



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2023 – 05:22 PM JST

PDB ID : 5ZT0  
Title : Crystal Structure of Protein Phosphate 1 Complexed with PP1 binding domain of GL  
Authors : Yu, J.; Xiang, S.  
Deposited on : 2018-05-01  
Resolution : 3.32 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](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.

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)  
Xtrriage (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

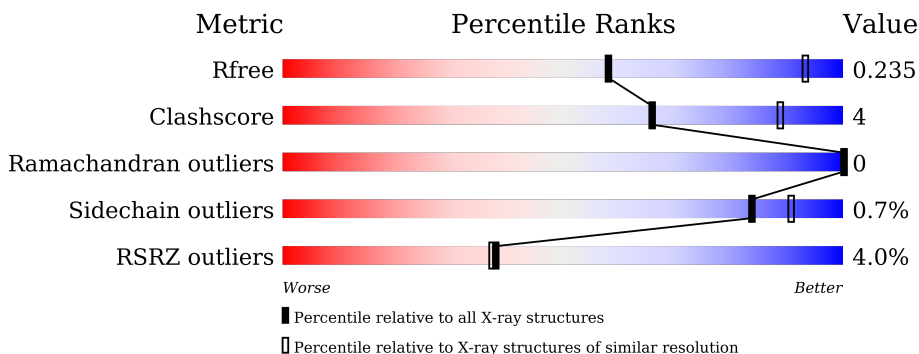
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.32 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	294	90% (green), 9% (yellow)
1	B	294	3% (red), 86% (green), 13% (yellow)
1	C	294	2% (red), 90% (green), 10% (yellow)
1	D	294	4% (red), 86% (green), 14% (yellow)
1	E	294	6% (red), 89% (green), 10% (yellow)
1	F	294	9% (red), 88% (green), 12% (yellow)

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	G	75	<p>% 19% 7% 75%</p>
2	H	75	<p>% 17% 8% 75%</p>
2	I	75	<p>4% 19% 7% 75%</p>
2	J	75	<p>20% 5% 75%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14774 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 Serine/threonine-protein phosphatase PP1-alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2358	1510	397	433	18	0	0	0
1	B	293	2358	1510	397	433	18	0	0	0
1	C	293	2358	1510	397	433	18	0	0	0
1	D	293	2358	1510	397	433	18	0	0	0
1	E	293	2358	1510	397	433	18	0	0	0
1	F	293	2358	1510	397	433	18	0	0	0

- Molecule 2 is a protein called Protein phosphatase 1 regulatory subunit 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	19	146	93	27	25	1	0	0	0
2	H	19	146	93	27	25	1	0	0	0
2	I	19	146	93	27	25	1	0	0	0
2	J	19	146	93	27	25	1	0	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

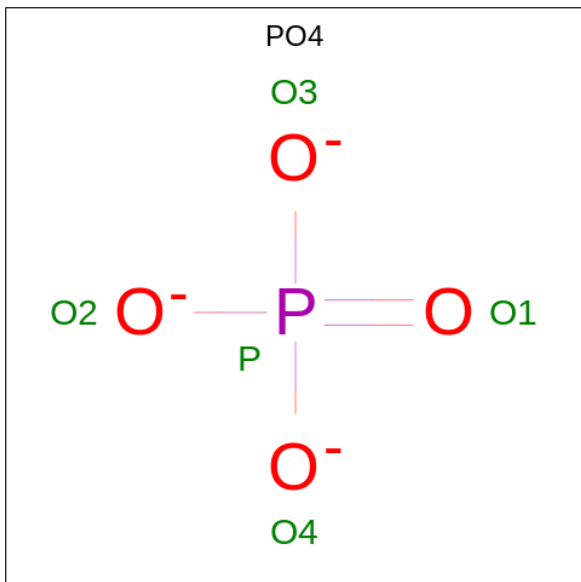
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mn	0	0
			2	2		
3	C	2	Total	Mn	0	0
			2	2		
3	D	2	Total	Mn	0	0
			2	2		
3	E	2	Total	Mn	0	0
			2	2		
3	F	2	Total	Mn	0	0
			2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

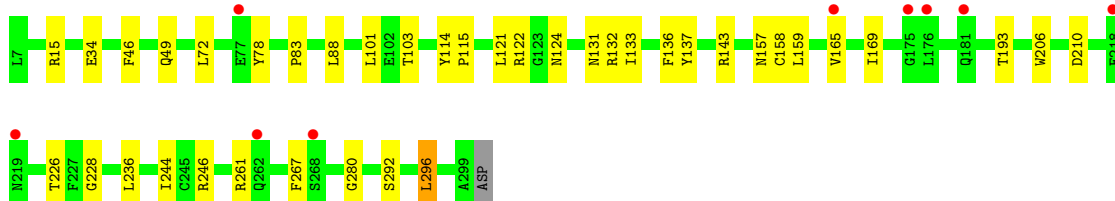
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit

Chain A:  90% 9%




- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit

Chain B:  3% 86% 13%




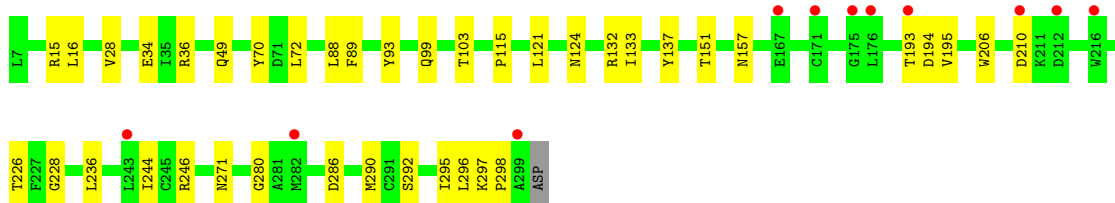
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit

Chain C:  2% 90% 10%

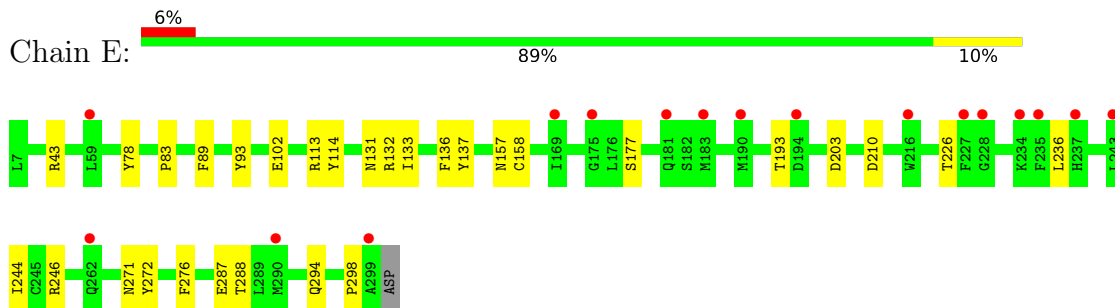


- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit

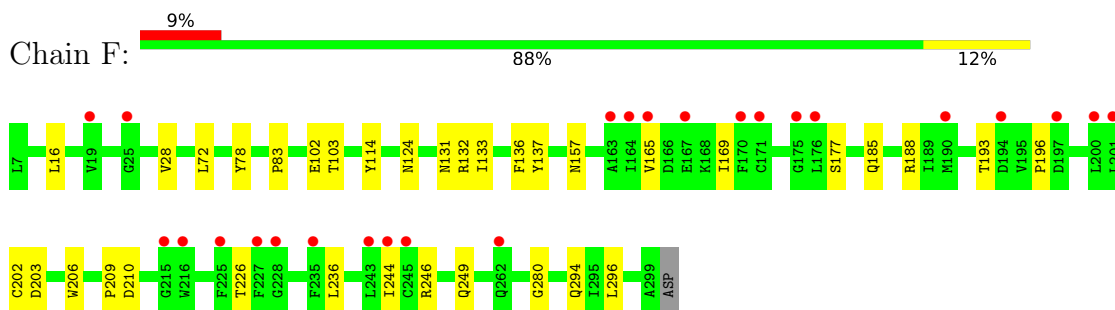
Chain D:  4% 86% 14%



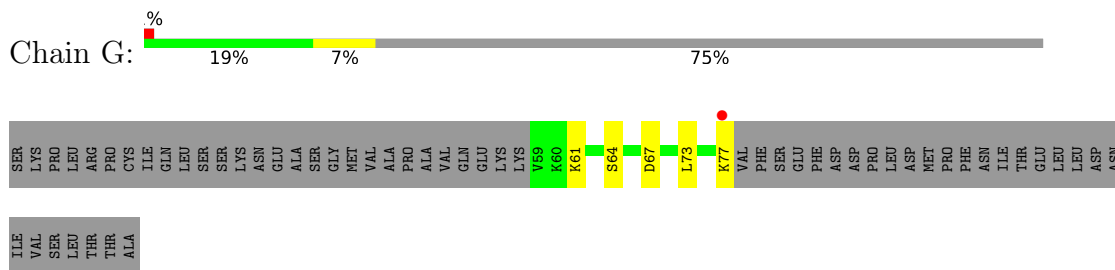
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



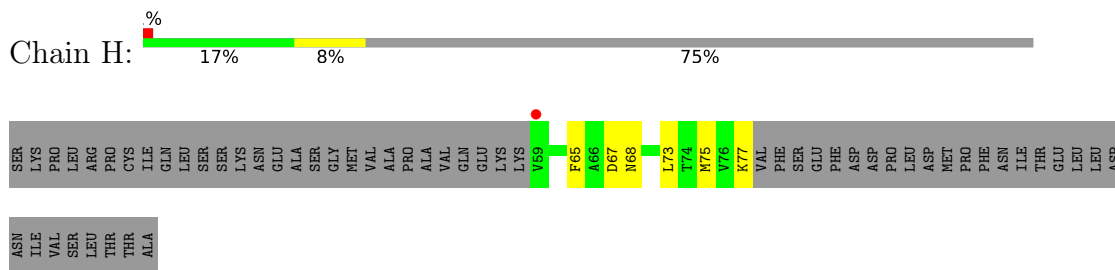
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



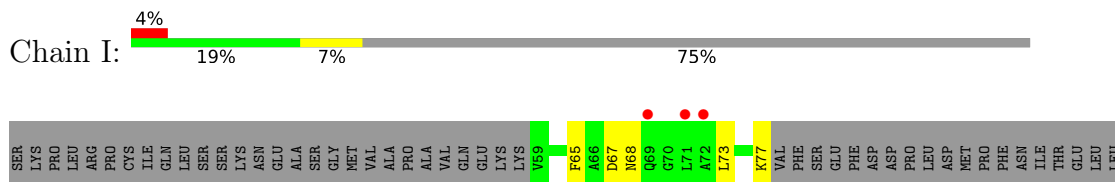
- Molecule 2: Protein phosphatase 1 regulatory subunit 3B



- Molecule 2: Protein phosphatase 1 regulatory subunit 3B



- Molecule 2: Protein phosphatase 1 regulatory subunit 3B



ASP  
ASN  
ILE  
VAL  
SER  
LEU  
THR  
THR  
ALA

● Molecule 2: Protein phosphatase 1 regulatory subunit 3B

Chain J:  20% 5% 75%

SER  
LYS  
PRO  
LEU  
LEU  
ARG  
PRO  
CYS  
ILE  
GLN  
LEU  
SER  
SER  
LYS  
ASN  
GLU  
ALA  
SER  
GLY  
MET  
VAL  
ALA  
PRO  
ALA  
VAL  
GLN  
GLU  
LYS  
LYS  
V59  
D67  
L73  
T74  
K77  
VAL  
PHE  
SER  
GLU  
PHE  
ASP  
ASP  
PRO  
LEU  
ASP  
MET  
PRO  
PHE  
ASN  
ILE  
THR  
GLU  
LEU  
LEU  
ASP  
ASN  
ILE  
VAL  
SER

LEU  
THR  
THR  
ALA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.53Å 106.53Å 187.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.79 – 3.32 41.79 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.79-3.32) 99.8 (41.79-3.32)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.32Å)	Xtrriage
Refinement program	REFMAC 5.8.0222, PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.200 , 0.233 0.209 , 0.235	Depositor DCC
$R_{free}$ test set	1748 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.4	Xtrriage
Anisotropy	0.332	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l 0.013 for h,-h-k,-l 0.207 for -k,-h,-l	Xtrriage
Reported twinning fraction	0.410 for H, K, L 0.103 for K, H, -L 0.097 for -h,-k,l 0.390 for -K, -H, -L	Depositor
Outliers	0 of 35074 reflections	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: MN, PO4

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	0.25	0/2412	0.43	0/3259
1	B	0.25	0/2412	0.42	0/3259
1	C	0.25	0/2412	0.42	0/3259
1	D	0.25	0/2412	0.42	0/3259
1	E	0.25	0/2412	0.42	0/3259
1	F	0.25	0/2412	0.42	0/3259
2	G	0.37	0/146	0.50	0/193
2	H	0.32	0/146	0.51	0/193
2	I	0.29	0/146	0.58	0/193
2	J	0.28	0/146	0.50	0/193
All	All	0.25	0/15056	0.43	0/20326

