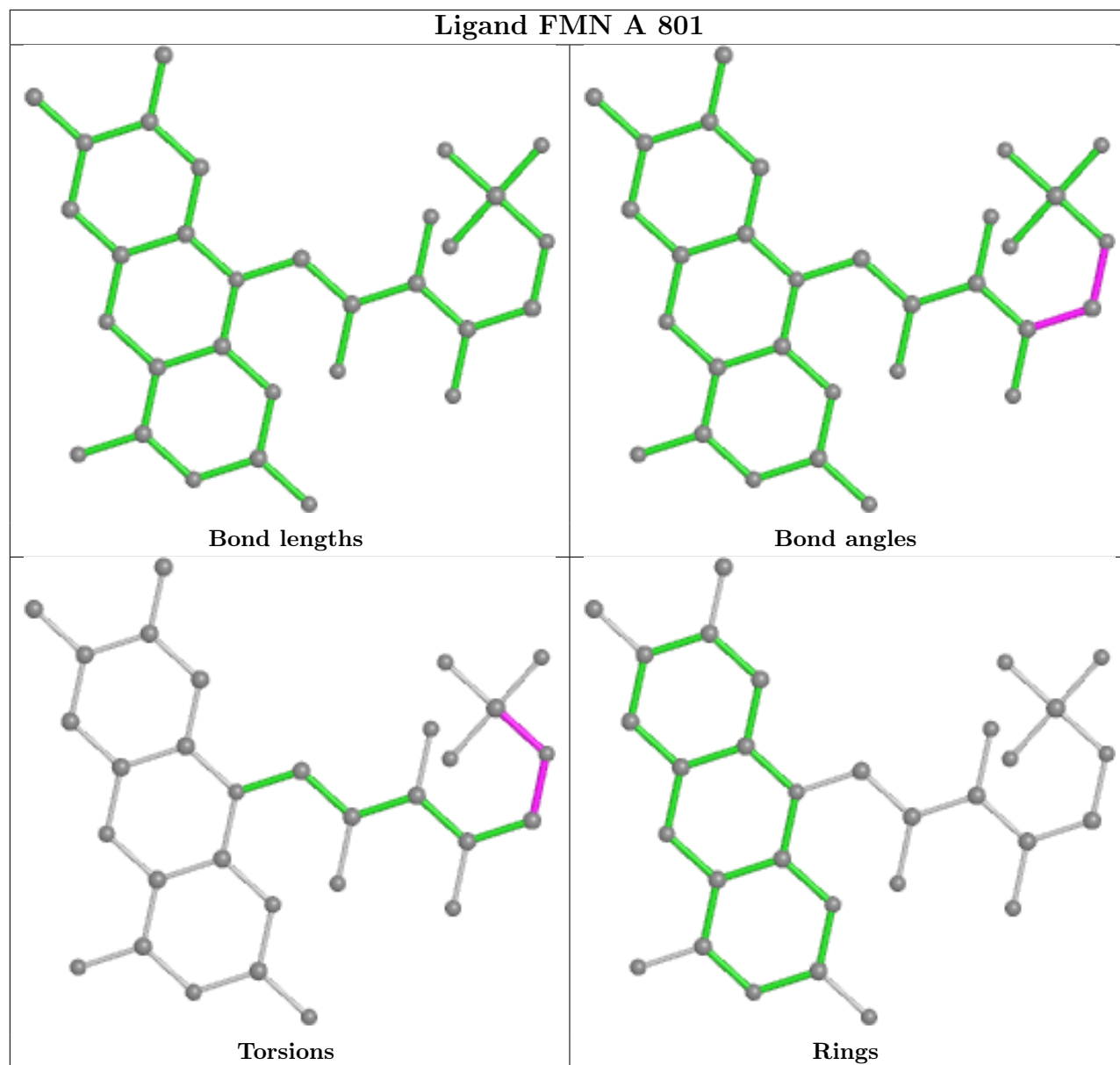
2 monomers are involved in 1 short contact:

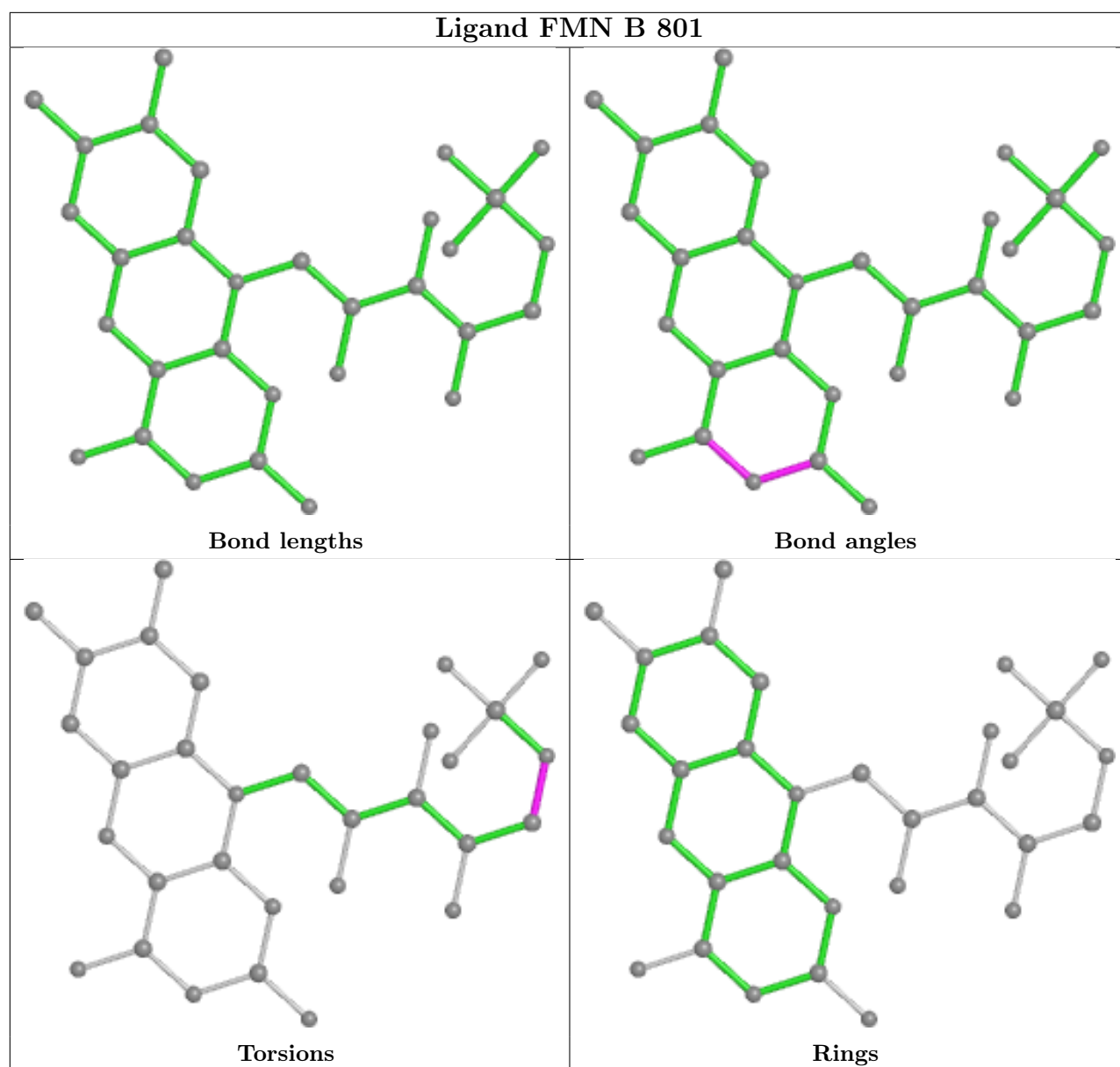
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	PYR	1	0
2	A	801	FMN	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	368/736 (50%)	1.25	70 (19%) 1 0	12, 20, 44, 119	0
1	B	368/736 (50%)	2.62	82 (22%) 0 0	12, 20, 93, 206	0
All	All	736/1472 (50%)	1.93	152 (20%) 1 0	12, 20, 62, 206	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	LEU	71.5
1	B	326	LEU	43.5
1	B	330	GLY	40.5
1	B	32	VAL	40.1
1	B	206	ALA	37.1

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](#)

