



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:36 AM BST

PDB ID : 6VST  
Title : Arginase from *Medicago truncatula* in complex with ornithine  
Authors : Sekula, B.  
Deposited on : 2020-02-11  
Resolution : 2.12 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 : 2.13  
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) : 2.13

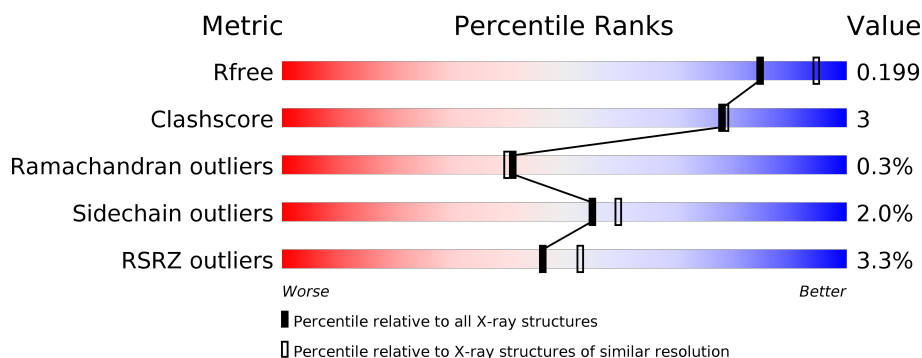
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 on 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	341	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
1	B	341	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>7%</div> </div> </div>
1	C	341	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	341	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> </div>
1	E	341	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> </div>
1	F	341	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	341	<div><div>%</div><div><div></div><div>87%</div><div>7%</div><div>6%</div></div></div>
1	H	341	<div><div>5%</div><div><div></div><div>86%</div><div>8%</div><div>6%</div></div></div>
1	I	341	<div><div>6%</div><div><div></div><div>82%</div><div>10%</div><div>7%</div></div></div>
1	J	341	<div><div>3%</div><div><div></div><div>87%</div><div>6%</div><div>7%</div></div></div>
1	K	341	<div><div>3%</div><div><div></div><div>85%</div><div>8%</div><div>7%</div></div></div>
1	L	341	<div><div>%</div><div><div></div><div>85%</div><div>8%</div><div>6%</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30999 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 Arginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	1	0
			2458	1542	440	469	7			
1	B	318	Total	C	N	O	S	0	1	0
			2464	1545	441	471	7			
1	C	318	Total	C	N	O	S	0	0	0
			2455	1537	441	470	7			
1	D	320	Total	C	N	O	S	0	2	0
			2484	1558	446	473	7			
1	E	319	Total	C	N	O	S	0	0	0
			2462	1542	442	471	7			
1	F	320	Total	C	N	O	S	0	0	0
			2470	1546	444	473	7			
1	G	320	Total	C	N	O	S	0	1	0
			2479	1554	444	474	7			
1	H	320	Total	C	N	O	S	0	0	0
			2470	1546	444	473	7			
1	I	317	Total	C	N	O	S	0	0	0
			2449	1534	440	468	7			
1	J	318	Total	C	N	O	S	0	1	0
			2464	1545	441	471	7			
1	K	318	Total	C	N	O	S	0	0	0
			2455	1537	441	470	7			
1	L	319	Total	C	N	O	S	0	1	0
			2471	1550	442	472	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7JFU5
A	-1	ASN	-	expression tag	UNP G7JFU5
A	0	ALA	-	expression tag	UNP G7JFU5
B	-2	SER	-	expression tag	UNP G7JFU5
B	-1	ASN	-	expression tag	UNP G7JFU5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP G7JFU5
C	-2	SER	-	expression tag	UNP G7JFU5
C	-1	ASN	-	expression tag	UNP G7JFU5
C	0	ALA	-	expression tag	UNP G7JFU5
D	-2	SER	-	expression tag	UNP G7JFU5
D	-1	ASN	-	expression tag	UNP G7JFU5
D	0	ALA	-	expression tag	UNP G7JFU5
E	-2	SER	-	expression tag	UNP G7JFU5
E	-1	ASN	-	expression tag	UNP G7JFU5
E	0	ALA	-	expression tag	UNP G7JFU5
F	-2	SER	-	expression tag	UNP G7JFU5
F	-1	ASN	-	expression tag	UNP G7JFU5
F	0	ALA	-	expression tag	UNP G7JFU5
G	-2	SER	-	expression tag	UNP G7JFU5
G	-1	ASN	-	expression tag	UNP G7JFU5
G	0	ALA	-	expression tag	UNP G7JFU5
H	-2	SER	-	expression tag	UNP G7JFU5
H	-1	ASN	-	expression tag	UNP G7JFU5
H	0	ALA	-	expression tag	UNP G7JFU5
I	-2	SER	-	expression tag	UNP G7JFU5
I	-1	ASN	-	expression tag	UNP G7JFU5
I	0	ALA	-	expression tag	UNP G7JFU5
J	-2	SER	-	expression tag	UNP G7JFU5
J	-1	ASN	-	expression tag	UNP G7JFU5
J	0	ALA	-	expression tag	UNP G7JFU5
K	-2	SER	-	expression tag	UNP G7JFU5
K	-1	ASN	-	expression tag	UNP G7JFU5
K	0	ALA	-	expression tag	UNP G7JFU5
L	-2	SER	-	expression tag	UNP G7JFU5
L	-1	ASN	-	expression tag	UNP G7JFU5
L	0	ALA	-	expression tag	UNP G7JFU5

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

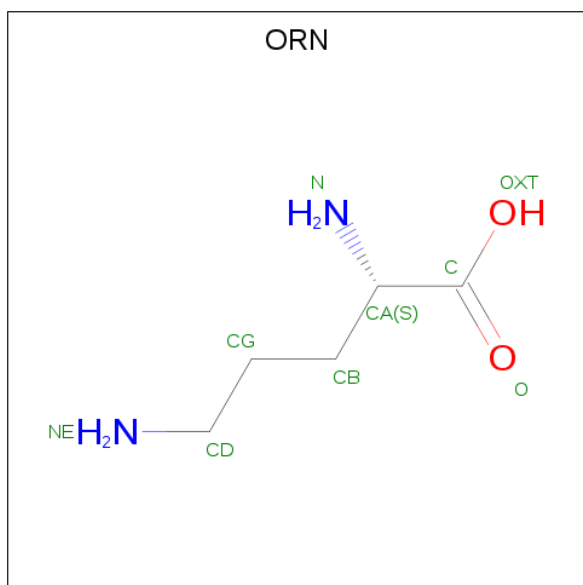
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Mn 2 2	0	0
2	J	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	H	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	I	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	L	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is L-ornithine (three-letter code: ORN) (formula:  $C_5H_{12}N_2O_2$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	5	2	2		
3	B	1	Total	C	N	O	0	0
			9	5	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			9	5	2	2		
3	F	1	Total	C	N	O	0	0
			9	5	2	2		
3	H	1	Total	C	N	O	0	0
			9	5	2	2		
3	J	1	Total	C	N	O	0	0
			9	5	2	2		
3	L	1	Total	C	N	O	0	0
			9	5	2	2		

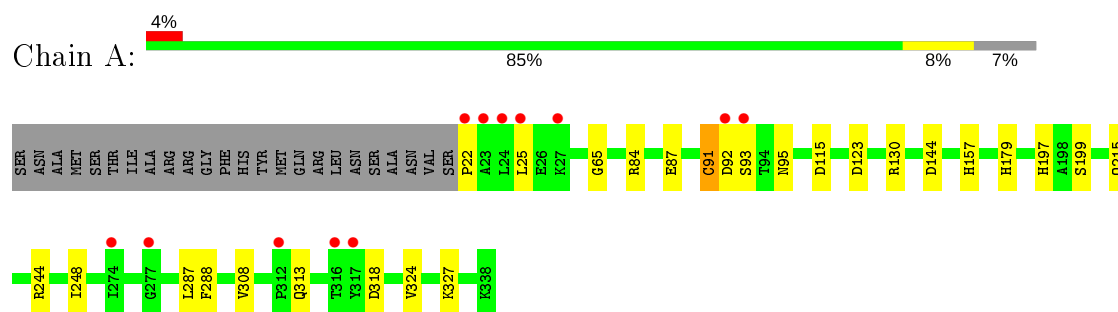
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	156	Total	O	0	0
			156	156		
4	B	166	Total	O	0	0
			166	166		
4	C	135	Total	O	0	0
			135	135		
4	D	99	Total	O	0	0
			99	99		
4	E	139	Total	O	0	0
			139	139		
4	F	115	Total	O	0	0
			115	115		
4	G	93	Total	O	0	0
			93	93		
4	H	56	Total	O	0	0
			56	56		
4	I	40	Total	O	0	0
			40	40		
4	J	151	Total	O	0	0
			151	151		
4	K	79	Total	O	0	0
			79	79		
4	L	102	Total	O	0	0
			102	102		

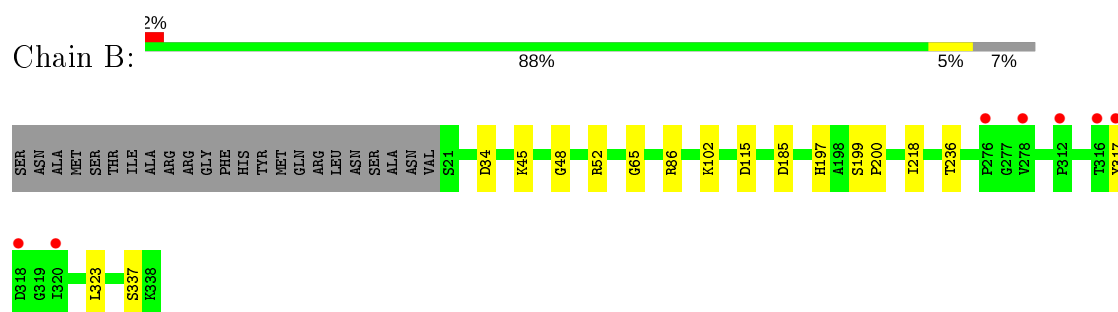
### 3 Residue-property plots [i](#)

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.