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	2358	0	2318	17	0
1	B	2358	0	2318	23	0
1	C	2358	0	2318	17	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2358	0	2318	23	0
1	E	2358	0	2318	17	0
1	F	2358	0	2318	19	0
2	G	146	0	161	4	0
2	H	146	0	161	4	0
2	I	146	0	161	5	0
2	J	146	0	161	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
All	All	14774	0	14552	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 117 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:C:294:GLN:HA	2:H:75:MET:HB2	1.60	0.82
1:A:133:ILE:HG23	1:E:133:ILE:HG23	1.64	0.79
1:C:133:ILE:HG23	1:F:133:ILE:HG23	1.65	0.77
1:B:78:TYR:CE1	2:I:77:LYS:HD2	2.23	0.74
1:B:133:ILE:HG23	1:D:133:ILE:HG23	1.71	0.72

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	291/294 (99%)	272 (94%)	19 (6%)	0	100	100
1	B	291/294 (99%)	273 (94%)	18 (6%)	0	100	100
1	C	291/294 (99%)	269 (92%)	22 (8%)	0	100	100
1	D	291/294 (99%)	270 (93%)	21 (7%)	0	100	100
1	E	291/294 (99%)	270 (93%)	21 (7%)	0	100	100
1	F	291/294 (99%)	273 (94%)	18 (6%)	0	100	100
2	G	17/75 (23%)	17 (100%)	0	0	100	100
2	H	17/75 (23%)	16 (94%)	1 (6%)	0	100	100
2	I	17/75 (23%)	16 (94%)	1 (6%)	0	100	100
2	J	17/75 (23%)	16 (94%)	1 (6%)	0	100	100
All	All	1814/2064 (88%)	1692 (93%)	122 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/259 (100%)	256 (99%)	2 (1%)	81	89
1	B	258/259 (100%)	256 (99%)	2 (1%)	81	89
1	C	258/259 (100%)	256 (99%)	2 (1%)	81	89
1	D	258/259 (100%)	257 (100%)	1 (0%)	91	95

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	258/259 (100%)	257 (100%)	1 (0%)	91	95
1	F	258/259 (100%)	257 (100%)	1 (0%)	91	95
2	G	16/67 (24%)	16 (100%)	0	100	100
2	H	16/67 (24%)	16 (100%)	0	100	100
2	I	16/67 (24%)	16 (100%)	0	100	100
2	J	16/67 (24%)	14 (88%)	2 (12%)	4	19
All	All	1612/1822 (88%)	1601 (99%)	11 (1%)	84	91

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	246	ARG
1	F	246	ARG
2	J	67	ASP
2	J	59	VAL
1	C	246	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	D	403	3	4,4,4	0.83	0	6,6,6	0.44	0
4	PO4	B	403	3	4,4,4	0.91	0	6,6,6	0.46	0
4	PO4	A	403	3	4,4,4	0.89	0	6,6,6	0.38	0
4	PO4	C	403	3	4,4,4	0.83	0	6,6,6	0.47	0
4	PO4	E	403	3	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	F	403	3	4,4,4	0.89	0	6,6,6	0.47	0

There are no bond length outliers.

There are no bond angle outliers.

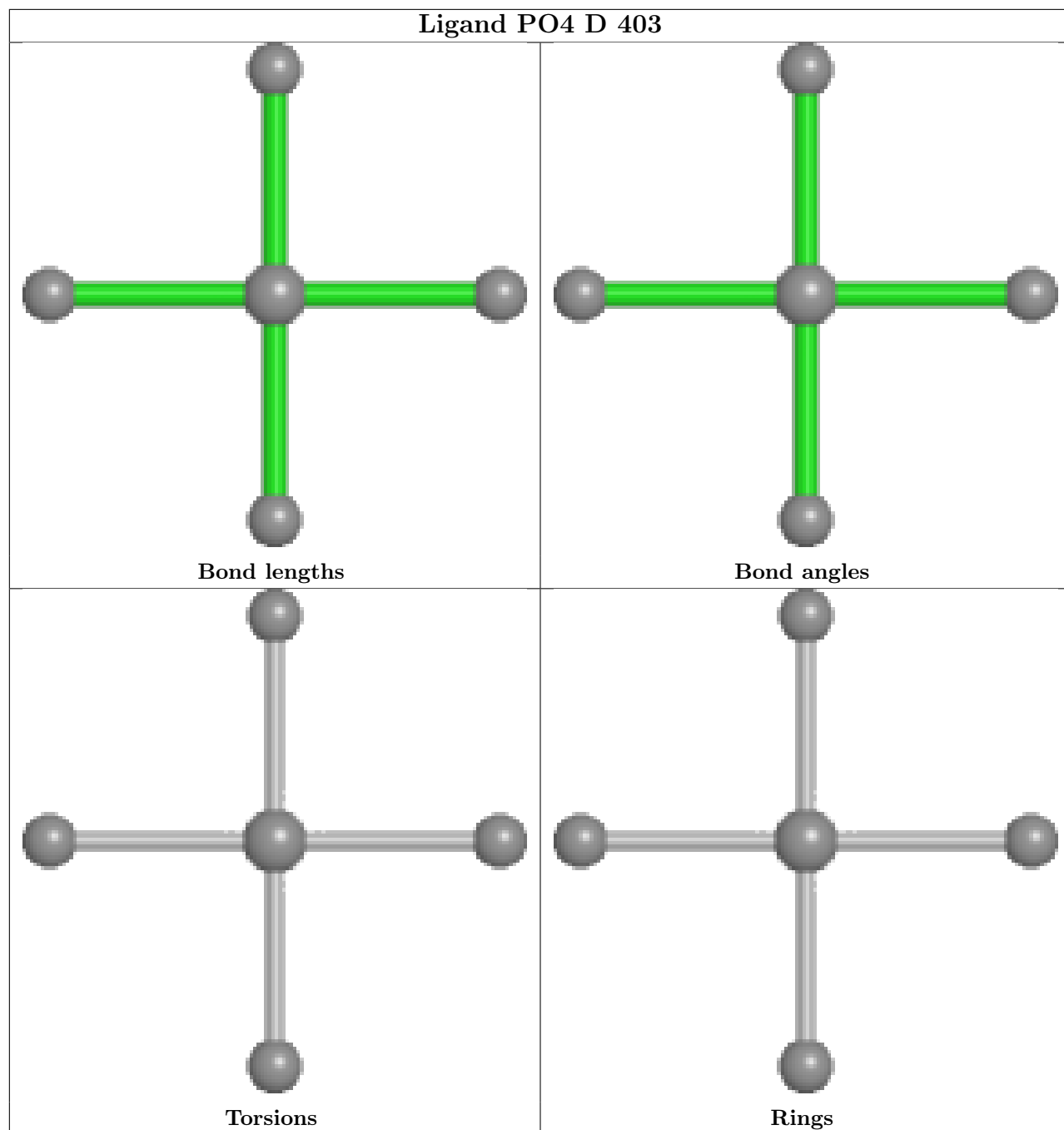
There are no chirality outliers.

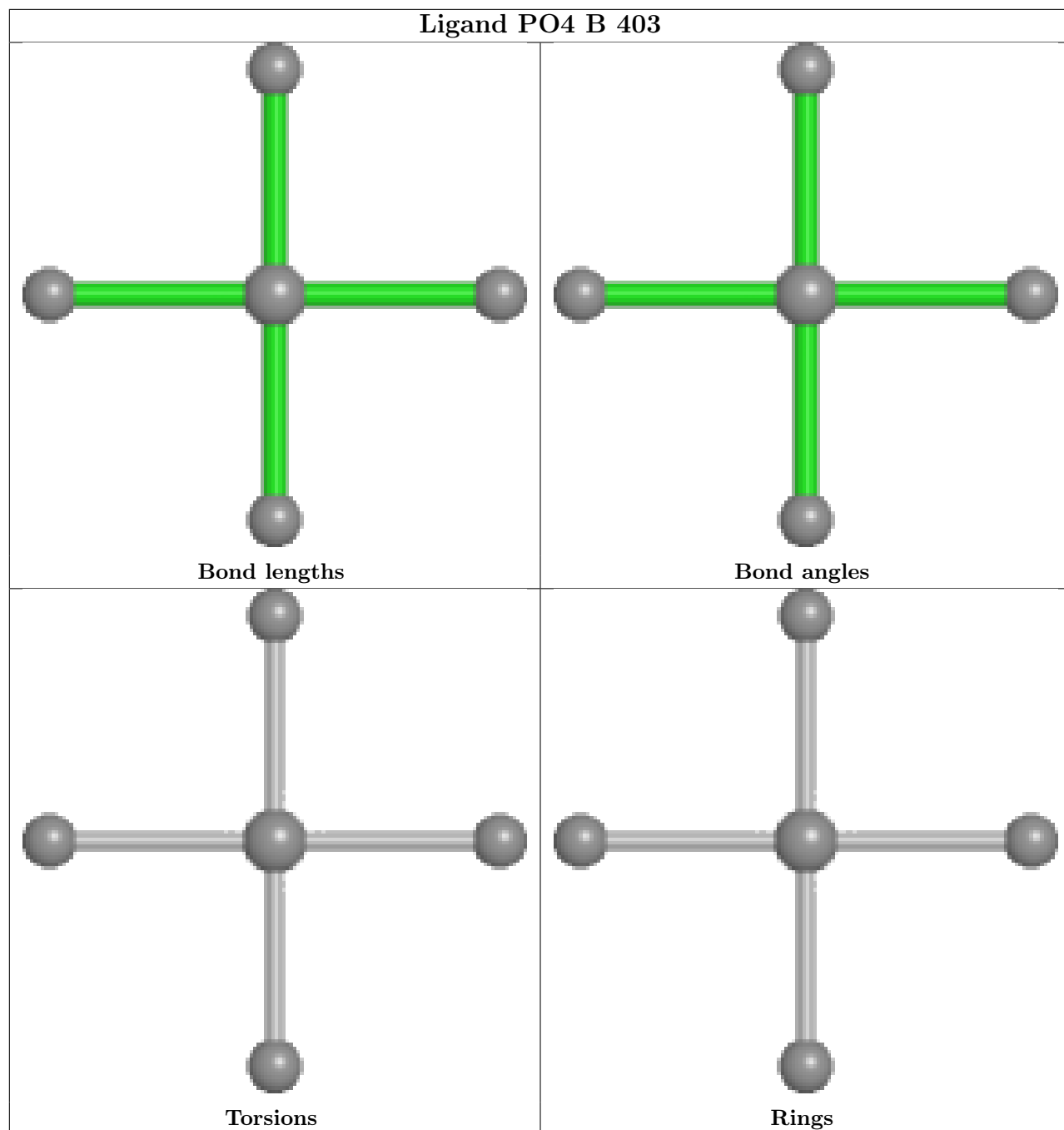
There are no torsion outliers.

There are no ring outliers.

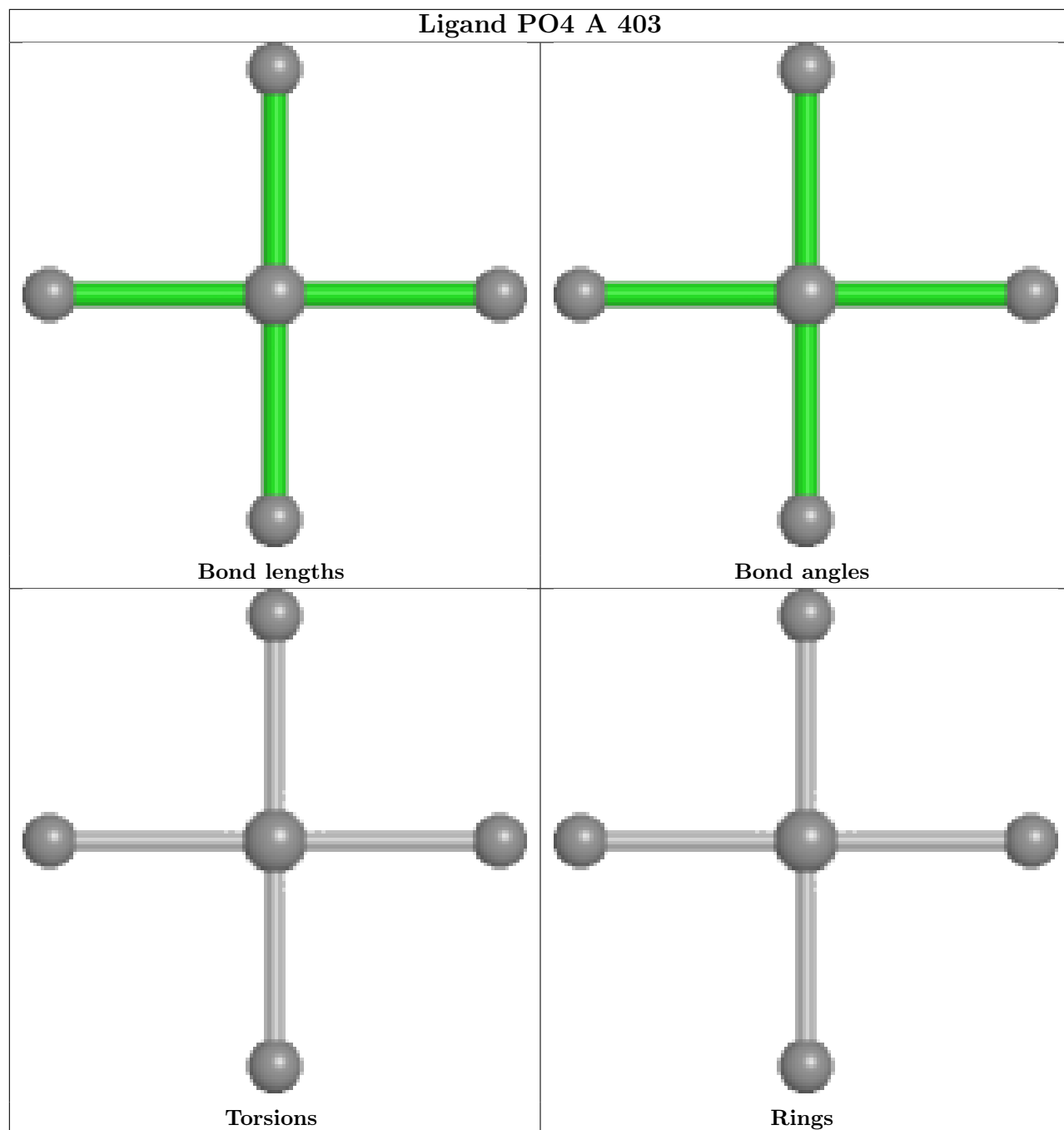
No monomer is involved in short contacts.