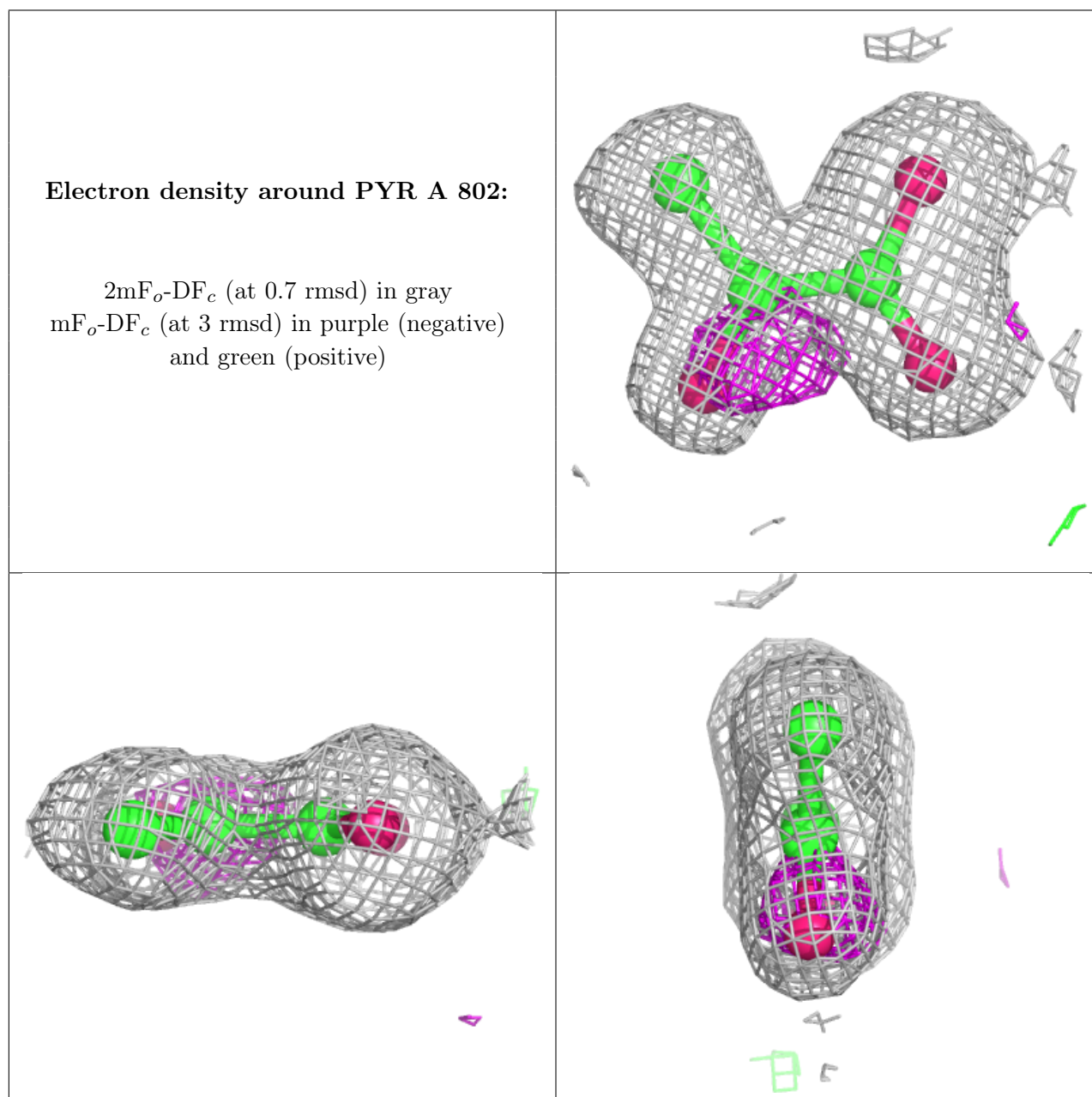
There are no monosaccharides in this entry.