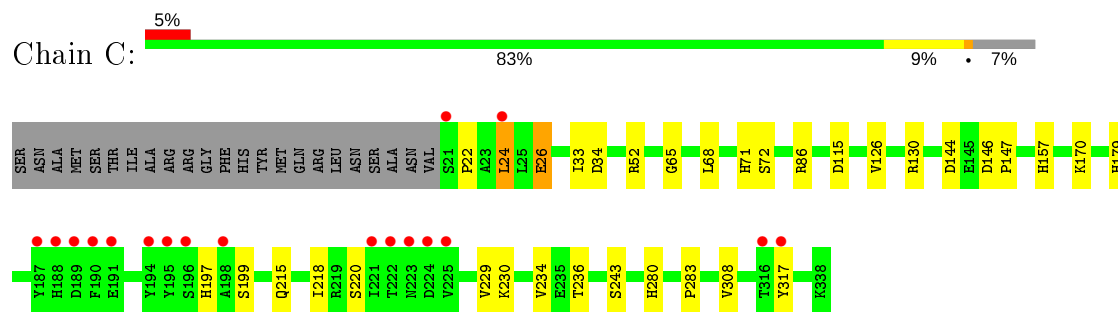
#### • Molecule 1: Arginase



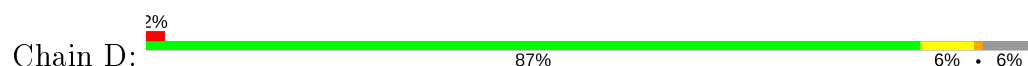
#### • Molecule 1: Arginase



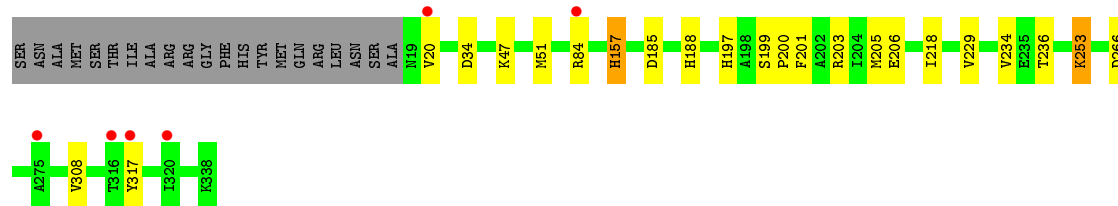
#### • Molecule 1: Arginase



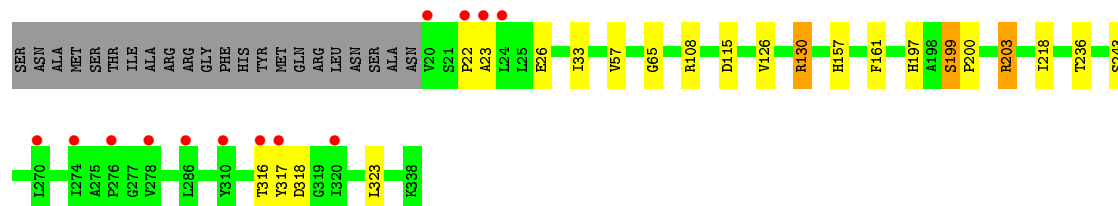
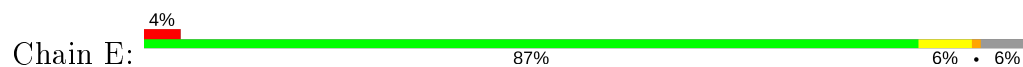
#### • Molecule 1: Arginase



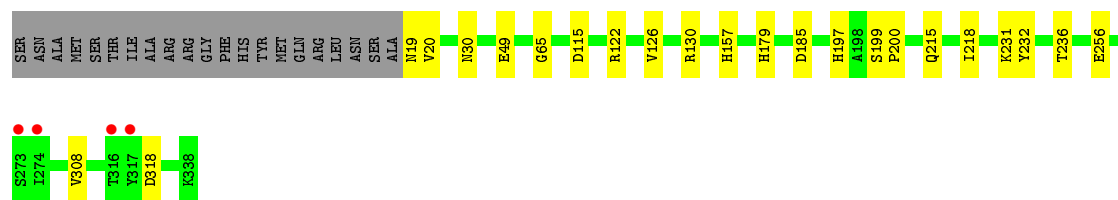
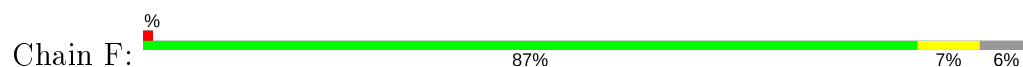




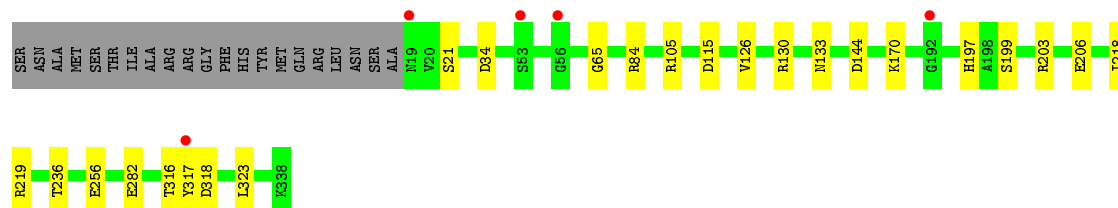
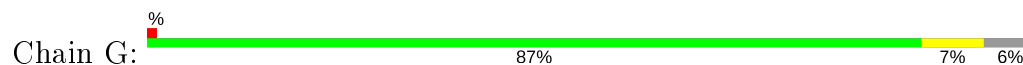
• Molecule 1: Arginase



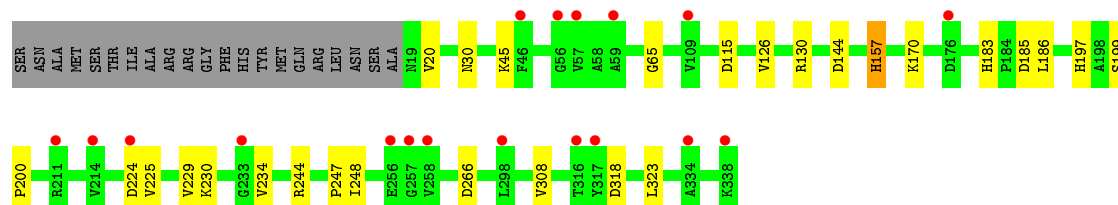
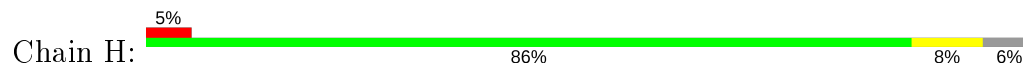
• Molecule 1: Arginase



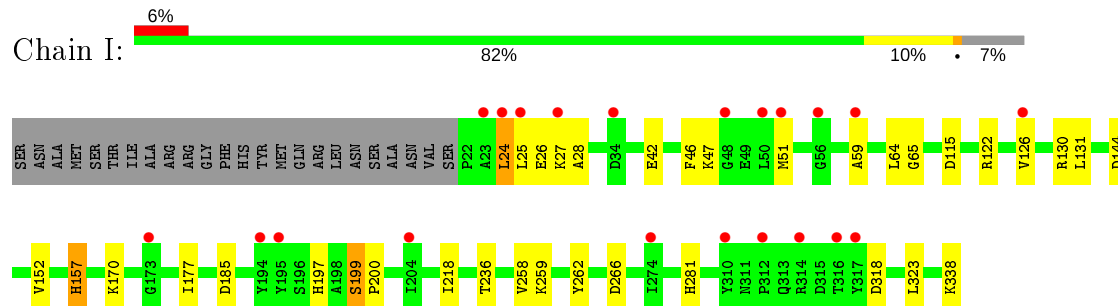
• Molecule 1: Arginase



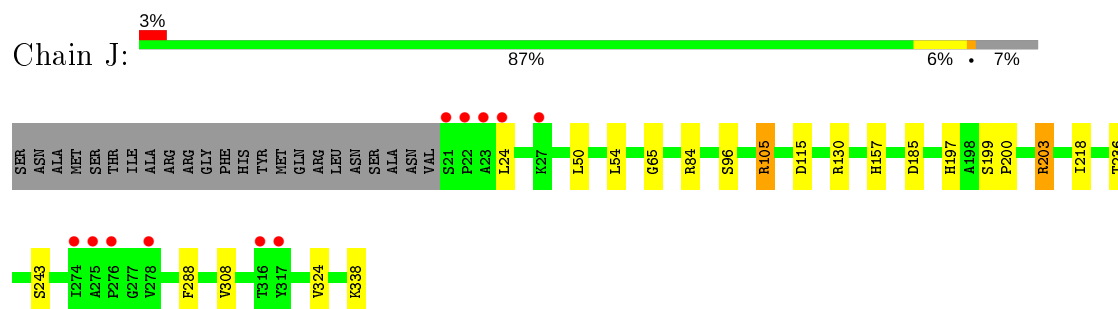
• Molecule 1: Arginase



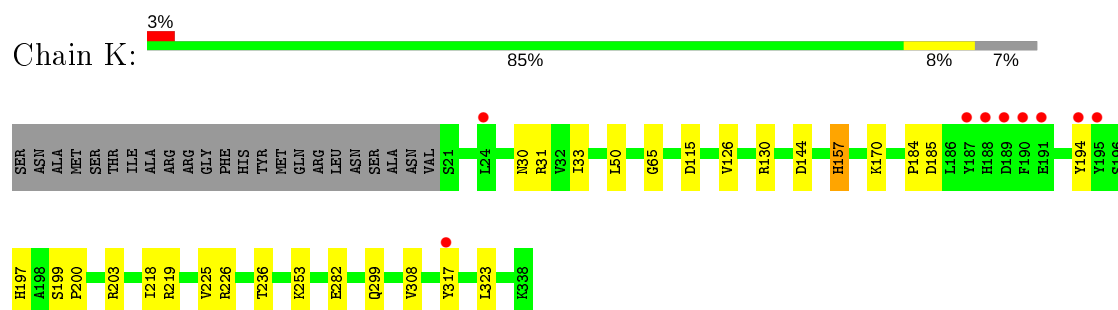
- Molecule 1: Arginase



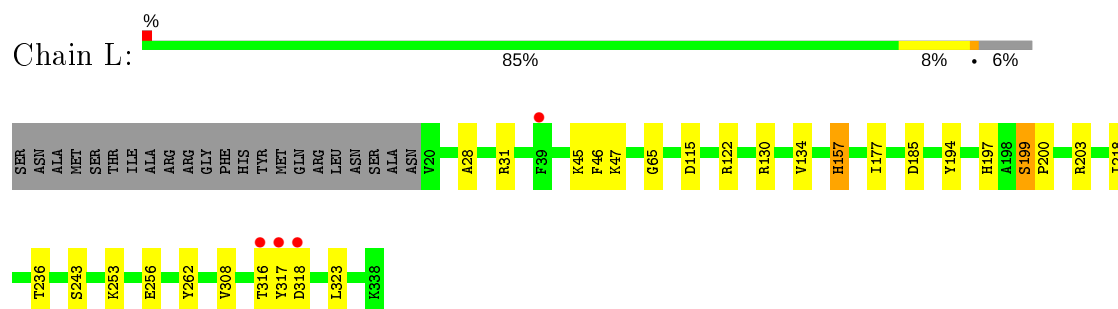
- Molecule 1: Arginase



- Molecule 1: Arginase



- Molecule 1: Arginase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.67Å 166.07Å 150.88Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	41.52 – 2.12 48.00 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.52-2.12) 99.7 (48.00-2.12)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.160 , 0.199 0.160 , 0.199	Depositor DCC
$R_{free}$ test set	1020 reflections (0.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	30999	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ORN, MN

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	0.40	0/2507	0.58	0/3393
1	B	0.43	0/2513	0.58	0/3402
1	C	0.41	0/2500	0.57	0/3384
1	D	0.35	0/2536	0.54	0/3433
1	E	0.40	0/2507	0.56	0/3394
1	F	0.38	0/2515	0.54	0/3405
1	G	0.35	0/2528	0.53	0/3423
1	H	0.33	0/2515	0.51	0/3405
1	I	0.33	0/2494	0.52	0/3375
1	J	0.41	0/2513	0.58	0/3402
1	K	0.35	0/2500	0.52	0/3384
1	L	0.39	0/2520	0.54	0/3412
All	All	0.38	0/30148	0.55	0/40812

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 [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	2458	0	2456	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2464	0	2460	9	0
1	C	2455	0	2451	22	0
1	D	2484	0	2484	14	0
1	E	2462	0	2460	15	0
1	F	2470	0	2466	10	0
1	G	2479	0	2475	12	0
1	H	2470	0	2466	14	0
1	I	2449	0	2447	30	0
1	J	2464	0	2460	10	0
1	K	2455	0	2451	15	0
1	L	2471	0	2469	22	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	9	0	11	1	0
3	B	9	0	11	1	0
3	D	9	0	11	1	0
3	F	9	0	11	0	0
3	H	9	0	11	1	0
3	J	9	0	11	1	0
3	L	9	0	11	0	0
4	A	156	0	0	1	0
4	B	166	0	0	3	0
4	C	135	0	0	3	0
4	D	99	0	0	3	0
4	E	139	0	0	0	0
4	F	115	0	0	1	0
4	G	93	0	0	1	0
4	H	56	0	0	0	0
4	I	40	0	0	0	0
4	J	151	0	0	3	0
4	K	79	0	0	0	0
4	L	102	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30999	0	29622	173	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 3.