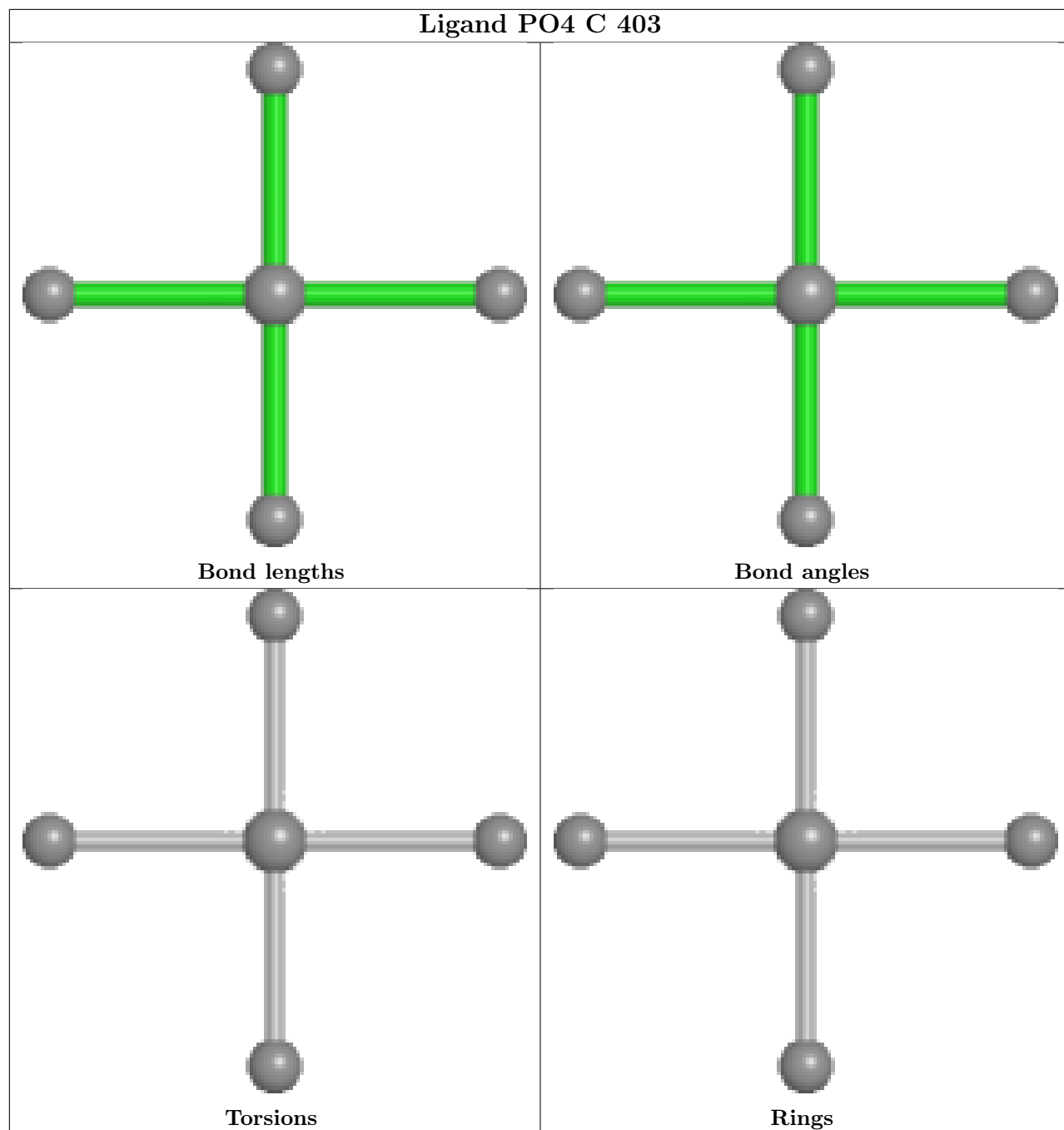
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be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

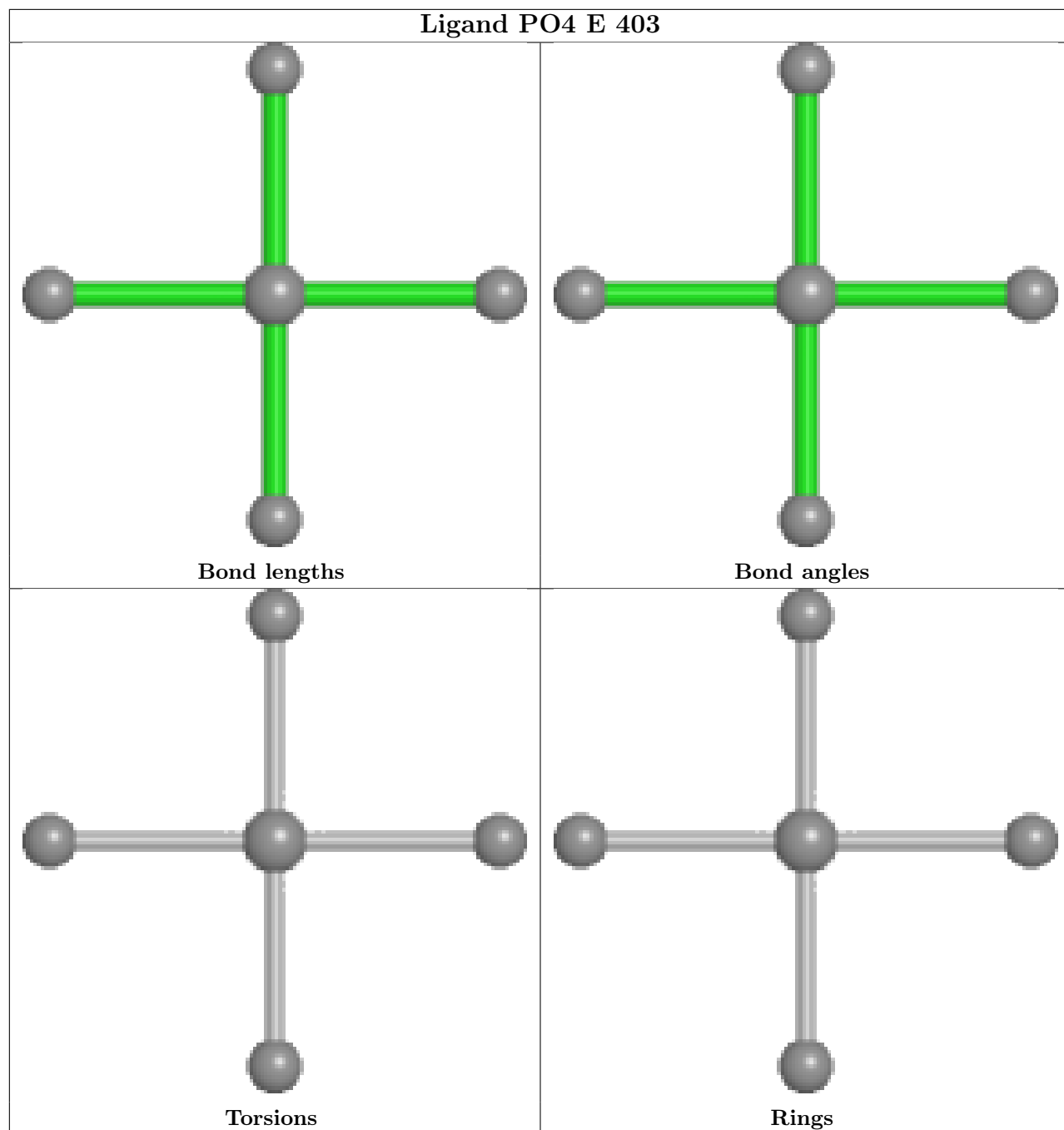


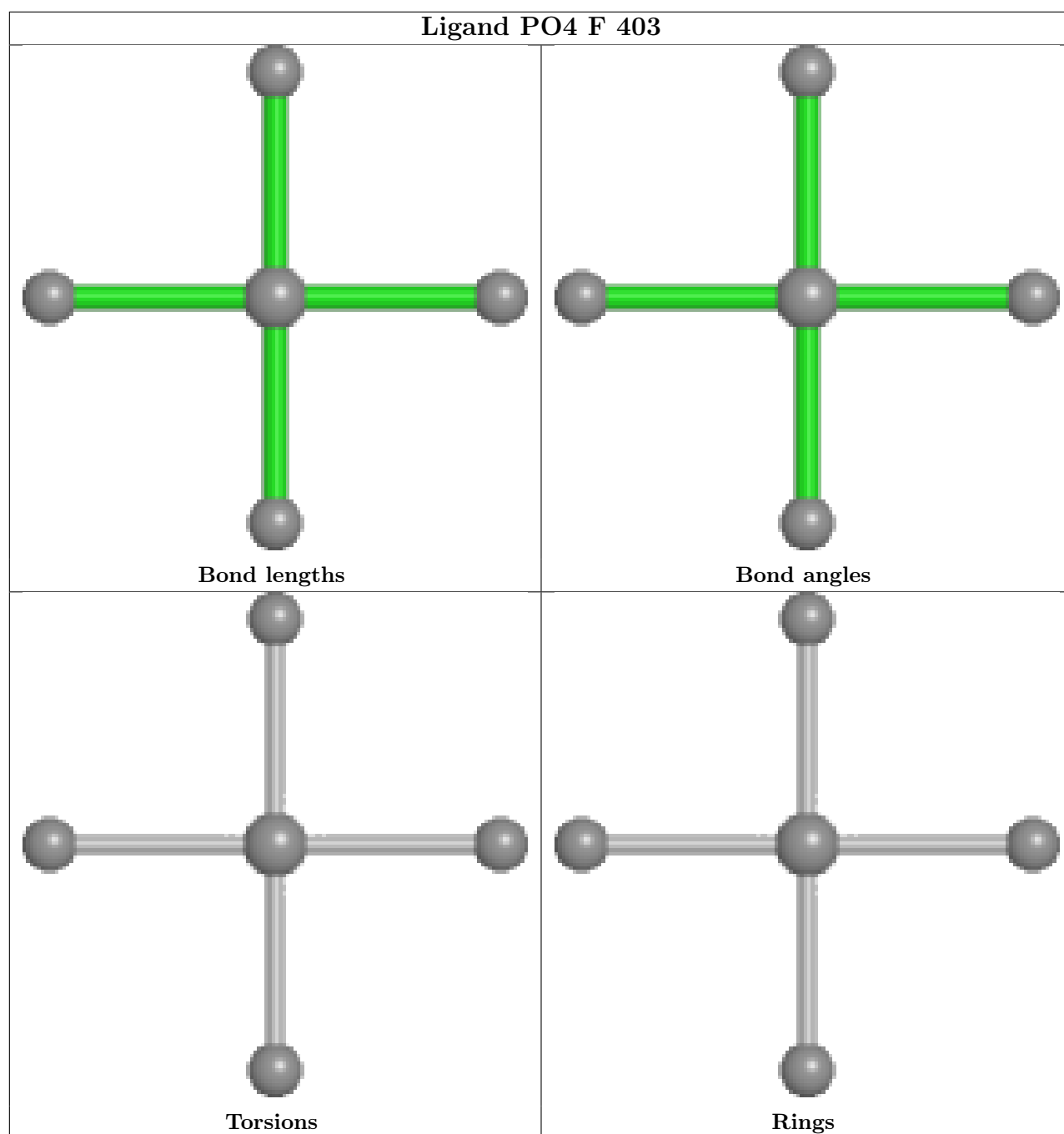












### 5.7 Other polymers [i](#)

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, 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	293/294 (99%)	-0.00	1 (0%) 94 95	69, 96, 124, 155	0
1	B	293/294 (99%)	0.10	9 (3%) 49 48	69, 107, 142, 204	0
1	C	293/294 (99%)	0.00	5 (1%) 70 68	65, 92, 124, 143	0
1	D	293/294 (99%)	0.07	11 (3%) 40 39	72, 104, 132, 153	0
1	E	293/294 (99%)	0.19	17 (5%) 23 24	74, 111, 155, 194	0
1	F	293/294 (99%)	0.31	25 (8%) 10 11	76, 116, 163, 214	0
2	G	19/75 (25%)	0.57	1 (5%) 26 26	90, 113, 135, 139	0
2	H	19/75 (25%)	0.61	1 (5%) 26 26	86, 108, 140, 141	0
2	I	19/75 (25%)	0.57	3 (15%) 2 1	104, 120, 143, 151	0
2	J	19/75 (25%)	0.31	0 100 100	102, 114, 128, 132	0
All	All	1834/2064 (88%)	0.13	73 (3%) 38 37	65, 104, 146, 214	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	176	LEU	7.5
1	F	243	LEU	6.5
1	C	291	CYS	5.7
1	D	175	GLY	5.6
1	E	216	TRP	5.5