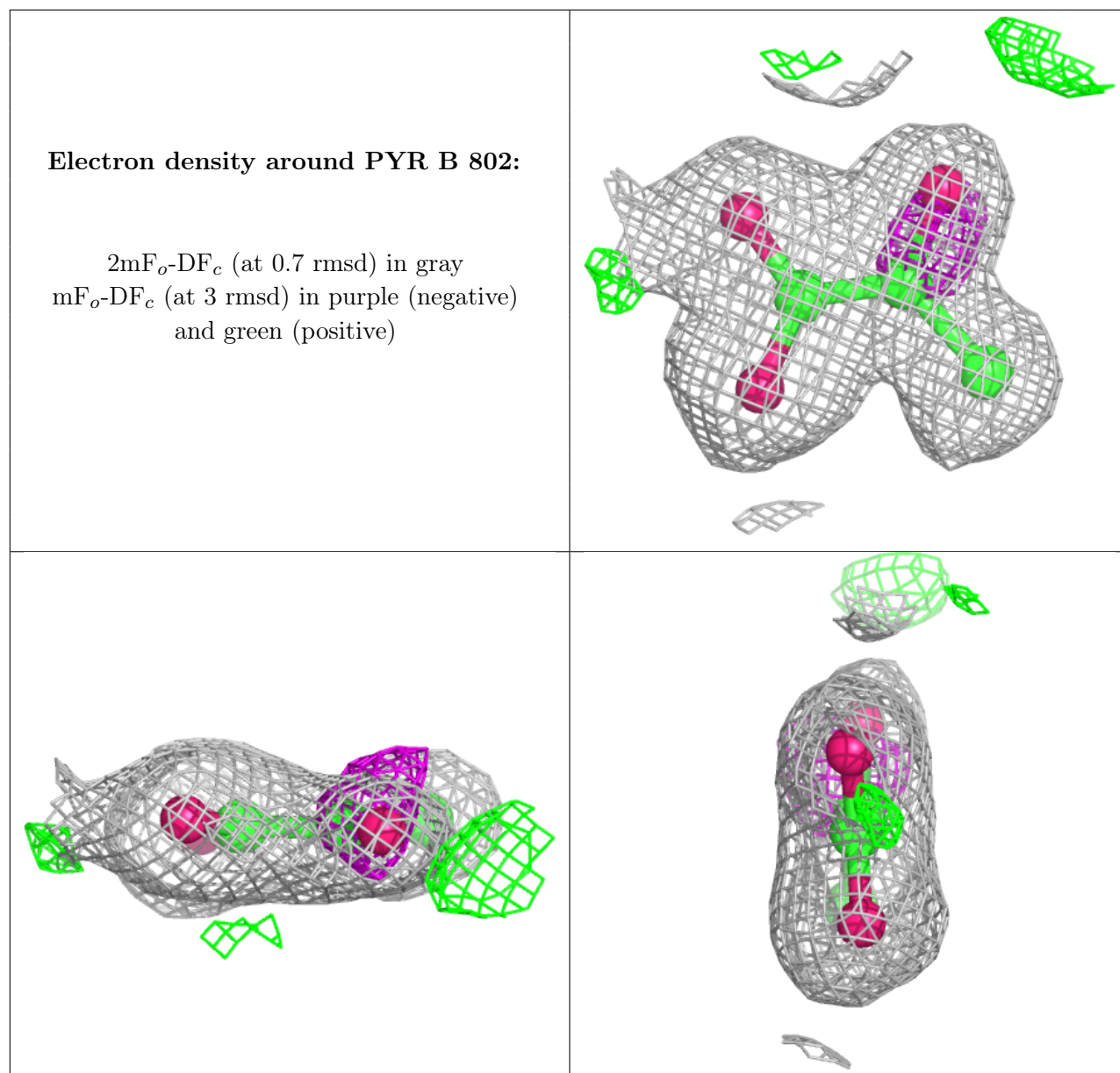
6.4 Ligands [i](#)

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, 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(\AA^2)	Q<0.9
3	PYR	A	802	6/6	0.81	0.14	24,26,28,30	0
3	PYR	B	802	6/6	0.83	0.17	26,28,29,31	0
2	FMN	A	801	31/31	0.96	0.08	13,15,18,19	0
2	FMN	B	801	31/31	0.96	0.09	13,15,18,18	0

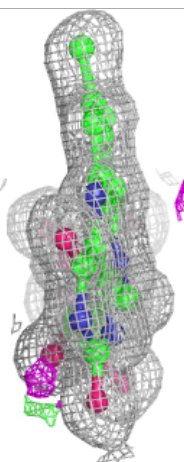
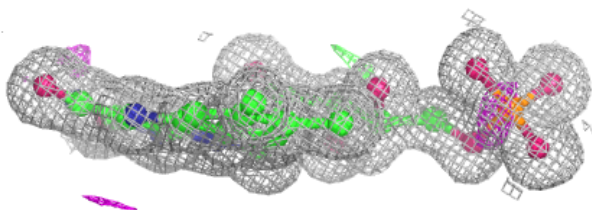
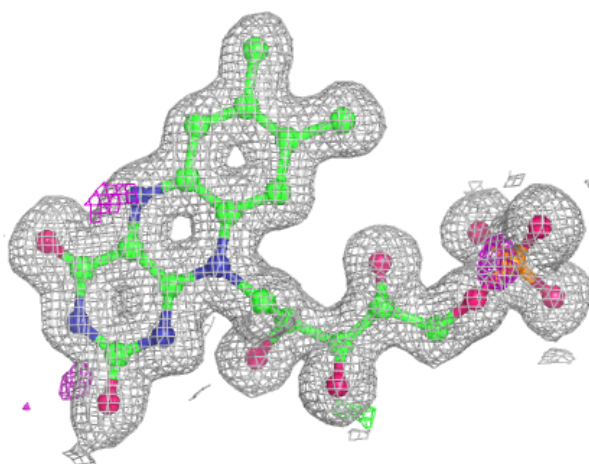
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