All (173) 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:I:24:LEU:O	1:I:28:ALA:CB	2.23	0.87
1:I:28:ALA:HB1	1:L:46:PHE:HD1	1.41	0.85
1:I:24:LEU:O	1:I:28:ALA:HB3	1.79	0.83
1:E:130:ARG:HG2	1:E:130:ARG:HH11	1.45	0.81
1:I:24:LEU:O	1:I:24:LEU:HD12	1.82	0.80
1:I:28:ALA:HB1	1:L:46:PHE:CD1	2.21	0.75
1:C:24:LEU:HD21	1:F:49:GLU:OE1	1.86	0.75
1:E:130:ARG:HG2	1:E:130:ARG:NH1	1.98	0.75
1:I:130:ARG:HH21	1:I:130:ARG:HG2	1.52	0.74
1:C:86:ARG:NH1	4:C:501:HOH:O	2.22	0.72
1:E:23:ALA:HA	1:E:26:GLU:OE1	1.91	0.70
1:D:84[A]:ARG:NH2	4:D:501:HOH:O	2.24	0.70
1:I:24:LEU:O	1:I:28:ALA:HB2	1.91	0.69
1:A:95:ASN:ND2	1:C:220:SER:OG	2.25	0.69
3:B:403:ORN:NE	4:B:501:HOH:O	2.24	0.68
1:G:317[A]:TYR:OH	1:L:318:ASP:HB3	1.93	0.68
1:D:203:ARG:NH1	1:D:206:GLU:OE2	2.27	0.67
1:G:144:ASP:OD1	1:G:170:LYS:NZ	2.26	0.66
1:H:229:VAL:HG13	1:H:234:VAL:HB	1.77	0.66
1:K:144:ASP:OD1	1:K:170:LYS:NZ	2.29	0.66
1:D:185:ASP:HB3	1:D:200:PRO:HD2	1.77	0.65
1:I:46:PHE:HD2	1:L:28:ALA:HB1	1.62	0.63
1:A:87:GLU:O	1:A:91:CYS:HB3	1.98	0.63
1:F:19:ASN:N	4:F:501:HOH:O	2.31	0.62
1:I:130:ARG:HG2	1:I:130:ARG:NH2	2.14	0.62
1:B:218:ILE:HG13	1:B:236:THR:HG23	1.83	0.61
1:E:22:PRO:O	1:E:26:GLU:HG2	2.02	0.58
1:F:30:ASN:OD1	1:F:130:ARG:NH2	2.36	0.58
3:D:403:ORN:NE	4:D:502:HOH:O	2.27	0.58
1:I:144:ASP:OD1	1:I:170:LYS:NZ	2.28	0.58
1:C:218:ILE:HG13	1:C:236:THR:HG23	1.85	0.58
3:A:403:ORN:NE	4:A:502:HOH:O	2.32	0.57
1:A:84:ARG:HD3	4:D:501:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ILE:H	1:A:248:ILE:HD12	1.70	0.56
1:L:185:ASP:HB3	1:L:200:PRO:HD2	1.89	0.55
1:C:126:VAL:HG13	1:C:130:ARG:HB3	1.89	0.54
1:D:229:VAL:HG13	1:D:234:VAL:HB	1.89	0.54
1:K:126:VAL:HG13	1:K:130:ARG:HB3	1.90	0.54
1:C:144:ASP:OD1	1:C:170:LYS:NZ	2.21	0.53
1:C:157:HIS:CE1	1:C:179:HIS:HE2	2.27	0.53
1:A:288:PHE:HE1	1:A:324:VAL:HG13	1.73	0.53
1:K:218:ILE:HG13	1:K:236:THR:HG23	1.91	0.53
1:C:157:HIS:HE1	1:C:179:HIS:HE2	1.57	0.52
1:K:30:ASN:OD1	1:K:130:ARG:NH2	2.42	0.52
1:A:327:LYS:HD3	1:C:283:PRO:HG2	1.90	0.52
1:B:65:GLY:HA3	1:B:115:ASP:OD1	2.09	0.52
1:A:22:PRO:N	1:A:25:LEU:HG	2.25	0.52
1:H:30:ASN:OD1	1:H:130:ARG:NH2	2.42	0.52
1:H:65:GLY:HA3	1:H:115:ASP:OD1	2.09	0.52
1:K:219:ARG:HG3	1:K:282:GLU:HG3	1.91	0.52
1:E:57:VAL:HB	1:E:108:ARG:HD2	1.91	0.52
1:H:126:VAL:HG13	1:H:130:ARG:HB3	1.92	0.51
1:B:317[A]:TYR:CD1	1:D:317[A]:TYR:CD1	2.98	0.51
1:H:157:HIS:CE1	1:H:266:ASP:HB2	2.45	0.51
1:I:42:GLU:OE2	1:L:31:ARG:NH2	2.44	0.51
1:H:20:VAL:HG22	1:K:50:LEU:HD11	1.94	0.50
1:G:317[A]:TYR:CD1	1:L:317[A]:TYR:CD1	3.00	0.50
1:I:65:GLY:HA3	1:I:115:ASP:OD1	2.12	0.50
1:J:96:SER:OG	1:J:105:ARG:HD2	2.13	0.49
1:E:161:PHE:CD1	1:E:203:ARG:HB3	2.47	0.49
1:J:185:ASP:HB3	1:J:200:PRO:HD2	1.93	0.49
1:A:130:ARG:HG2	1:A:130:ARG:HH21	1.78	0.49
1:G:84:ARG:HD3	4:G:501:HOH:O	2.13	0.48
1:K:33:ILE:HD11	1:K:126:VAL:HG21	1.95	0.48
1:G:65:GLY:HA3	1:G:115:ASP:OD1	2.14	0.48
1:L:253:LYS:HE3	1:L:256:GLU:HG3	1.95	0.48
1:B:86:ARG:NH1	4:B:504:HOH:O	2.46	0.48
1:J:218:ILE:HG13	1:J:236:THR:HG23	1.95	0.48
1:G:203:ARG:NH2	1:G:206:GLU:OE2	2.47	0.48
1:A:93:SER:HB2	1:C:280:HIS:ND1	2.29	0.48
1:C:230:LYS:HE2	4:C:626:HOH:O	2.14	0.48
1:E:316:THR:OG1	1:E:318:ASP:OD1	2.30	0.48
1:B:185:ASP:HB3	1:B:200:PRO:HD2	1.96	0.48
1:D:201:PHE:O	1:D:205:MET:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:ALA:HB3	1:I:338:LYS:HG2	1.95	0.47
1:H:144:ASP:OD1	1:H:170:LYS:NZ	2.32	0.47
1:I:126:VAL:HG13	1:I:130:ARG:HB3	1.96	0.47
1:C:317:TYR:CD1	1:E:317:TYR:CD1	3.03	0.47
1:E:33:ILE:HD11	1:E:126:VAL:HG21	1.96	0.47
1:G:219:ARG:HG3	1:G:282:GLU:HG2	1.95	0.47
1:C:52:ARG:NH1	1:C:146:ASP:O	2.47	0.46
1:F:231:LYS:HE2	1:F:232:TYR:CZ	2.50	0.46
1:K:194:TYR:CZ	1:K:203:ARG:HD2	2.50	0.46
1:L:316:THR:OG1	1:L:318:ASP:OD1	2.30	0.46
1:C:229:VAL:HG13	1:C:234:VAL:HB	1.97	0.46
1:F:157:HIS:CD2	1:F:308:VAL:HG21	2.51	0.46
1:A:65:GLY:HA3	1:A:115:ASP:OD1	2.15	0.46
1:E:323:LEU:HA	1:E:323:LEU:HD23	1.78	0.45
1:G:323:LEU:HD12	1:I:281:HIS:HB2	1.96	0.45
1:E:23:ALA:HA	1:E:26:GLU:CG	2.47	0.45
1:I:259:LYS:HD3	1:I:259:LYS:HA	1.76	0.45
1:F:65:GLY:HA3	1:F:115:ASP:OD1	2.16	0.45
1:D:218:ILE:HG13	1:D:236:THR:HG23	1.99	0.45
1:H:186:LEU:HB2	1:H:225:VAL:HG13	1.98	0.45
1:I:318:ASP:HB3	1:K:317:TYR:OH	2.17	0.45
1:L:130:ARG:O	1:L:134:VAL:HG23	2.17	0.45
1:J:84:ARG:HD3	4:J:510:HOH:O	2.16	0.45
1:C:157:HIS:CD2	1:C:308:VAL:HG21	2.51	0.45
1:I:177:ILE:HG12	1:I:262:TYR:HB3	1.99	0.44
1:I:157:HIS:CE1	1:I:266:ASP:HB2	2.52	0.44
1:E:65:GLY:HA3	1:E:115:ASP:OD1	2.17	0.44
1:G:316:THR:OG1	1:G:318:ASP:OD1	2.31	0.44
1:H:244:ARG:O	1:H:247:PRO:HD2	2.17	0.44
1:K:185:ASP:HB3	1:K:200:PRO:HD2	1.99	0.44
1:I:218:ILE:HG13	1:I:236:THR:HG23	1.99	0.44
1:G:126:VAL:HG13	1:G:130:ARG:HB3	2.00	0.44
1:E:218:ILE:HG13	1:E:236:THR:HG23	2.00	0.44
1:H:323:LEU:HD23	1:H:323:LEU:HA	1.83	0.44
1:D:157:HIS:CE1	1:D:266:ASP:HB2	2.52	0.44
1:H:230:LYS:HB2	1:H:230:LYS:HE3	1.84	0.44
1:D:157:HIS:CD2	1:D:308:VAL:HG21	2.53	0.43
1:E:130:ARG:CG	1:E:130:ARG:HH11	2.16	0.43
1:B:102:LYS:NZ	1:B:337:SER:O	2.51	0.43
1:F:126:VAL:HG13	1:F:130:ARG:HB3	2.00	0.43
1:J:338:LYS:HE2	4:J:514:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:185:ASP:HB3	1:H:200:PRO:HD2	2.00	0.43
1:K:323:LEU:HD23	1:K:323:LEU:HA	1.87	0.43
1:L:218:ILE:HG13	1:L:236:THR:HG23	2.00	0.43
1:B:48:GLY:O	1:B:52:ARG:HG3	2.19	0.43
1:E:199:SER:N	1:E:200:PRO:CD	2.81	0.43
3:J:403:ORN:NE	4:J:502:HOH:O	2.37	0.43
1:G:317[B]:TYR:CD2	1:L:317[B]:TYR:CD2	3.06	0.43
1:C:22:PRO:O	1:C:26:GLU:HG3	2.18	0.43
1:K:184:PRO:HG2	1:K:225:VAL:HG11	1.99	0.43
1:I:130:ARG:CG	1:I:130:ARG:NH2	2.81	0.43
1:C:179:HIS:O	1:C:215:GLN:HA	2.18	0.43
1:C:72:SER:HB3	4:C:545:HOH:O	2.18	0.43
1:L:157:HIS:CD2	1:L:308:VAL:HG21	2.54	0.43
1:H:183:HIS:CD2	3:H:403:ORN:HB2	2.54	0.43
1:C:68:LEU:HD21	1:C:71:HIS:CD2	2.55	0.42
1:I:46:PHE:CD2	1:L:28:ALA:HB1	2.48	0.42
1:L:45:LYS:HB2	1:L:45:LYS:NZ	2.34	0.42
1:J:203:ARG:HA	1:J:203:ARG:HD3	1.72	0.42
1:D:188:HIS:O	1:D:203:ARG:NH2	2.36	0.42
1:I:24:LEU:HD12	1:I:28:ALA:HB2	2.01	0.42
1:I:323:LEU:HD23	1:I:323:LEU:HA	1.79	0.42
1:F:185:ASP:HB3	1:F:200:PRO:HD2	2.03	0.41
1:J:288:PHE:HE1	1:J:324:VAL:HG13	1.85	0.41
1:K:253:LYS:HG2	1:K:299:GLN:HB2	2.03	0.41
1:L:157:HIS:CG	1:L:308:VAL:HG21	2.55	0.41
1:H:157:HIS:CD2	1:H:308:VAL:HG21	2.56	0.41
1:J:157:HIS:CD2	1:J:308:VAL:HG21	2.56	0.41
1:B:323:LEU:HA	1:B:323:LEU:HD23	1.88	0.41
1:J:65:GLY:HA3	1:J:115:ASP:OD1	2.19	0.41
1:L:177:ILE:HG12	1:L:262:TYR:HB3	2.01	0.41
1:I:64:LEU:O	1:I:152:VAL:HA	2.21	0.41
1:D:253:LYS:HE2	1:D:253:LYS:HB3	1.84	0.41
1:F:218:ILE:HG13	1:F:236:THR:HG23	2.02	0.41
1:A:91:CYS:SG	1:A:92:ASP:N	2.92	0.41
1:C:65:GLY:HA3	1:C:115:ASP:OD1	2.20	0.41
1:I:199:SER:N	1:I:200:PRO:CD	2.83	0.41
1:A:123:ASP:OD2	1:D:47:LYS:NZ	2.44	0.41
1:A:327:LYS:CD	1:C:283:PRO:HG2	2.50	0.41
1:B:45:LYS:NZ	4:B:509:HOH:O	2.54	0.41
1:I:47:LYS:O	1:I:51:MET:HG2	2.20	0.41
1:A:157:HIS:CG	1:A:308:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:GLY:HA3	1:L:115:ASP:OD1	2.21	0.41
1:A:179:HIS:O	1:A:215:GLN:HA	2.21	0.40
1:I:131:LEU:HD12	1:I:131:LEU:HA	1.92	0.40
1:I:185:ASP:HB3	1:I:200:PRO:HD2	2.03	0.40
1:D:47:LYS:O	1:D:51:MET:HG2	2.21	0.40
1:F:179:HIS:O	1:F:215:GLN:HA	2.21	0.40
1:I:170:LYS:HD2	1:I:170:LYS:HA	1.90	0.40
1:G:218:ILE:HG13	1:G:236:THR:HG23	2.04	0.40
1:K:157:HIS:CD2	1:K:308:VAL:HG21	2.56	0.40
1:A:313:GLN:HE21	1:D:84[B]:ARG:CZ	2.34	0.40
1:K:65:GLY:HA3	1:K:115:ASP:OD1	2.21	0.40
1:C:33:ILE:HD11	1:C:126:VAL:HG21	2.04	0.40
1:J:50:LEU:O	1:J:54:LEU:HG	2.22	0.40
1:L:194:TYR:CZ	1:L:203:ARG:HD2	2.56	0.40
1:L:199:SER:N	1:L:200:PRO:CD	2.85	0.40
1:L:323:LEU:HD23	1:L:323:LEU:HA	1.95	0.40
1:L:47:LYS:HD3	1:L:47:LYS:HA	1.84	0.40