### 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](#)

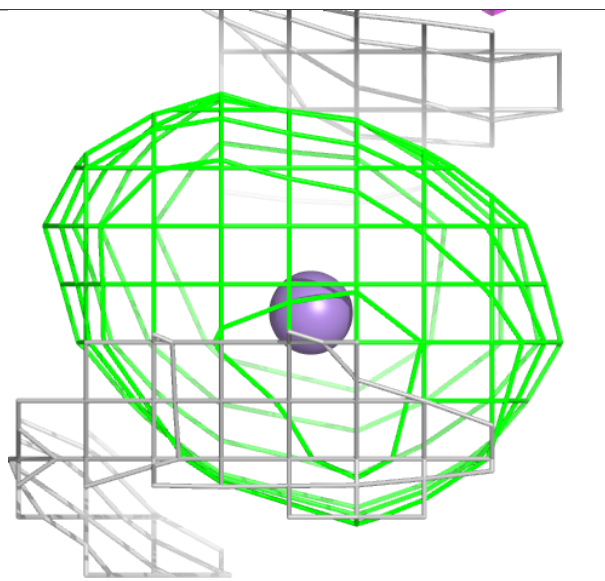
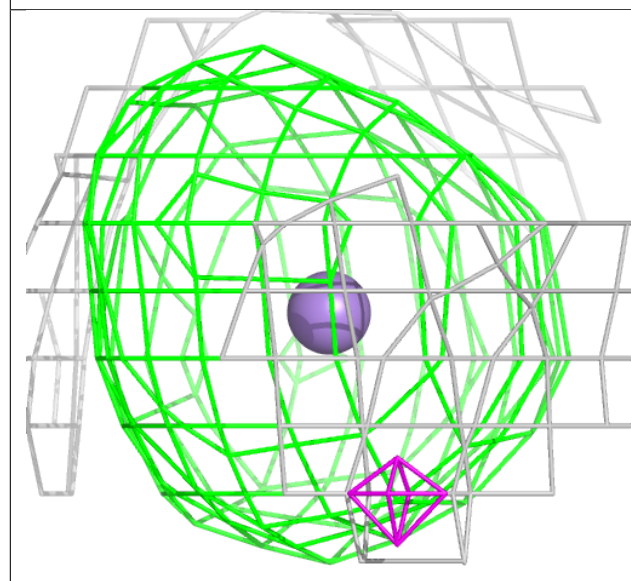
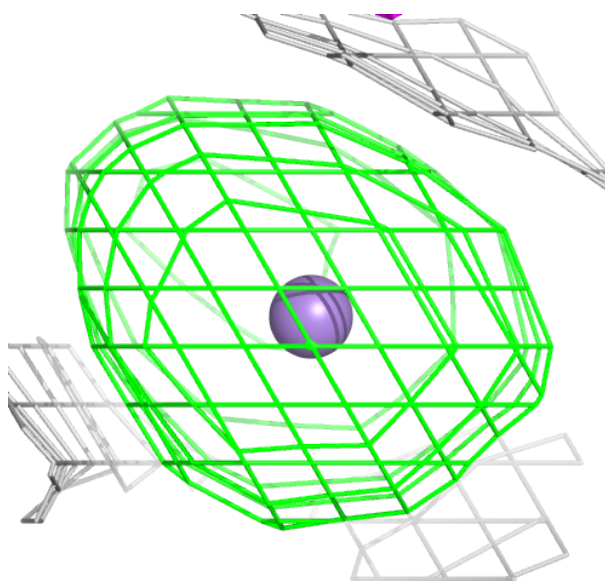
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MN	B	401	1/1	0.83	0.38	143,143,143,143	0
3	MN	B	402	1/1	0.90	0.22	54,54,54,54	1
4	PO4	B	403	5/5	0.90	0.25	18,61,71,83	5
3	MN	D	402	1/1	0.95	0.23	56,56,56,56	1
4	PO4	E	403	5/5	0.95	0.29	21,65,71,113	5
3	MN	F	402	1/1	0.97	0.30	49,49,49,49	1
4	PO4	C	403	5/5	0.97	0.33	18,64,77,111	5
4	PO4	D	403	5/5	0.97	0.19	25,49,65,102	5
4	PO4	A	403	5/5	0.97	0.23	29,34,58,66	5
3	MN	C	402	1/1	0.98	0.25	21,21,21,21	1
3	MN	E	402	1/1	0.98	0.34	44,44,44,44	1
4	PO4	F	403	5/5	0.98	0.23	20,41,82,92	5
3	MN	D	401	1/1	0.99	0.20	47,47,47,47	0
3	MN	A	402	1/1	0.99	0.25	31,31,31,31	1
3	MN	E	401	1/1	0.99	0.26	68,68,68,68	0
3	MN	C	401	1/1	0.99	0.26	65,65,65,65	0
3	MN	F	401	1/1	0.99	0.23	55,55,55,55	0
3	MN	A	401	1/1	0.99	0.23	47,47,47,47	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.

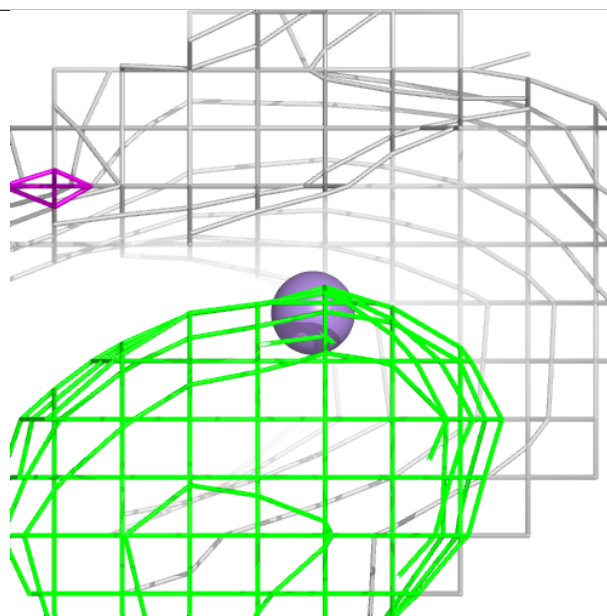
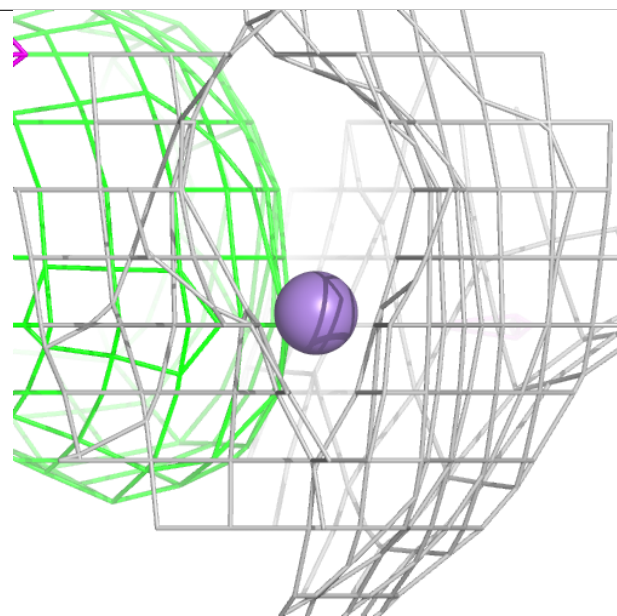
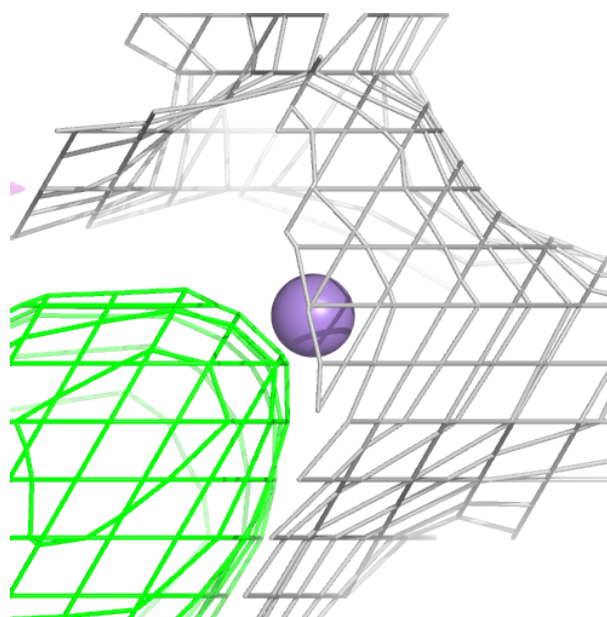
**Electron density around MN B 401:**

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



**Electron density around MN B 402:**

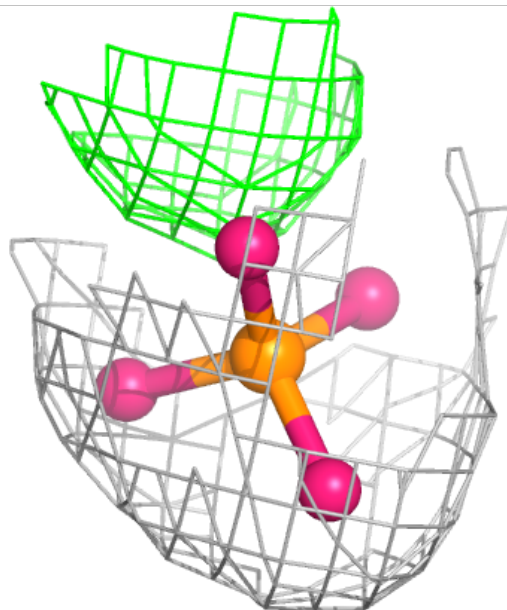
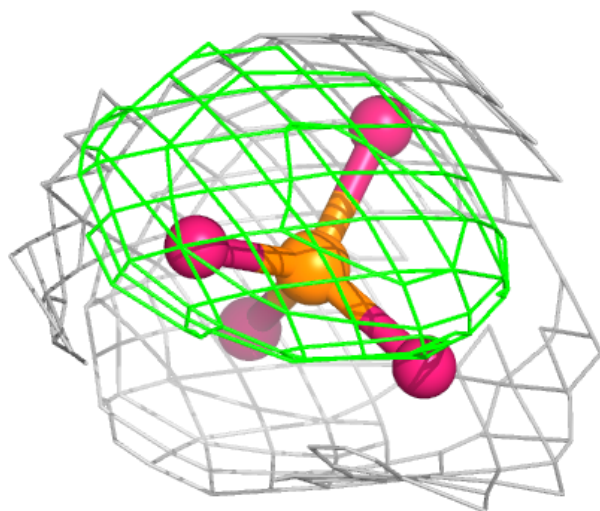
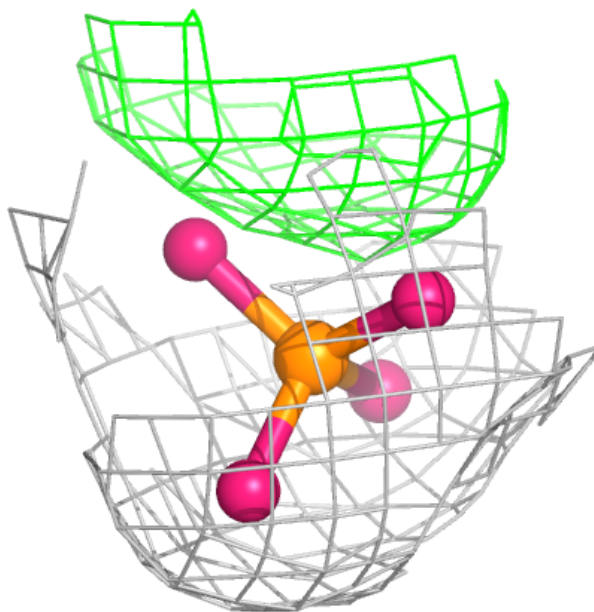
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