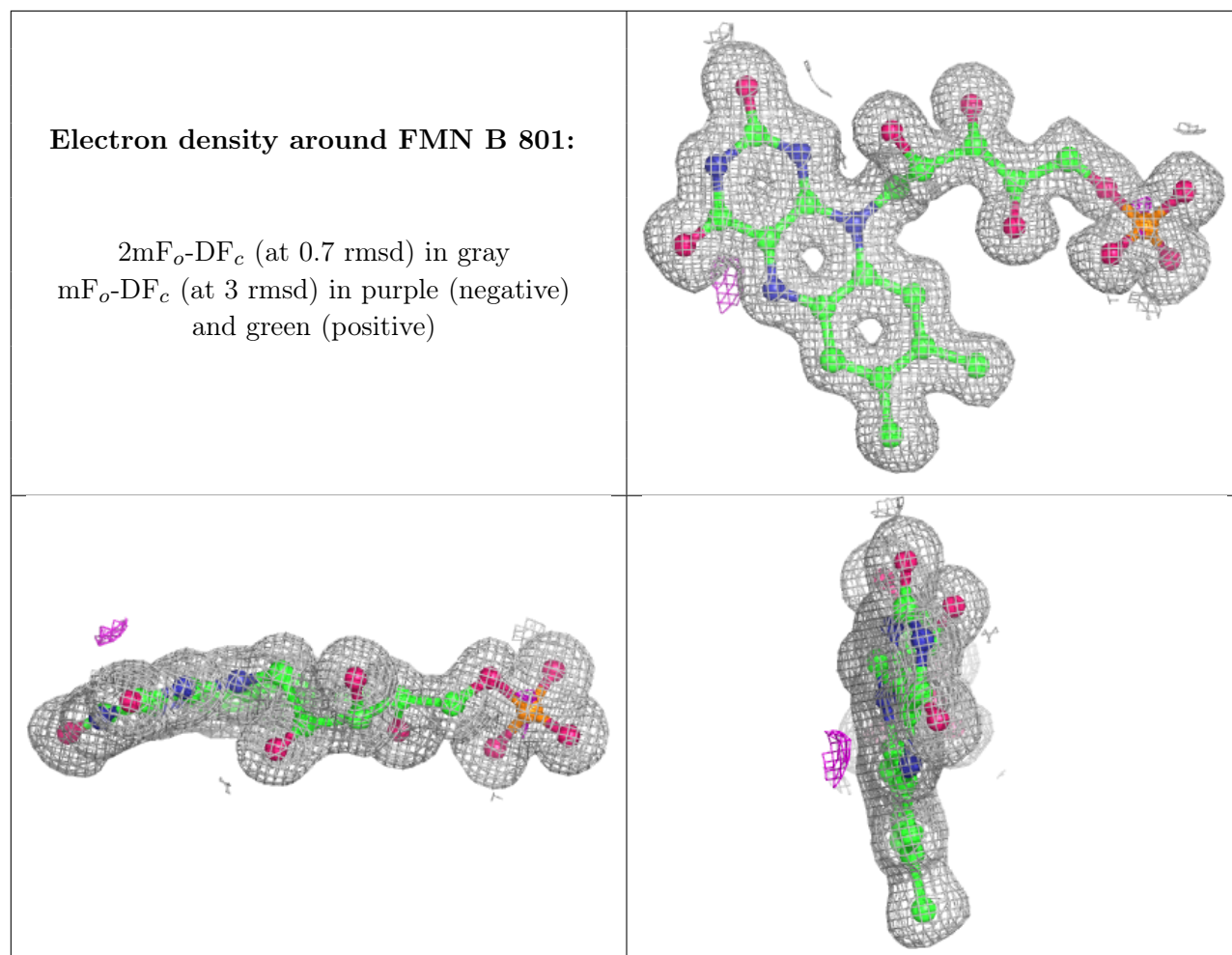




Electron density around FMN A 801:

$2mF_o-DF_c$ (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.