There are no symmetry-related clashes.

## 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	316/341 (93%)	306 (97%)	9 (3%)	1 (0%)	41	40
1	B	317/341 (93%)	309 (98%)	7 (2%)	1 (0%)	41	40
1	C	316/341 (93%)	310 (98%)	5 (2%)	1 (0%)	41	40
1	D	320/341 (94%)	314 (98%)	5 (2%)	1 (0%)	41	40
1	E	317/341 (93%)	310 (98%)	6 (2%)	1 (0%)	41	40
1	F	318/341 (93%)	312 (98%)	5 (2%)	1 (0%)	41	40
1	G	319/341 (94%)	311 (98%)	7 (2%)	1 (0%)	41	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	318/341 (93%)	310 (98%)	7 (2%)	1 (0%)	41	40
1	I	315/341 (92%)	309 (98%)	5 (2%)	1 (0%)	41	40
1	J	317/341 (93%)	308 (97%)	8 (2%)	1 (0%)	41	40
1	K	316/341 (93%)	307 (97%)	8 (2%)	1 (0%)	41	40
1	L	318/341 (93%)	310 (98%)	7 (2%)	1 (0%)	41	40
All	All	3807/4092 (93%)	3716 (98%)	79 (2%)	12 (0%)	41	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	199	SER
1	A	199	SER
1	B	199	SER
1	C	199	SER
1	D	199	SER
1	E	199	SER
1	F	199	SER
1	G	199	SER
1	H	199	SER
1	I	199	SER
1	L	199	SER
1	K	199	SER

### 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	267/286 (93%)	261 (98%)	6 (2%)	52	55
1	B	268/286 (94%)	266 (99%)	2 (1%)	84	88
1	C	267/286 (93%)	261 (98%)	6 (2%)	52	55
1	D	270/286 (94%)	265 (98%)	5 (2%)	57	61
1	E	268/286 (94%)	263 (98%)	5 (2%)	57	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	269/286 (94%)	264 (98%)	5 (2%)	57	61
1	G	270/286 (94%)	264 (98%)	6 (2%)	52	55
1	H	269/286 (94%)	263 (98%)	6 (2%)	52	55
1	I	266/286 (93%)	258 (97%)	8 (3%)	41	43
1	J	268/286 (94%)	262 (98%)	6 (2%)	52	55
1	K	267/286 (93%)	263 (98%)	4 (2%)	65	70
1	L	269/286 (94%)	265 (98%)	4 (2%)	65	70
All	All	3218/3432 (94%)	3155 (98%)	63 (2%)	55	59

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	CYS
1	A	144	ASP
1	A	197	HIS
1	A	244	ARG
1	A	287	LEU
1	A	318	ASP
1	B	34	ASP
1	B	197	HIS
1	C	24	LEU
1	C	26	GLU
1	C	34	ASP
1	C	147	PRO
1	C	197	HIS
1	C	243	SER
1	D	20	VAL
1	D	34	ASP
1	D	157	HIS
1	D	197	HIS
1	D	253	LYS
1	E	130	ARG
1	E	157	HIS
1	E	197	HIS
1	E	203	ARG
1	E	243	SER
1	F	20	VAL
1	F	122	ARG
1	F	197	HIS
1	F	256	GLU

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Mol	Chain	Res	Type
1	F	318	ASP
1	G	21	SER
1	G	34	ASP
1	G	105	ARG
1	G	133	ASN
1	G	197	HIS
1	G	256	GLU
1	H	45	LYS
1	H	157	HIS
1	H	197	HIS
1	H	224	ASP
1	H	248	ILE
1	H	318	ASP
1	I	24	LEU
1	I	25	LEU
1	I	26	GLU
1	I	27	LYS
1	I	122	ARG
1	I	157	HIS
1	I	197	HIS
1	I	258	VAL
1	J	24	LEU
1	J	105	ARG
1	J	130	ARG
1	J	197	HIS
1	J	203	ARG
1	J	243	SER
1	K	31	ARG
1	K	157	HIS
1	K	197	HIS
1	K	226	ARG
1	L	122	ARG
1	L	157	HIS
1	L	197	HIS
1	L	243	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 24 are monoatomic - leaving 7 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	$\# Z  > 2$
3	ORN	L	403	-	4,8,8	0.51	0	3,9,9	0.41	0
3	ORN	H	403	-	4,8,8	0.53	0	3,9,9	0.44	0
3	ORN	J	403	-	4,8,8	0.50	0	3,9,9	0.57	0
3	ORN	D	403	-	4,8,8	0.52	0	3,9,9	0.57	0
3	ORN	F	403	-	4,8,8	0.56	0	3,9,9	0.46	0
3	ORN	B	403	-	4,8,8	0.51	0	3,9,9	0.49	0
3	ORN	A	403	-	4,8,8	0.55	0	3,9,9	0.55	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
3	ORN	L	403	-	-	0/4/8/8	-
3	ORN	H	403	-	-	2/4/8/8	-
3	ORN	J	403	-	-	0/4/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ORN	D	403	-	-	0/4/8/8	-
3	ORN	F	403	-	-	0/4/8/8	-
3	ORN	B	403	-	-	0/4/8/8	-
3	ORN	A	403	-	-	1/4/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