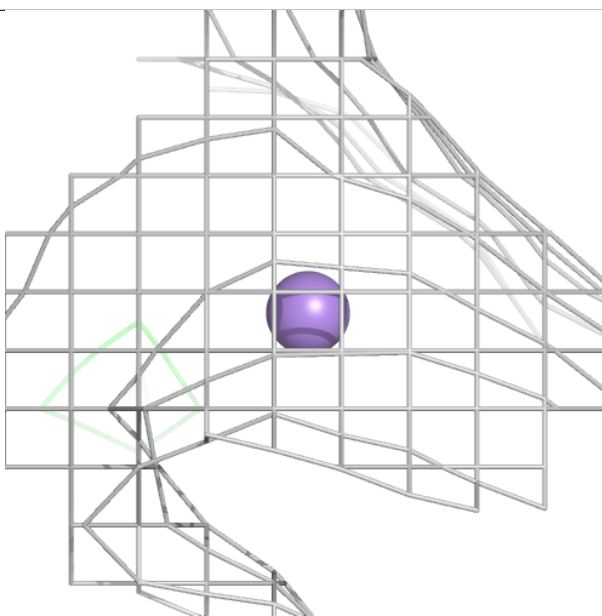
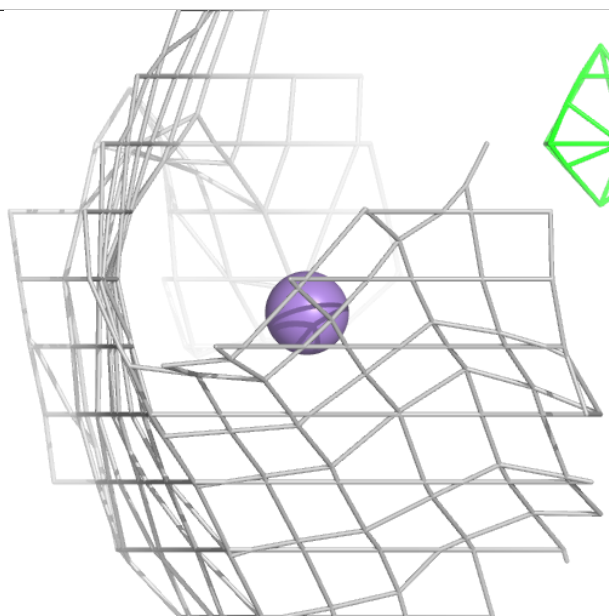
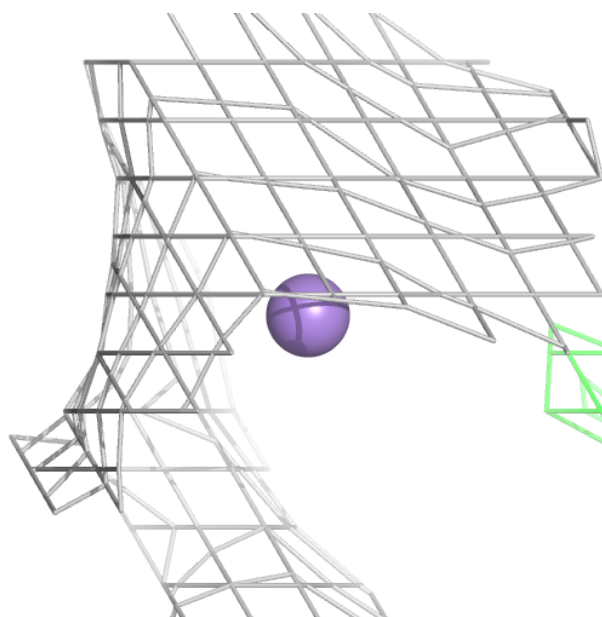
**Electron density around PO4 B 403:**

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



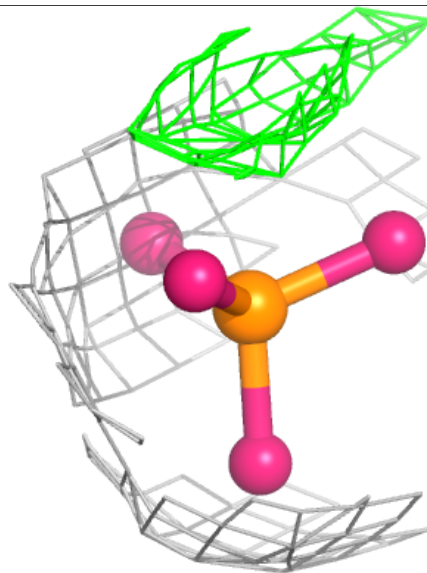
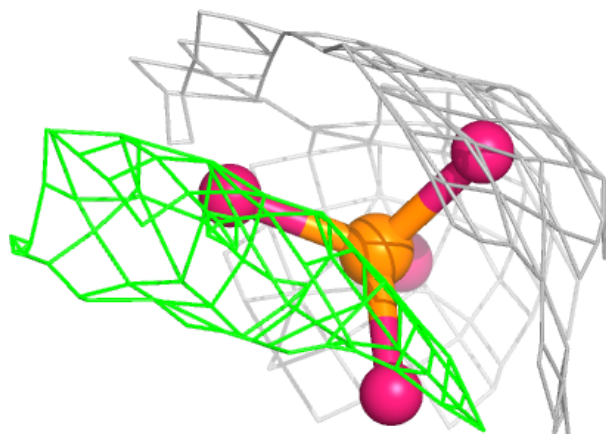
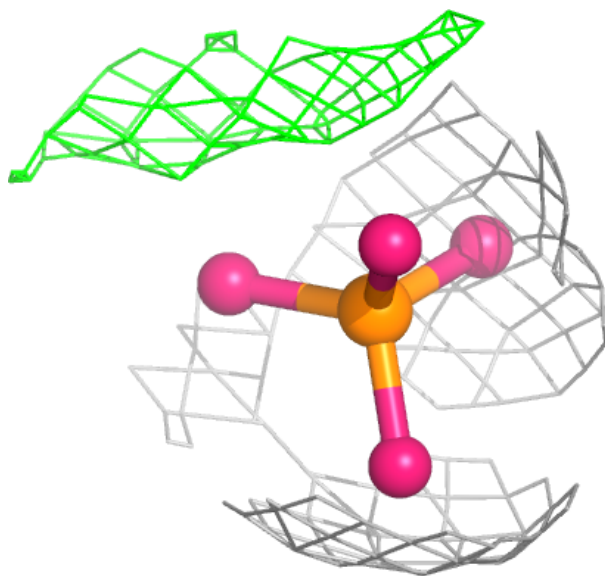
**Electron density around MN D 402:**

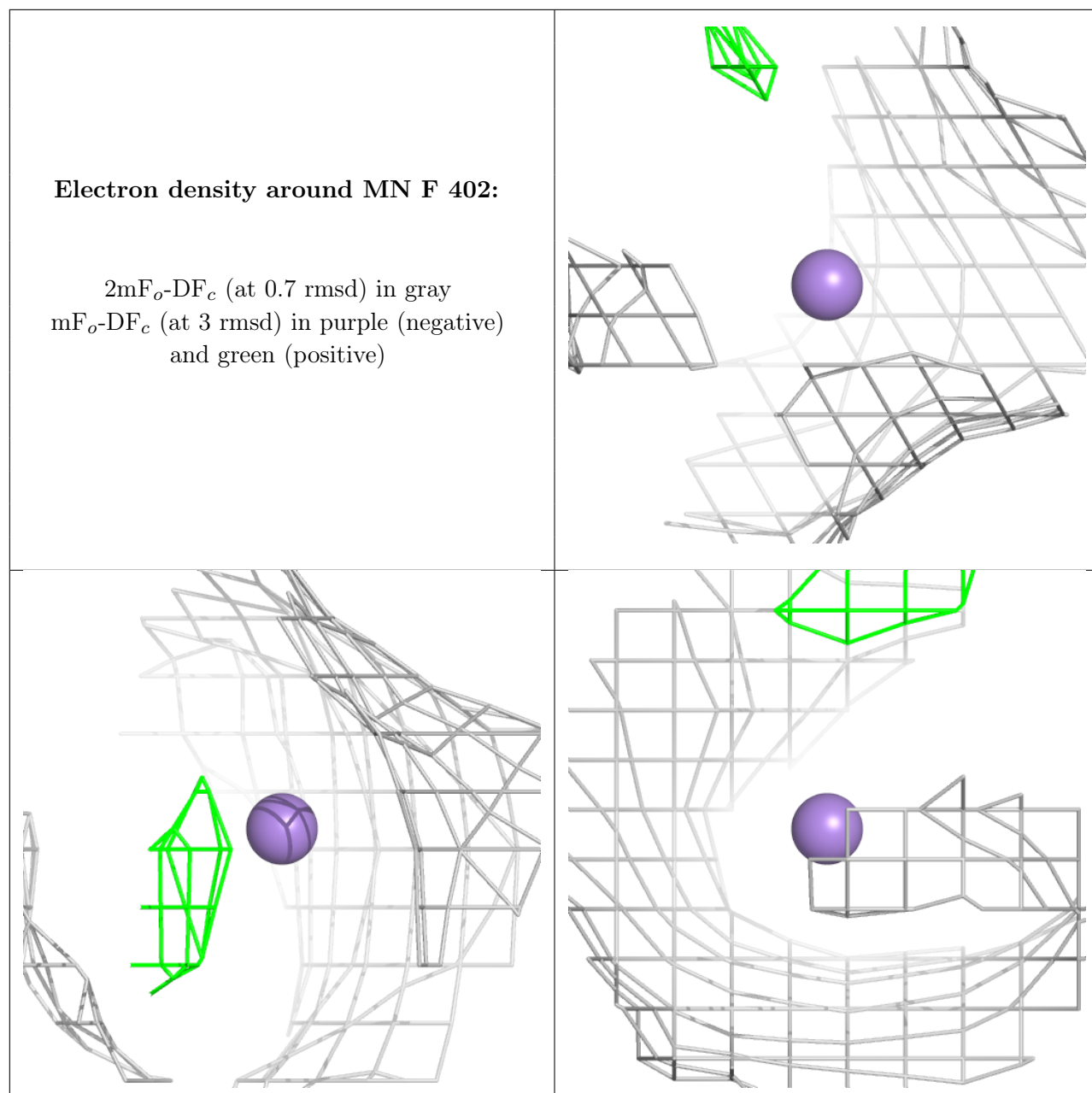
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PO4 E 403:**

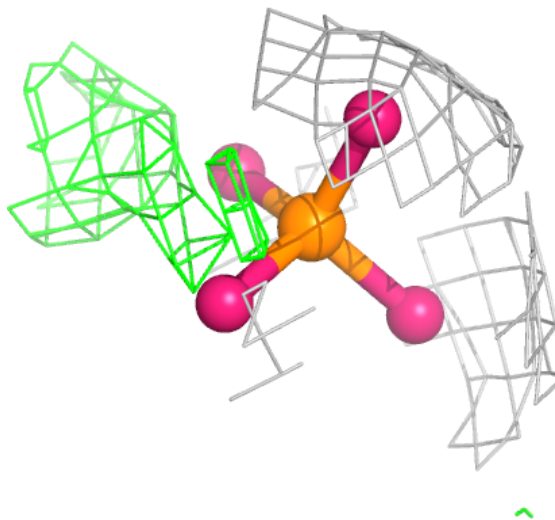
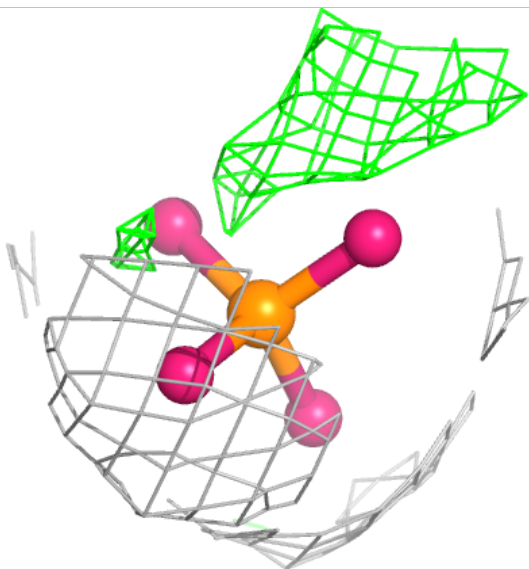
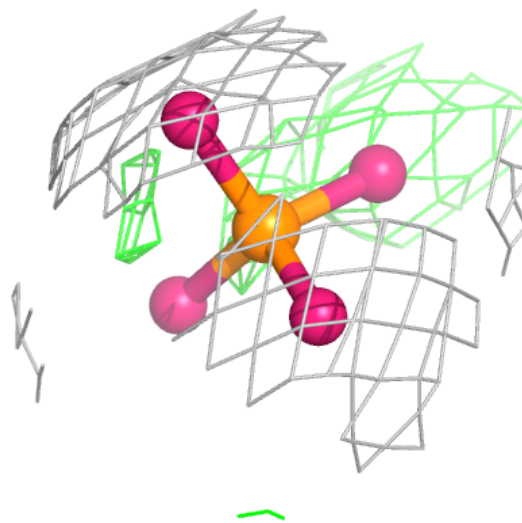
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