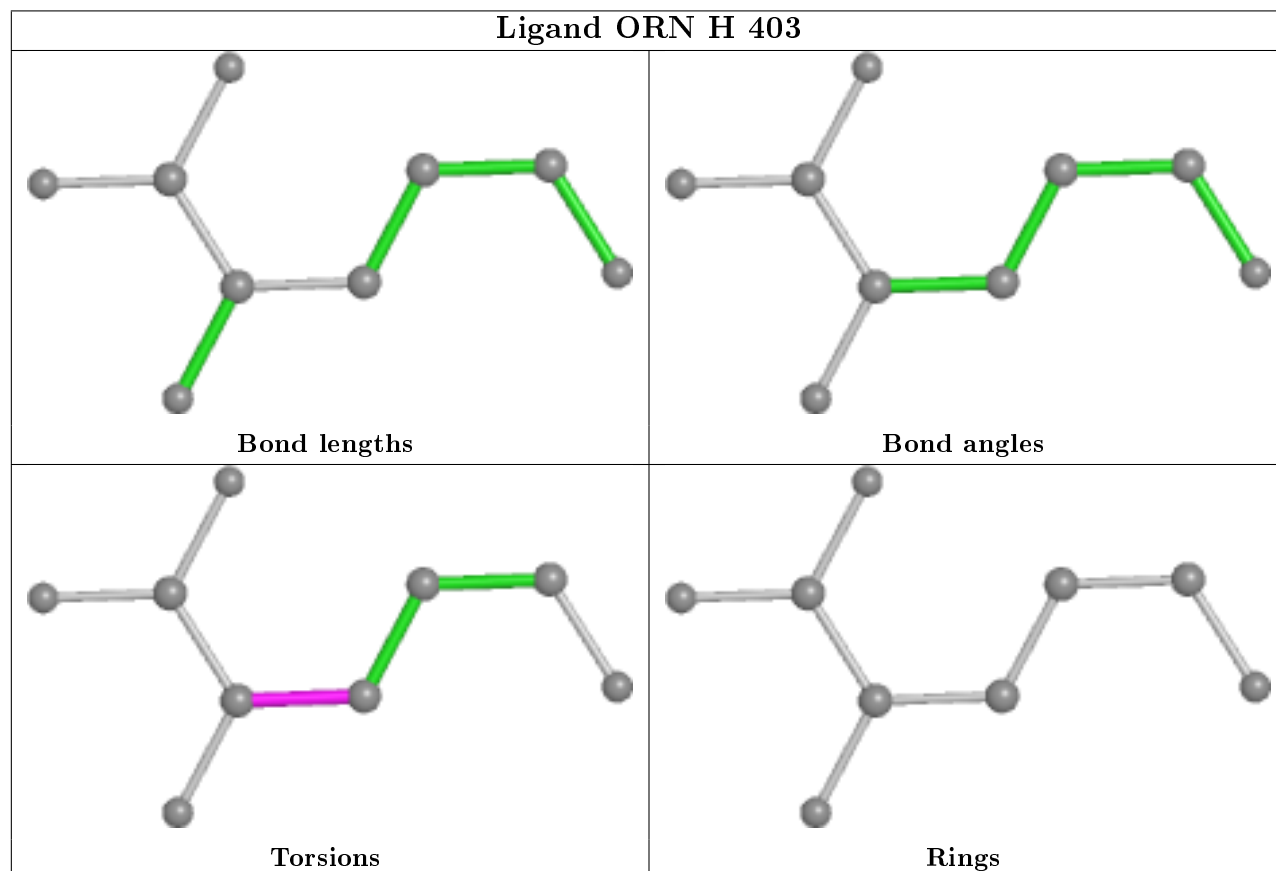
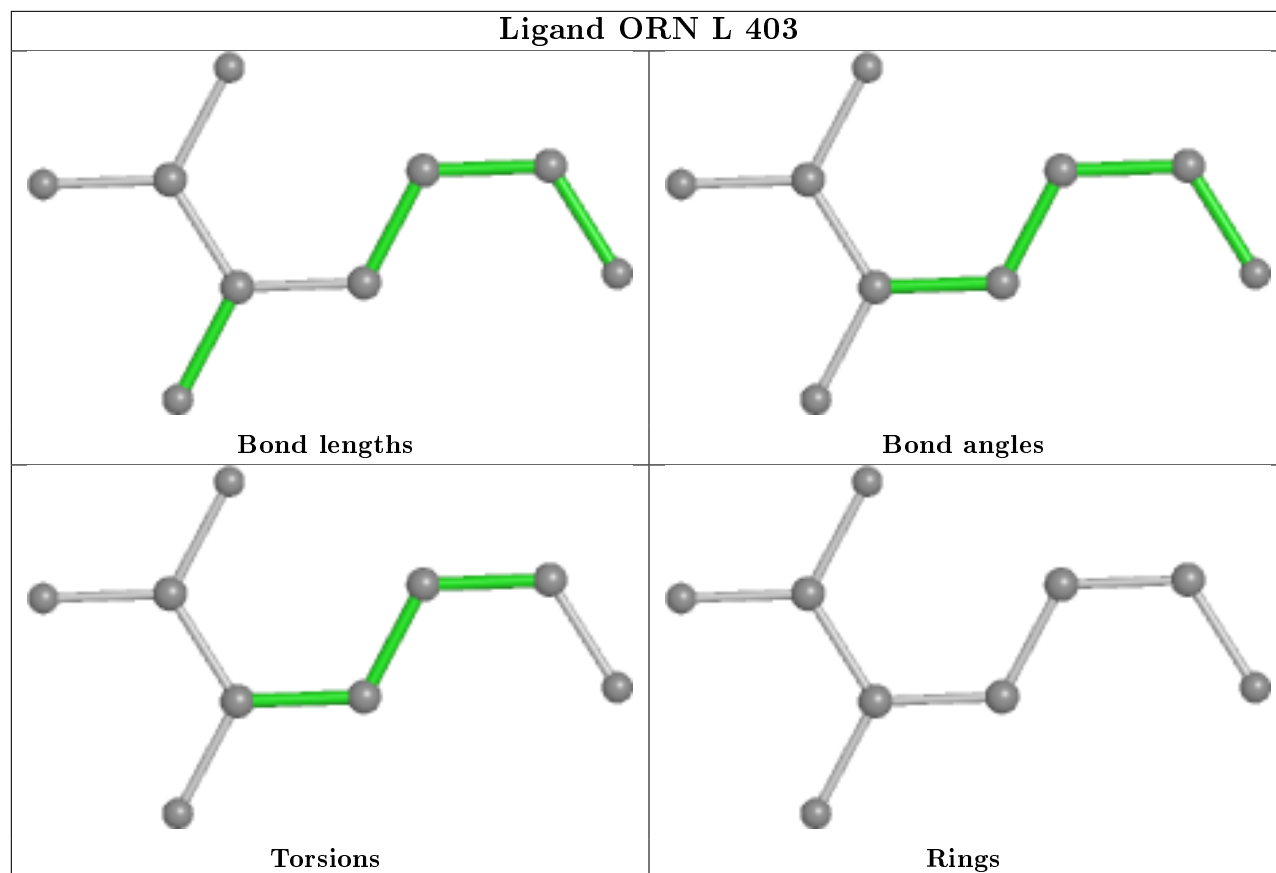
Mol	Chain	Res	Type	Atoms
3	H	403	ORN	N-CA-CB-CG
3	H	403	ORN	C-CA-CB-CG
3	A	403	ORN	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 5 short contacts:

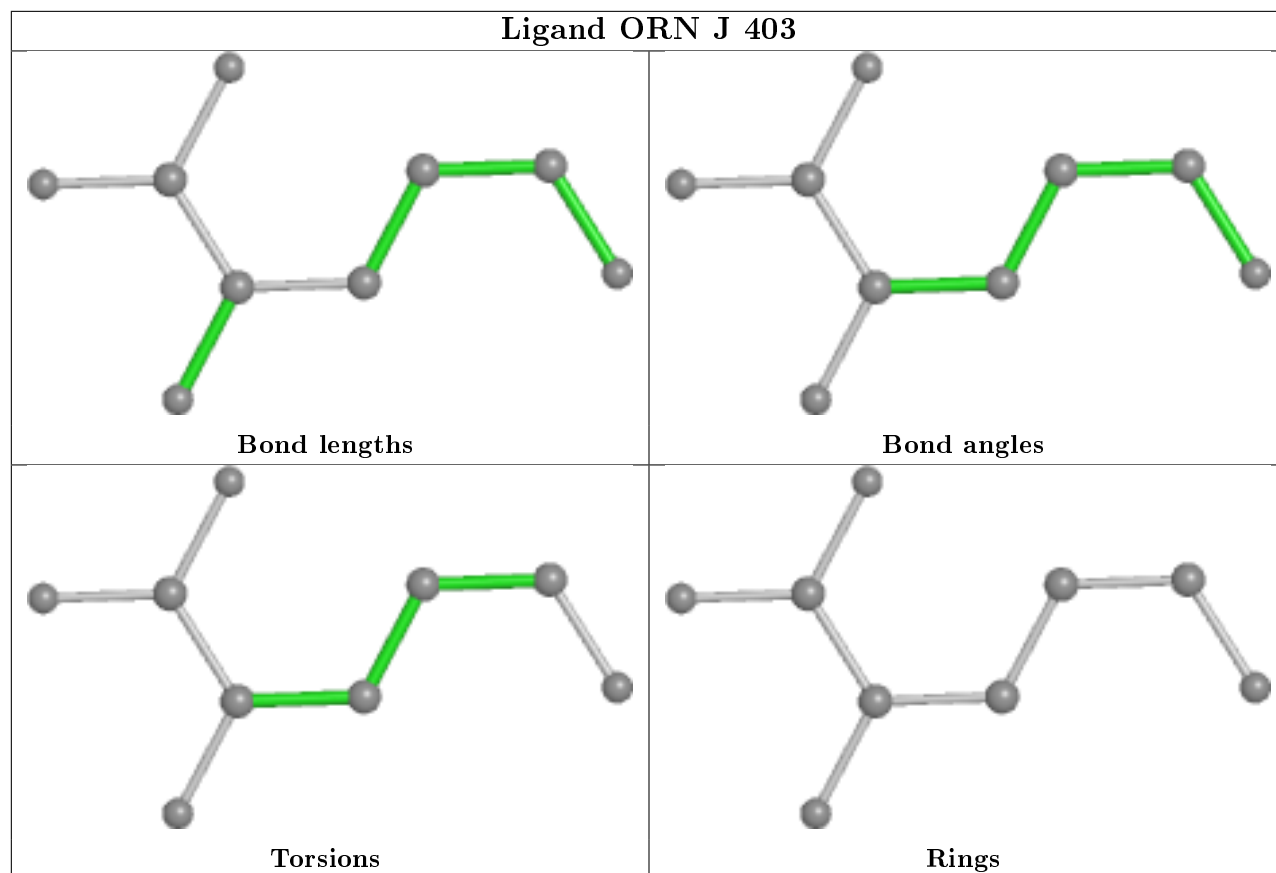
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	403	ORN	1	0
3	J	403	ORN	1	0
3	D	403	ORN	1	0
3	B	403	ORN	1	0
3	A	403	ORN	1	0

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.

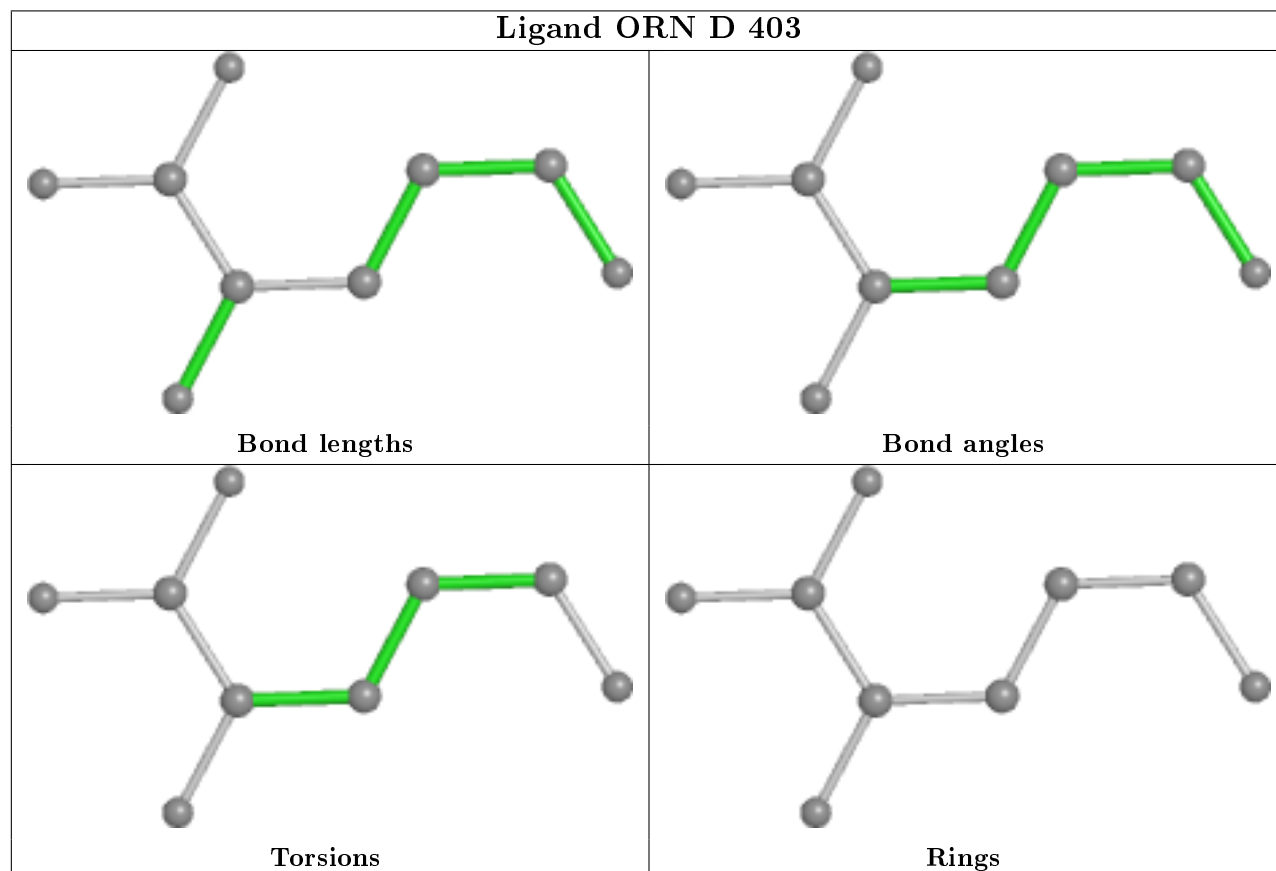


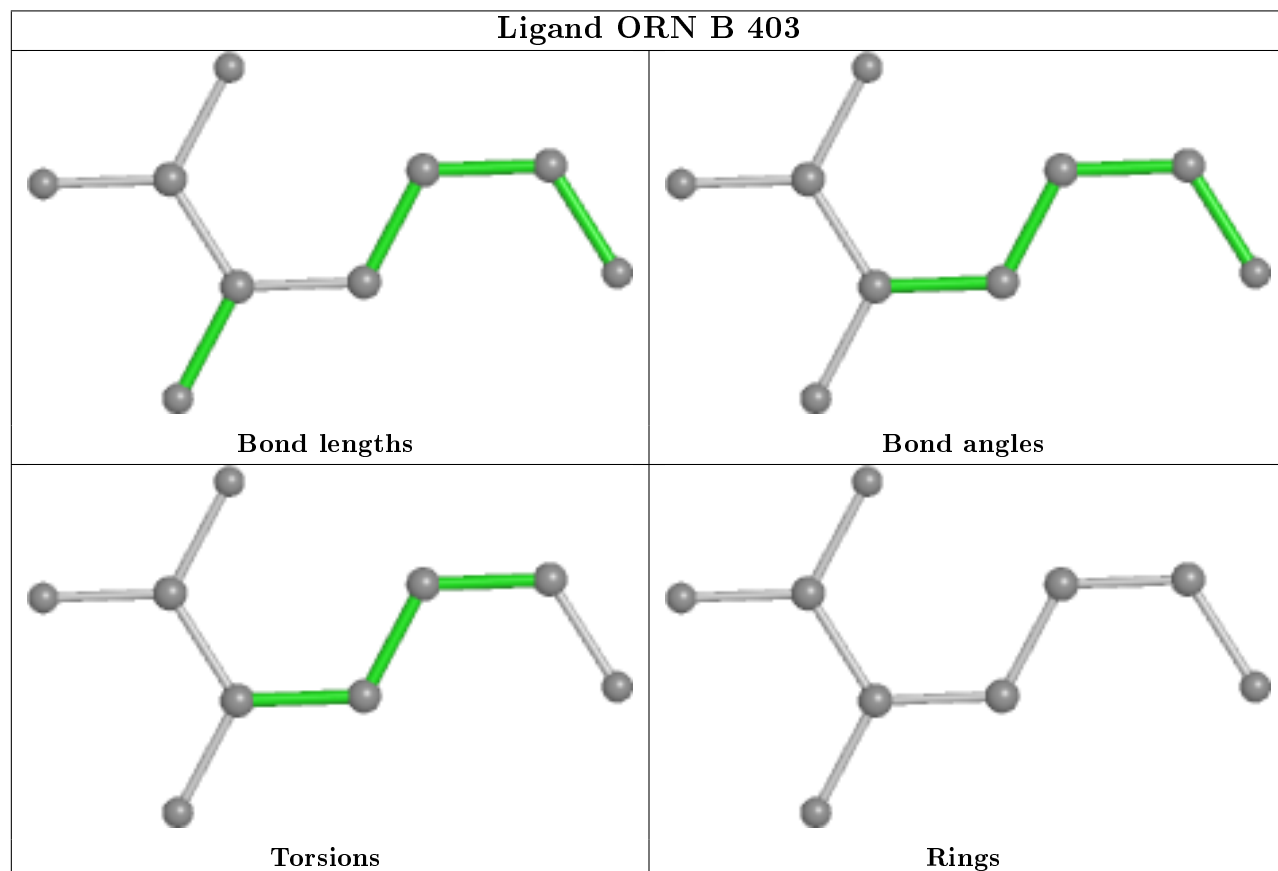
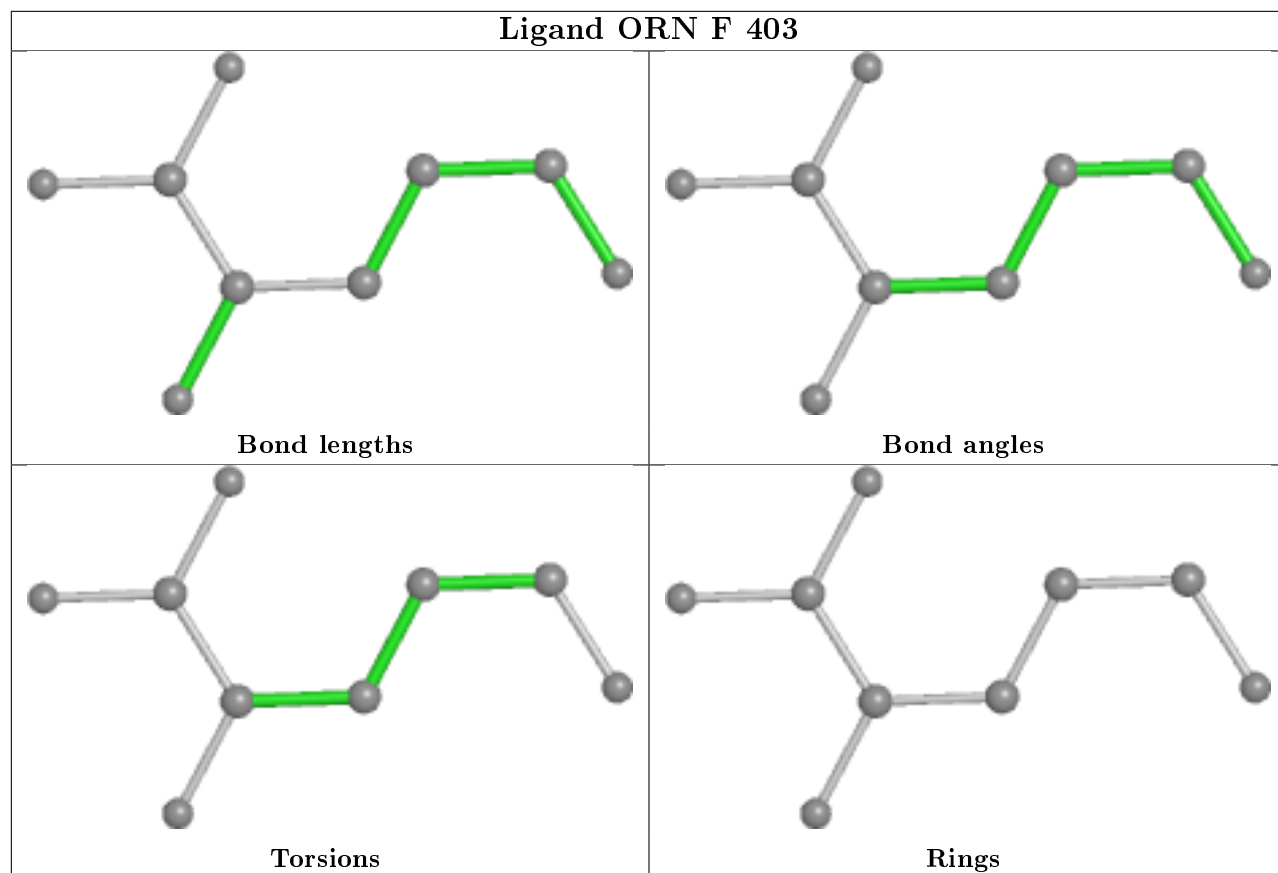