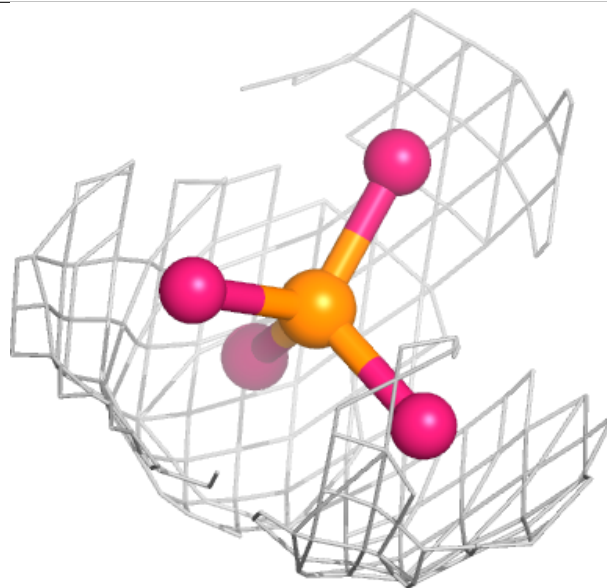
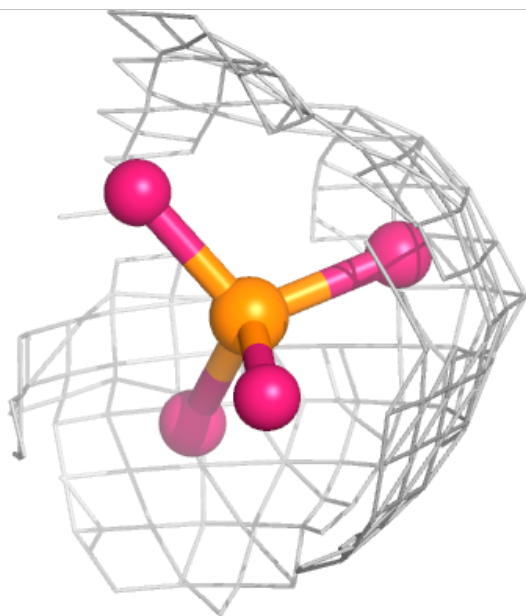
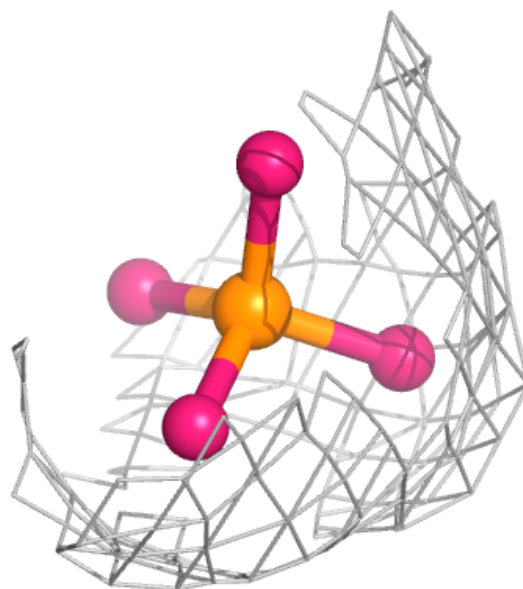
**Electron density around PO4 C 403:**

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



**Electron density around PO4 D 403:**

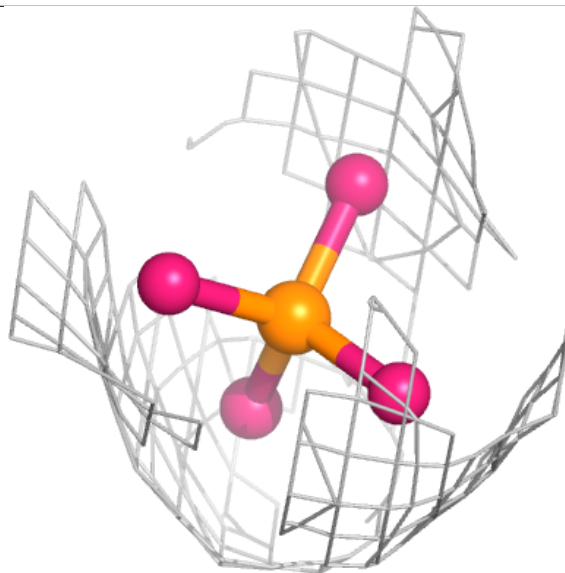
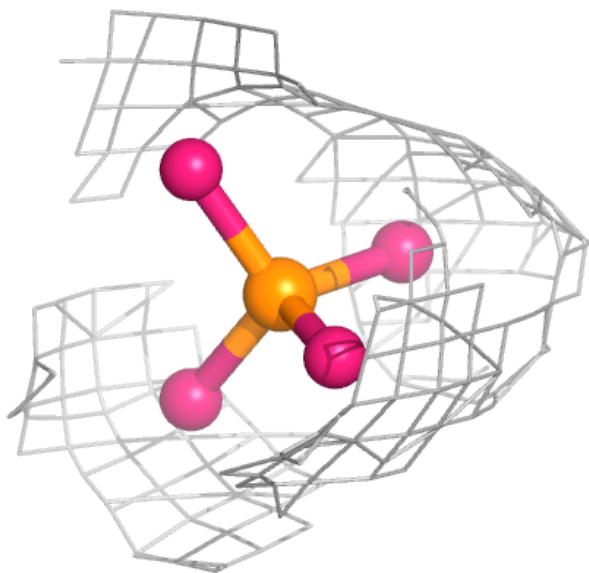
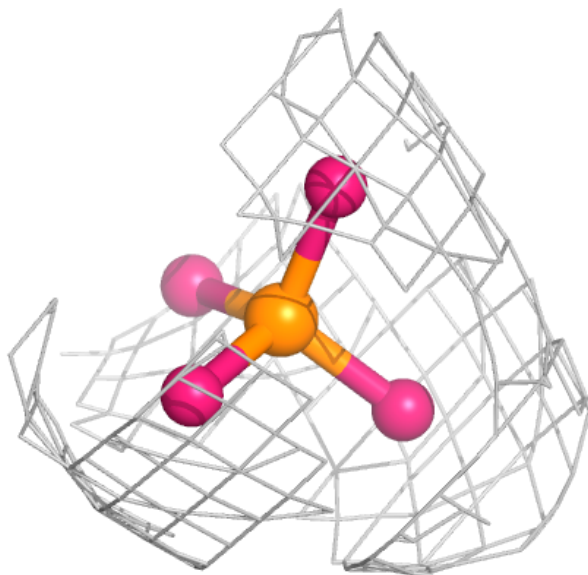
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

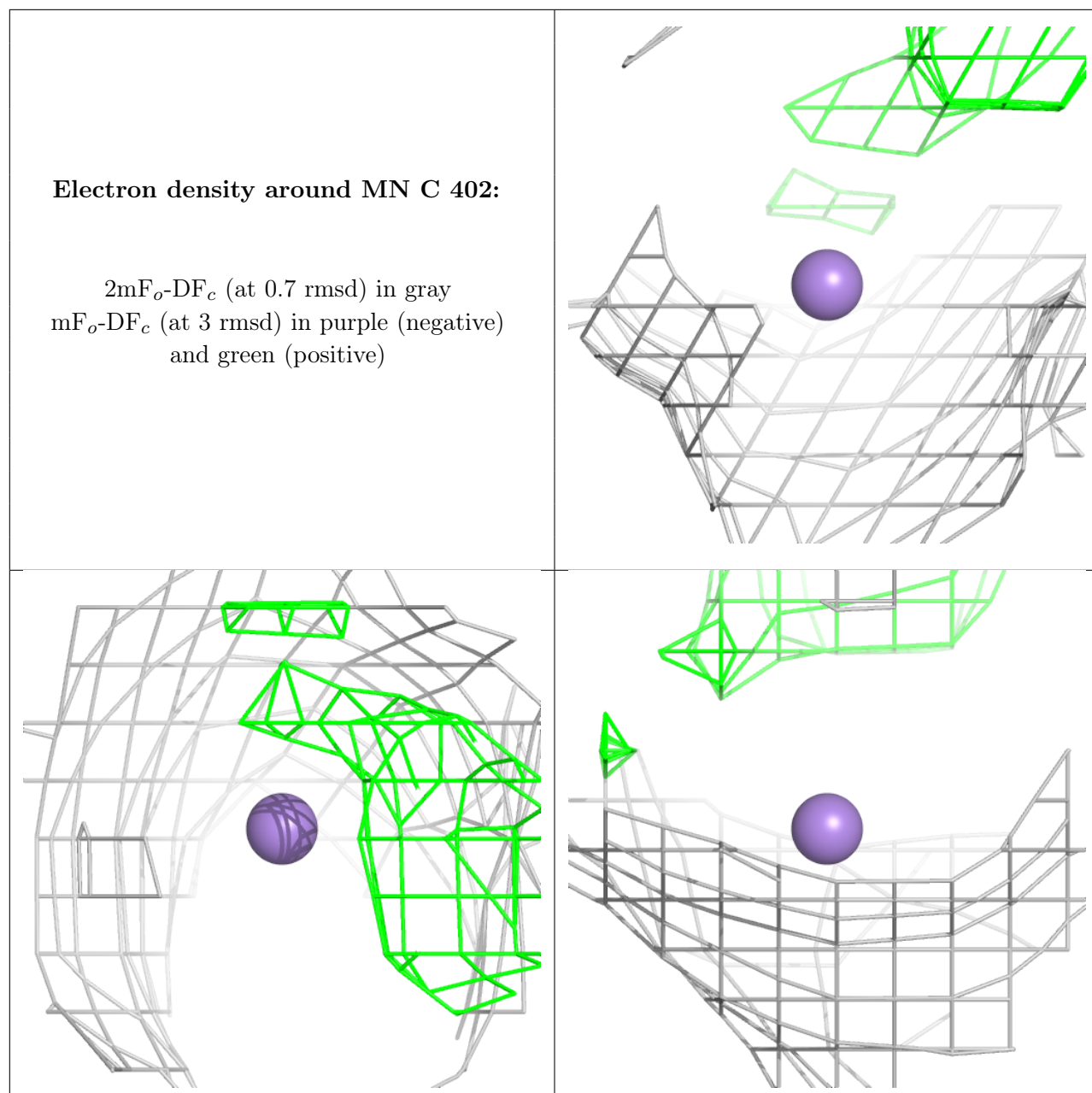




**Electron density around PO4 A 403:**

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

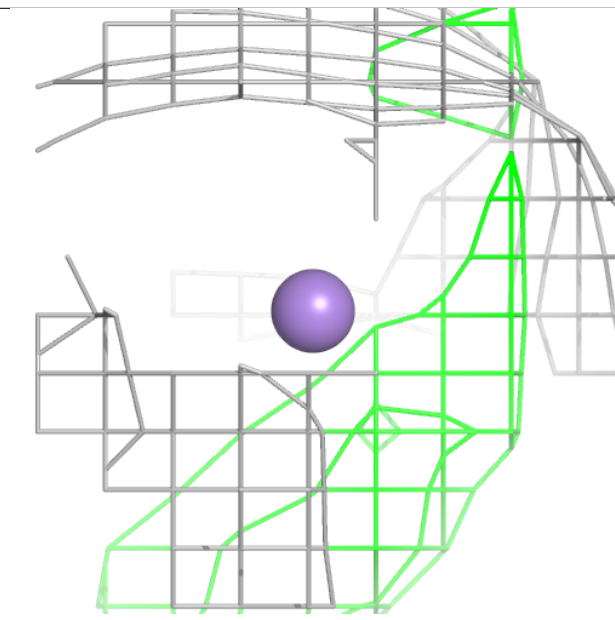
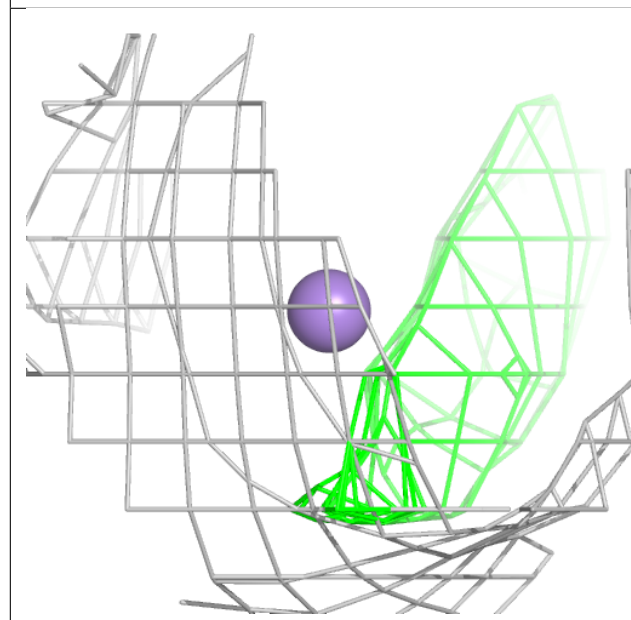
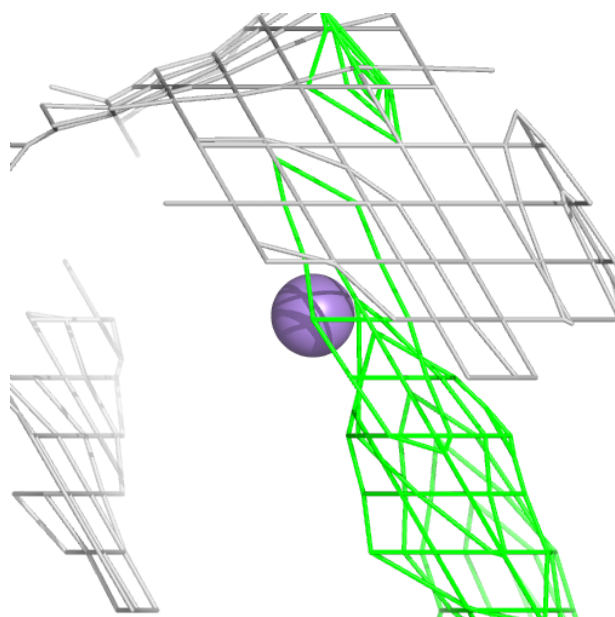






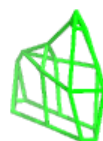
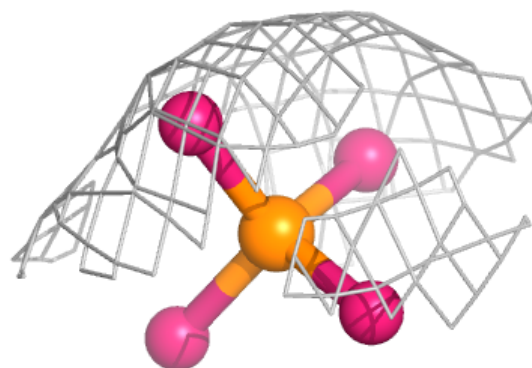
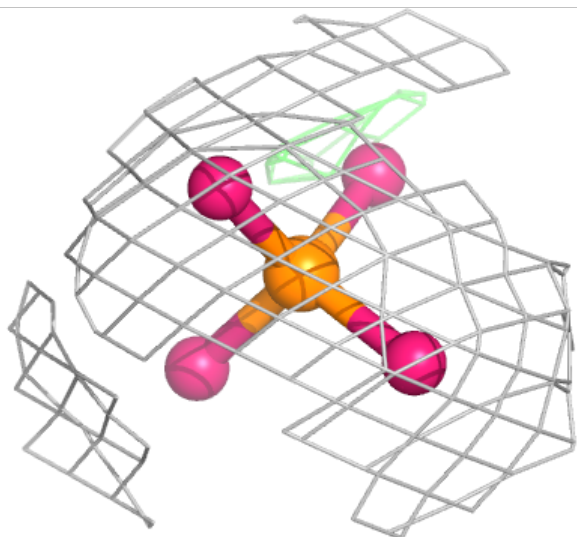
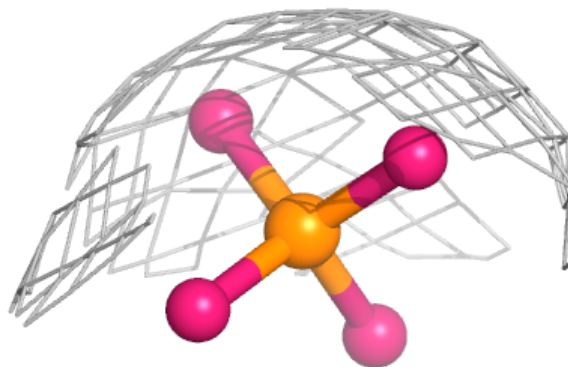
**Electron density around MN E 402:**

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



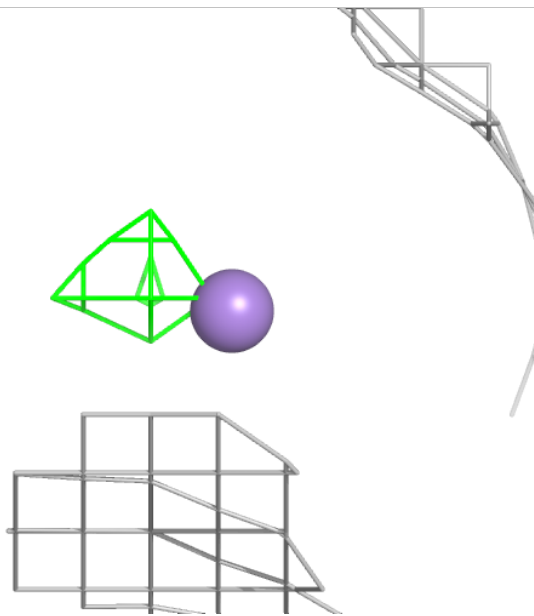
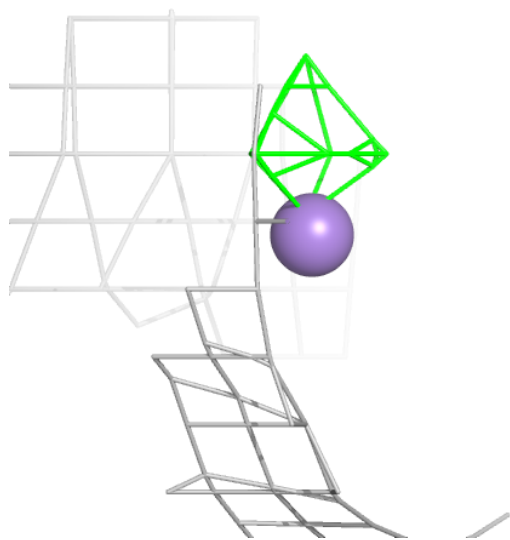
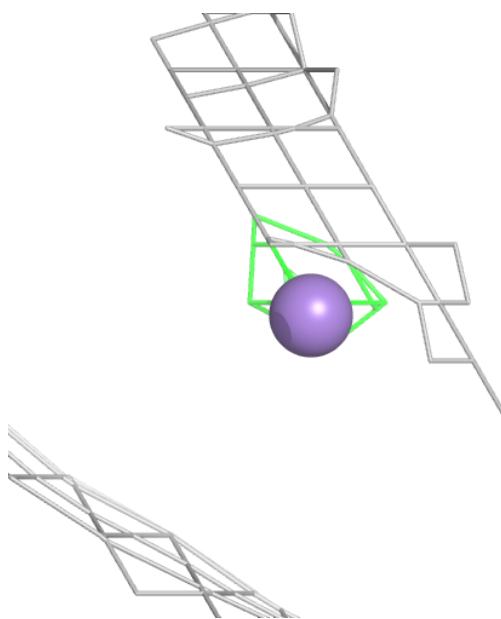
**Electron density around PO4 F 403:**

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



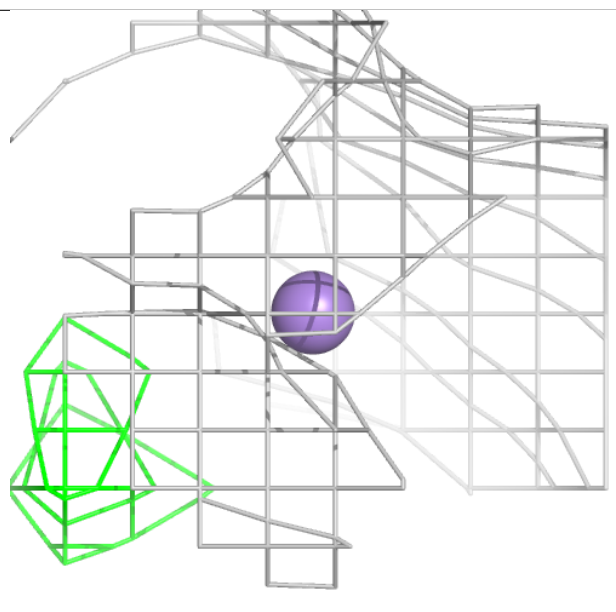
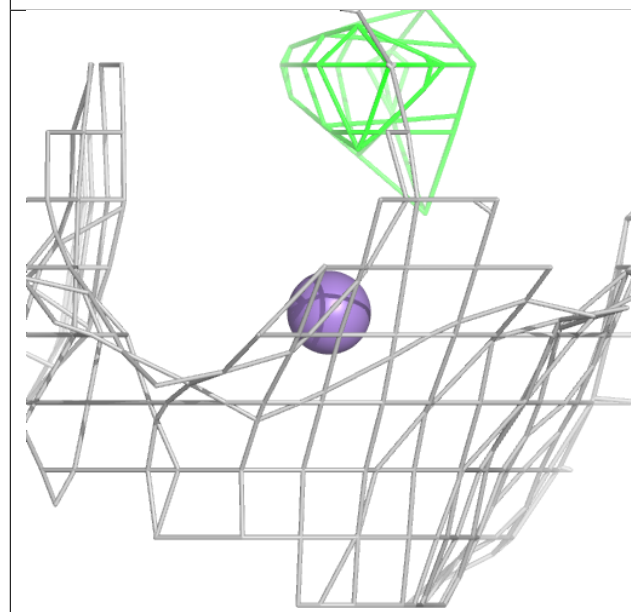
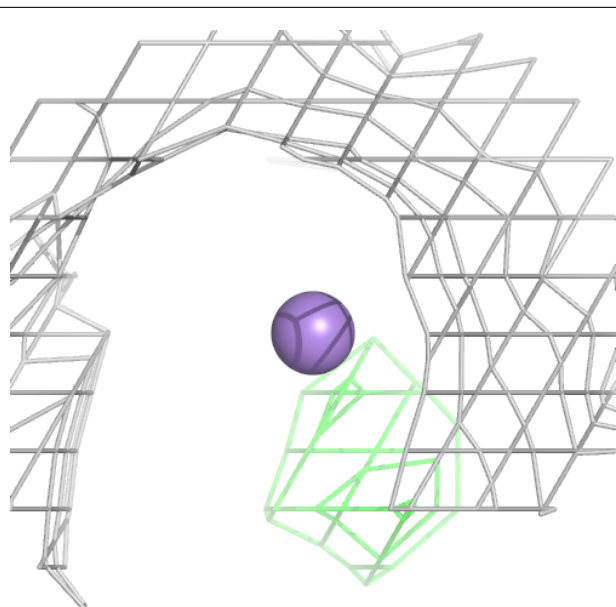
**Electron density around MN D 401:**