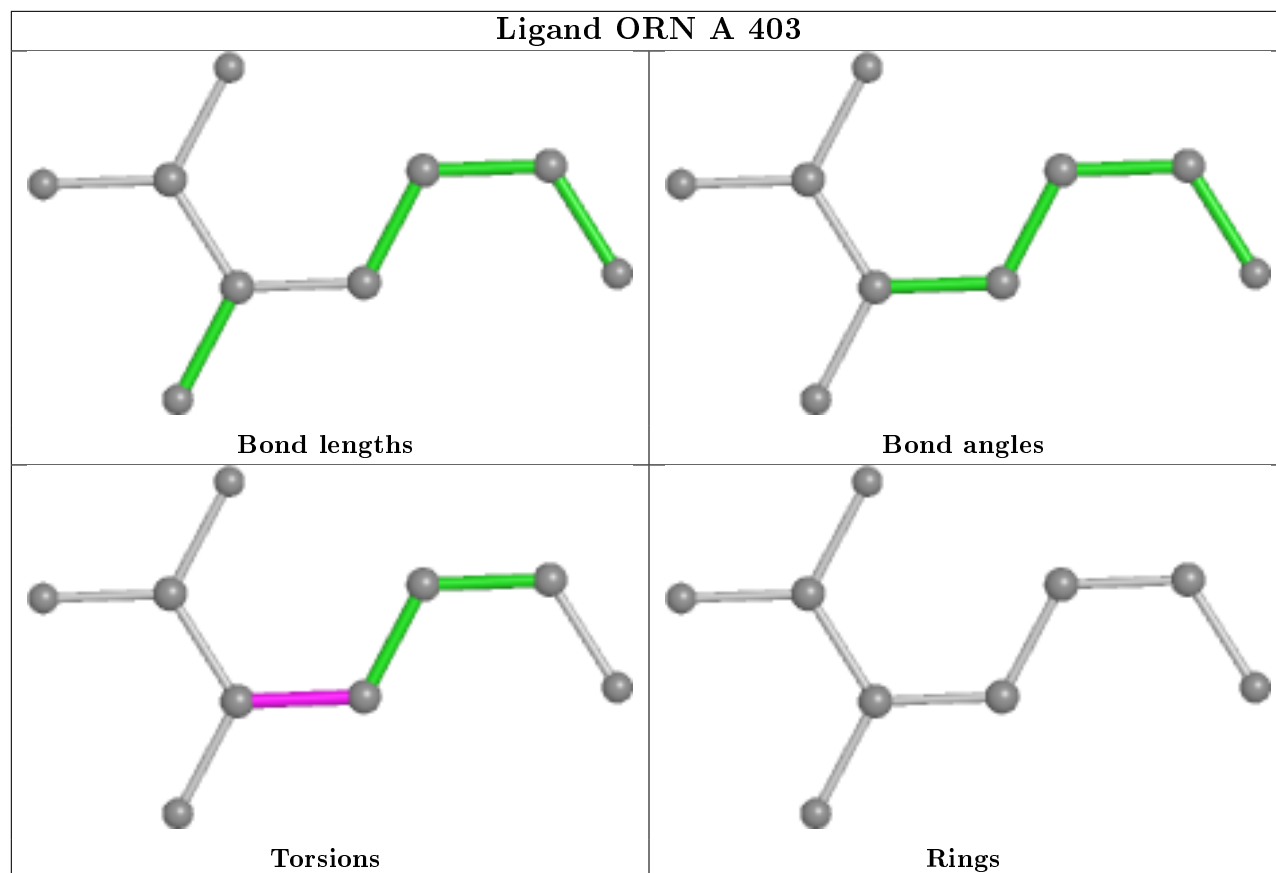
## Ligand ORN J 403



## Ligand ORN D 403







## 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	317/341 (92%)	-0.01	12 (3%) 40 46	27, 40, 69, 143	0
1	B	318/341 (93%)	-0.18	7 (2%) 62 66	25, 40, 59, 76	0
1	C	318/341 (93%)	-0.05	18 (5%) 23 28	26, 41, 74, 99	0
1	D	320/341 (93%)	-0.02	6 (1%) 66 71	34, 50, 72, 103	0
1	E	319/341 (93%)	0.02	13 (4%) 37 43	29, 44, 64, 111	0
1	F	320/341 (93%)	-0.11	4 (1%) 77 80	28, 45, 72, 105	0
1	G	320/341 (93%)	-0.09	5 (1%) 72 76	37, 53, 76, 114	0
1	H	320/341 (93%)	0.34	18 (5%) 24 29	41, 63, 91, 118	0
1	I	317/341 (92%)	0.33	21 (6%) 18 22	40, 65, 88, 130	0
1	J	318/341 (93%)	-0.10	11 (3%) 44 50	30, 42, 69, 118	0
1	K	318/341 (93%)	-0.10	9 (2%) 53 59	34, 54, 79, 118	0
1	L	319/341 (93%)	0.02	4 (1%) 77 80	32, 51, 69, 82	0
All	All	3824/4092 (93%)	0.01	128 (3%) 46 53	25, 49, 79, 143	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	317[A]	TYR	11.1
1	L	317[A]	TYR	10.6
1	J	317[A]	TYR	10.4
1	G	317[A]	TYR	10.1
1	A	317[A]	TYR	10.0
1	B	317[A]	TYR	8.8
1	A	25	LEU	8.0
1	I	24	LEU	7.8
1	E	24	LEU	7.4
1	I	25	LEU	5.7
1	A	93	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	190	PHE	5.2
1	J	24	LEU	4.9
1	E	317	TYR	4.7
1	A	92	ASP	4.5
1	G	19	ASN	4.3
1	C	24	LEU	4.3
1	K	190	PHE	4.2
1	B	316	THR	3.9
1	C	222	THR	3.9
1	A	24	LEU	3.8
1	I	317	TYR	3.8
1	I	23	ALA	3.8
1	K	24	LEU	3.8
1	C	224	ASP	3.6
1	H	257	GLY	3.6
1	C	196	SER	3.6
1	C	188	HIS	3.5
1	J	22	PRO	3.5
1	K	194	TYR	3.5
1	F	317	TYR	3.4
1	C	194	TYR	3.4
1	L	316	THR	3.4
1	K	317	TYR	3.3
1	A	27	LYS	3.3
1	C	317	TYR	3.2
1	E	20	VAL	3.2
1	H	256	GLU	3.1
1	C	195	TYR	3.0
1	I	27	LYS	3.0
1	I	50	LEU	3.0
1	C	191	GLU	3.0
1	H	109	VAL	2.9
1	I	312	PRO	2.9
1	G	56	GLY	2.9
1	C	225	VAL	2.9
1	E	274	ILE	2.9
1	A	316	THR	2.9
1	H	316	THR	2.9
1	A	23	ALA	2.8
1	F	316	THR	2.8
1	C	221	ILE	2.8
1	H	298	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	57	VAL	2.7
1	H	317	TYR	2.7
1	B	320	ILE	2.7
1	H	338	LYS	2.7
1	E	278	VAL	2.7
1	A	274	ILE	2.7
1	L	39	PHE	2.7
1	C	189	ASP	2.6
1	E	23	ALA	2.6
1	E	316	THR	2.5
1	I	204	ILE	2.5
1	L	318	ASP	2.5
1	H	214	VAL	2.5
1	J	316	THR	2.5
1	I	56	GLY	2.5
1	K	195	TYR	2.4
1	E	286	LEU	2.4
1	K	189	ASP	2.4
1	H	211	ARG	2.4
1	E	310	TYR	2.4
1	C	223	ASN	2.4
1	H	59	ALA	2.4
1	J	275	ALA	2.4
1	I	274	ILE	2.4
1	J	23	ALA	2.3
1	F	274	ILE	2.3
1	J	274	ILE	2.3
1	C	187	TYR	2.3
1	J	21	SER	2.3
1	D	316	THR	2.3
1	H	46	PHE	2.3
1	A	277	GLY	2.3
1	C	198	ALA	2.3
1	F	273	SER	2.3
1	H	233	GLY	2.3
1	H	224	ASP	2.3
1	J	27	LYS	2.3
1	C	21	SER	2.3
1	E	270	LEU	2.2
1	I	51	MET	2.2
1	H	258	VAL	2.2
1	I	314	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	176	ASP	2.2
1	K	188	HIS	2.2
1	G	53	SER	2.2
1	I	48	GLY	2.2
1	E	320	ILE	2.2
1	E	276	PRO	2.2
1	K	187	TYR	2.2
1	I	194	TYR	2.2
1	I	59	ALA	2.2
1	A	312	PRO	2.2
1	J	276	PRO	2.1
1	I	126	VAL	2.1
1	D	84[A]	ARG	2.1
1	I	195	TYR	2.1
1	B	312	PRO	2.1
1	G	192	GLY	2.1
1	A	22	PRO	2.1
1	K	191	GLU	2.1
1	D	320	ILE	2.1
1	B	276	PRO	2.1
1	C	316	THR	2.1
1	D	275	ALA	2.1
1	I	310	TYR	2.1
1	H	56	GLY	2.1
1	I	34	ASP	2.0
1	B	278	VAL	2.0
1	D	20	VAL	2.0
1	I	316	THR	2.0
1	H	334	ALA	2.0
1	J	278	VAL	2.0
1	B	318	ASP	2.0
1	E	22	PRO	2.0
1	I	173	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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.

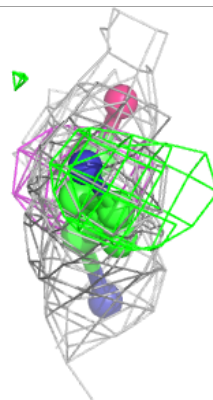
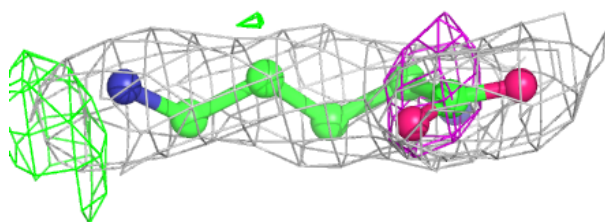
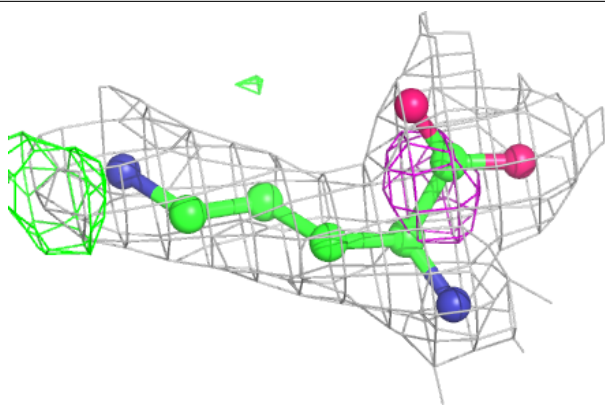
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ORN	A	403	9/9	0.66	0.24	48,54,57,57	0
3	ORN	D	403	9/9	0.72	0.29	62,69,78,78	0
3	ORN	F	403	9/9	0.76	0.20	56,60,67,69	0
3	ORN	H	403	9/9	0.77	0.25	70,75,83,84	0
3	ORN	B	403	9/9	0.77	0.17	50,56,59,64	0
3	ORN	L	403	9/9	0.80	0.19	58,62,66,67	0
3	ORN	J	403	9/9	0.87	0.18	53,59,60,60	0
2	MN	K	401	1/1	0.94	0.06	62,62,62,62	0
2	MN	G	401	1/1	0.96	0.04	62,62,62,62	0
2	MN	C	401	1/1	0.97	0.04	60,60,60,60	0
2	MN	I	401	1/1	0.97	0.05	56,56,56,56	0
2	MN	D	401	1/1	0.98	0.03	55,55,55,55	0
2	MN	K	402	1/1	0.99	0.06	42,42,42,42	0
2	MN	L	402	1/1	0.99	0.09	33,33,33,33	0
2	MN	C	402	1/1	0.99	0.04	42,42,42,42	0
2	MN	D	402	1/1	0.99	0.10	39,39,39,39	0
2	MN	I	402	1/1	0.99	0.06	44,44,44,44	0
2	MN	G	402	1/1	0.99	0.09	40,40,40,40	0
2	MN	E	401	1/1	0.99	0.09	43,43,43,43	0
2	MN	H	402	1/1	0.99	0.08	43,43,43,43	0
2	MN	F	401	1/1	0.99	0.09	41,41,41,41	0
2	MN	J	401	1/1	0.99	0.14	39,39,39,39	0
2	MN	H	401	1/1	0.99	0.05	55,55,55,55	0
2	MN	L	401	1/1	1.00	0.05	43,43,43,43	0
2	MN	B	402	1/1	1.00	0.12	28,28,28,28	0
2	MN	J	402	1/1	1.00	0.12	28,28,28,28	0
2	MN	B	401	1/1	1.00	0.08	36,36,36,36	0
2	MN	F	402	1/1	1.00	0.13	31,31,31,31	0
2	MN	A	401	1/1	1.00	0.13	34,34,34,34	0
2	MN	A	402	1/1	1.00	0.14	28,28,28,28	0
2	MN	E	402	1/1	1.00	0.12	34,34,34,34	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.

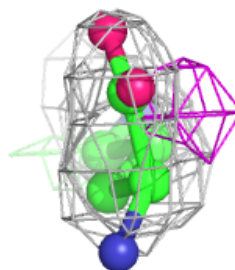
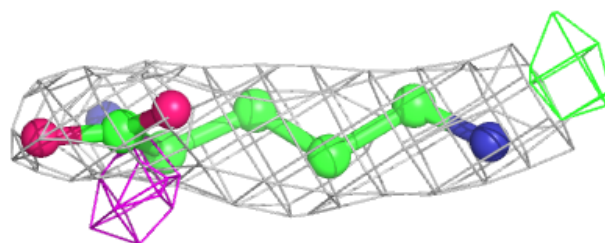
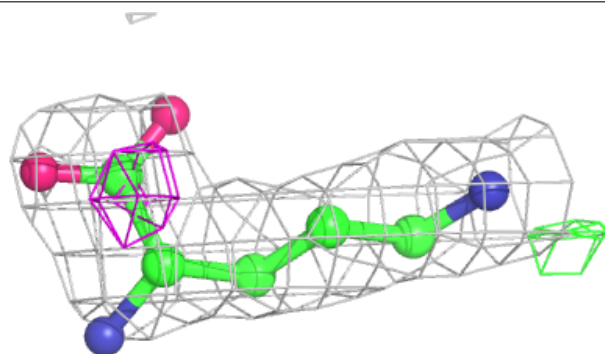