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



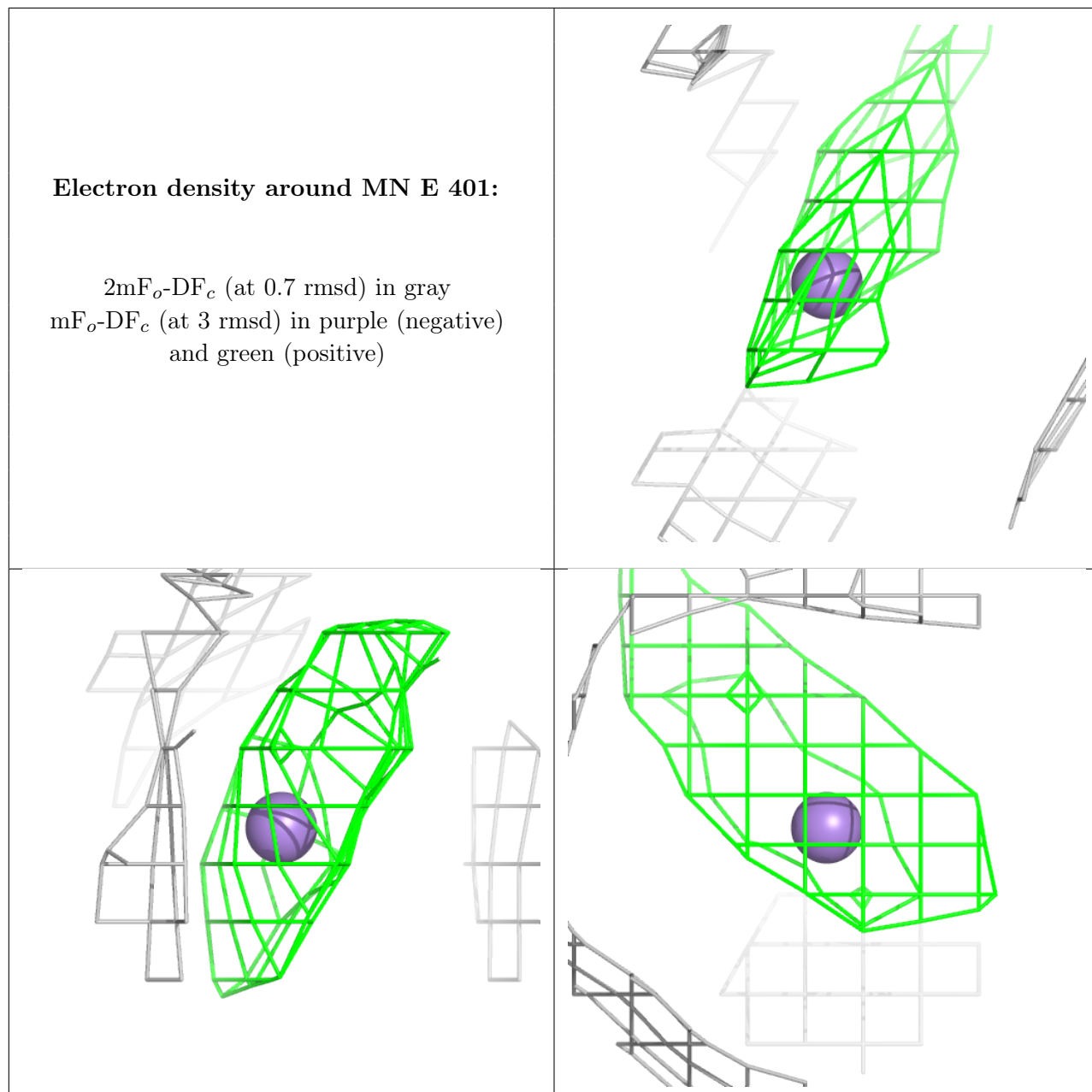
**Electron density around MN A 402:**

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



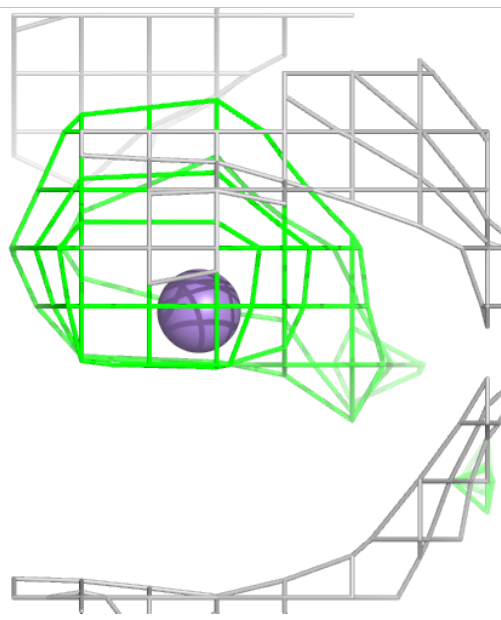
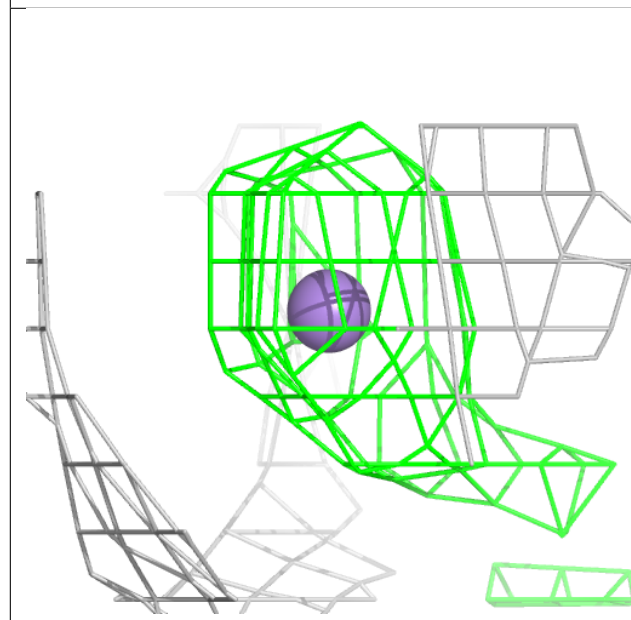
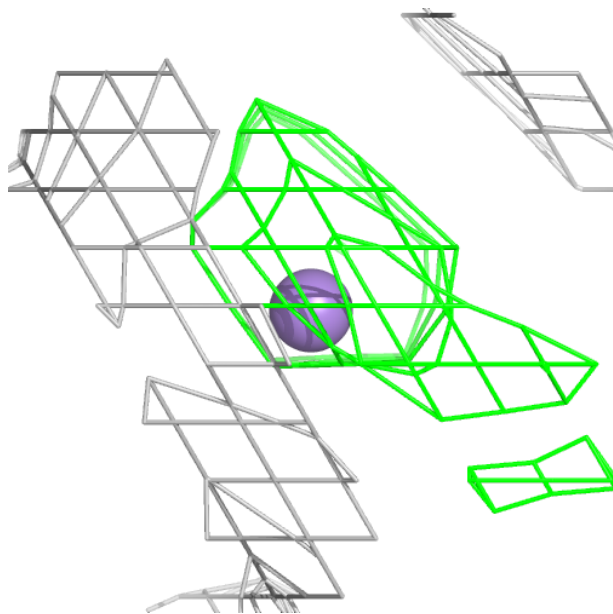
**Electron density around MN E 401:**

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



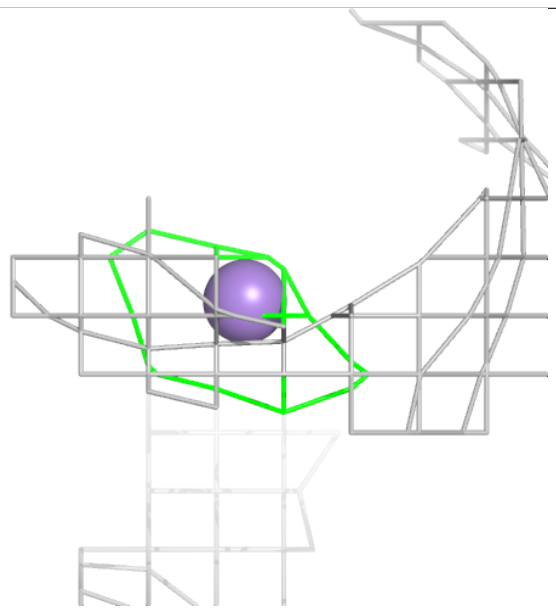
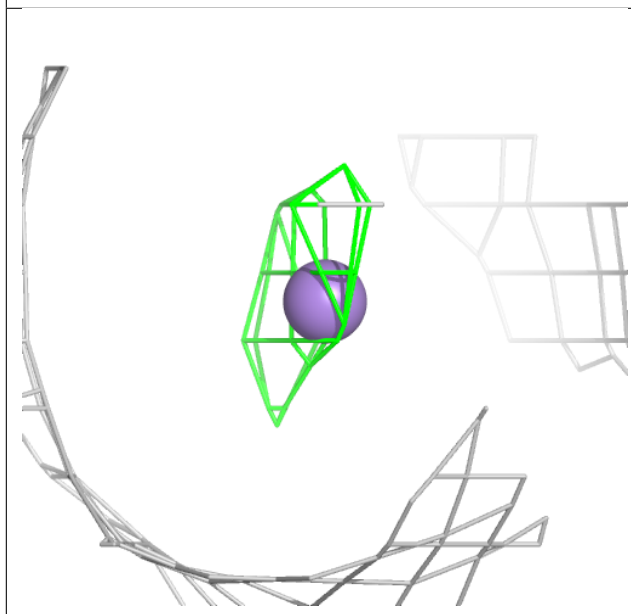
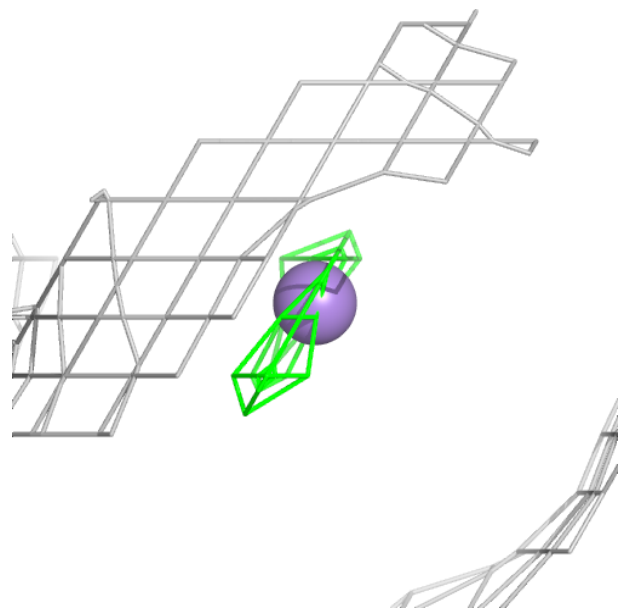
**Electron density around MN C 401:**

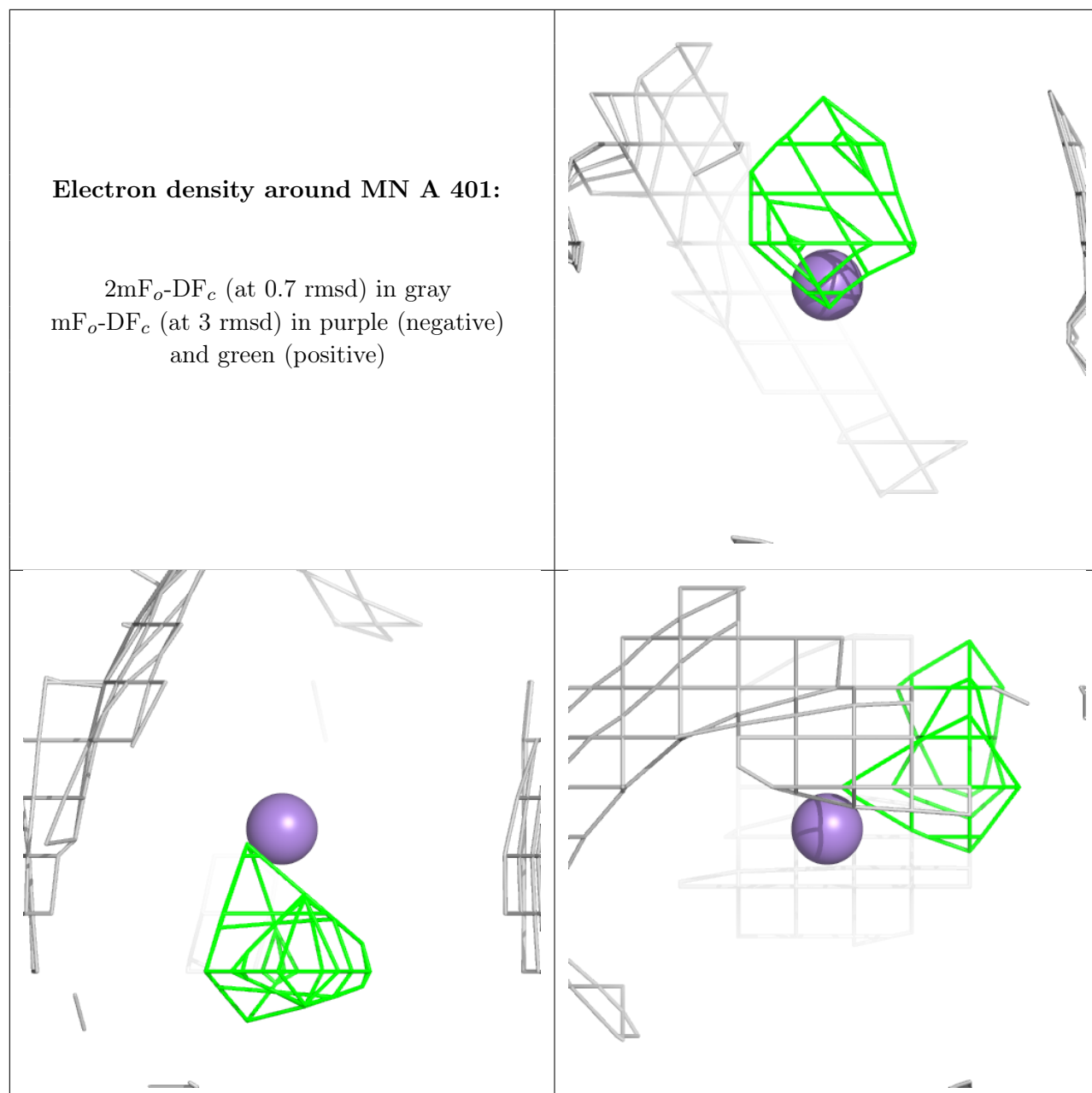
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MN F 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.