**Electron density around ORN A 403:**

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

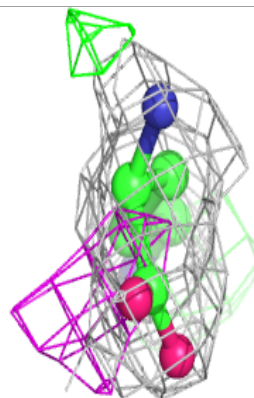
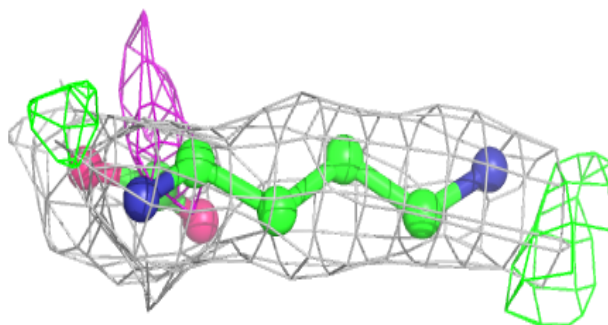
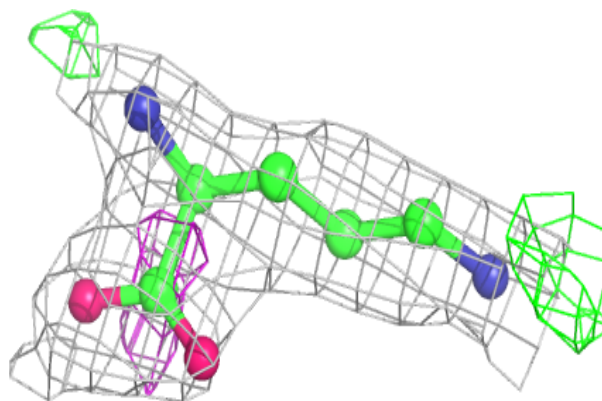
**Electron density around ORN D 403:**

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and green (positive)

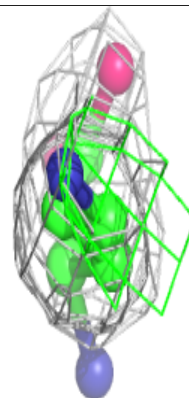
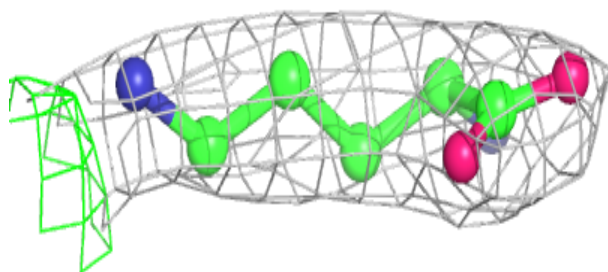
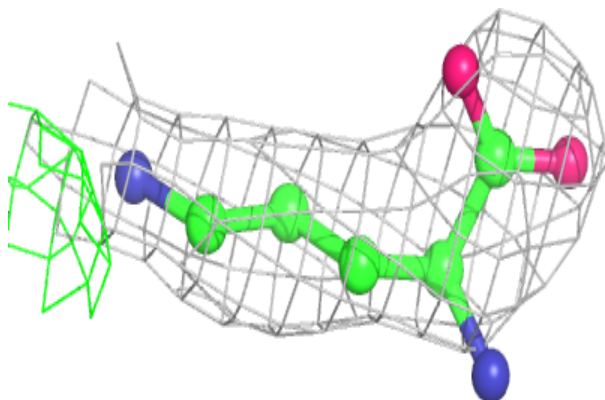


**Electron density around ORN F 403:**

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

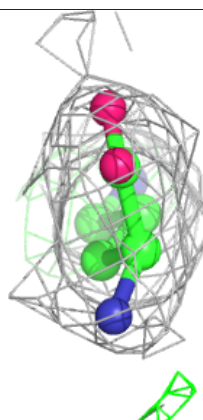
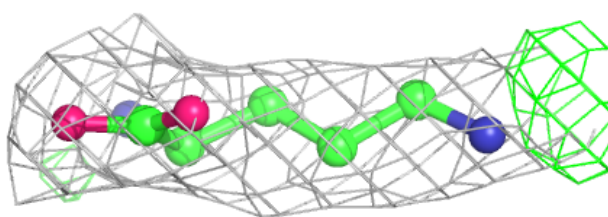
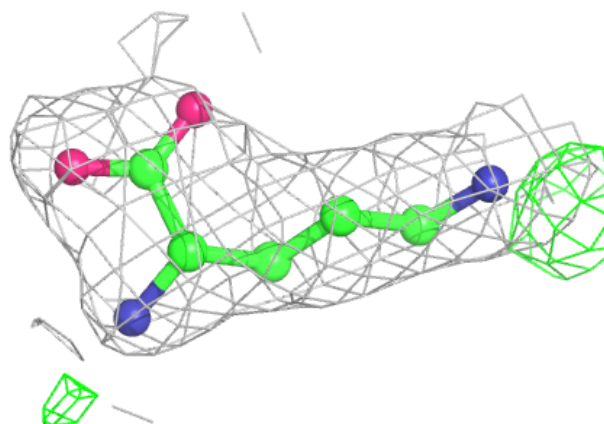
**Electron density around ORN H 403:**

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and green (positive)

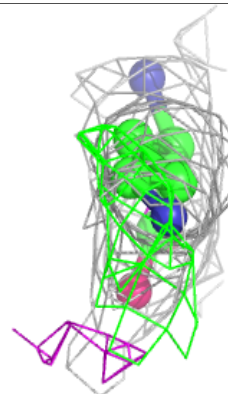
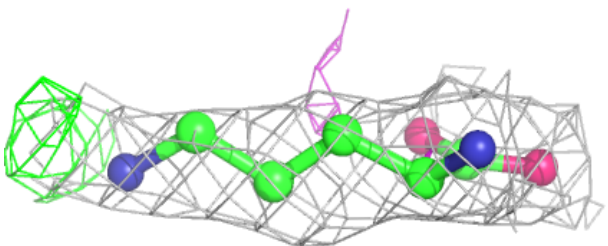
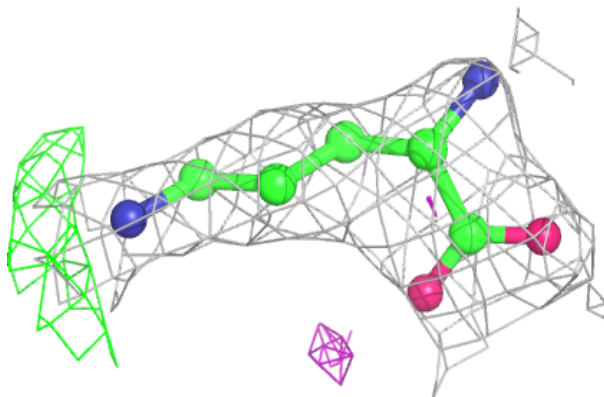


**Electron density around ORN B 403:**

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

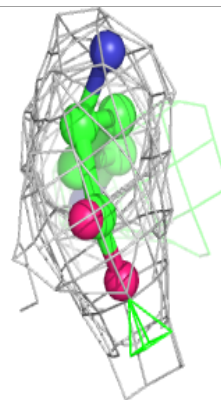
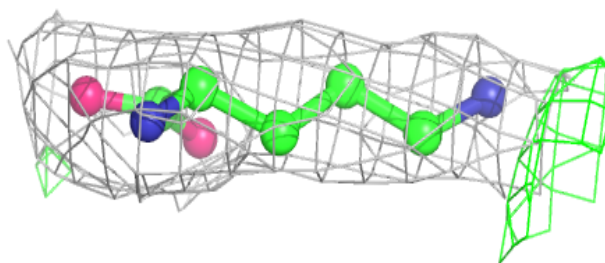
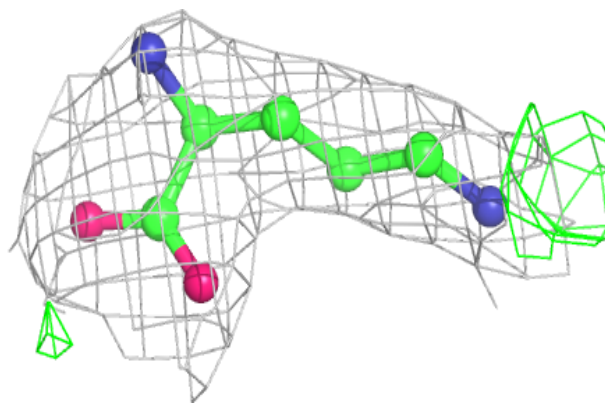
**Electron density around ORN L 403:**

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



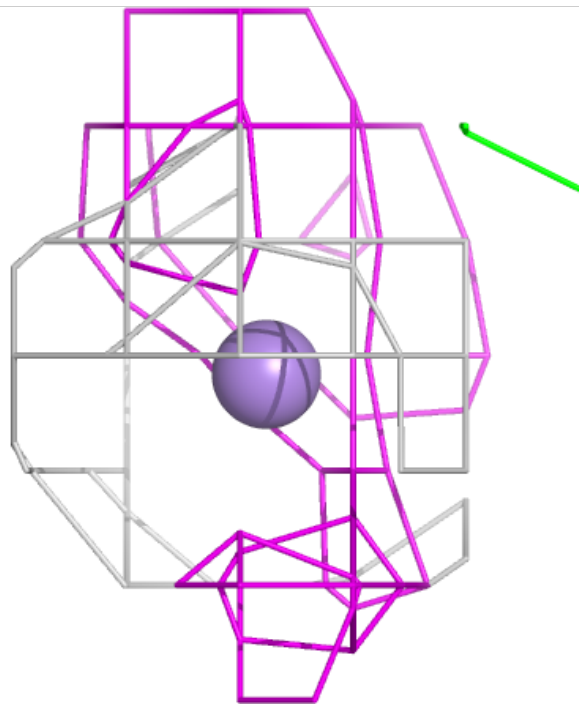
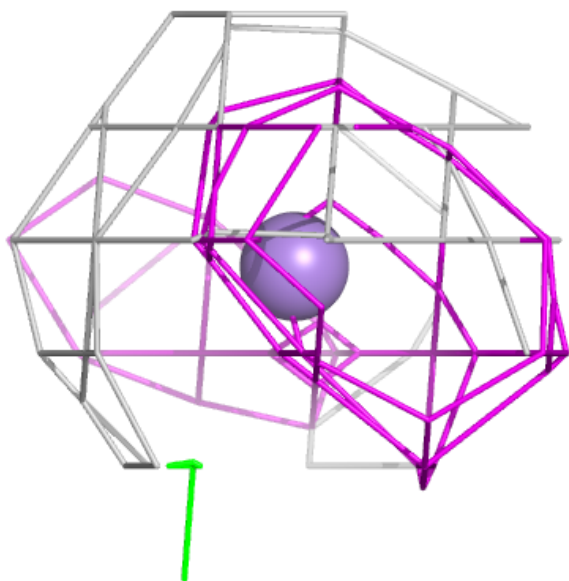
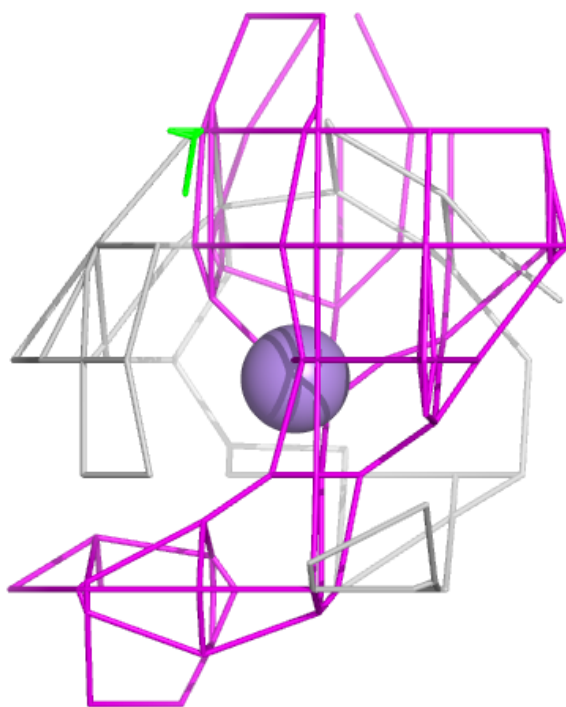
**Electron density around ORN J 403:**

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



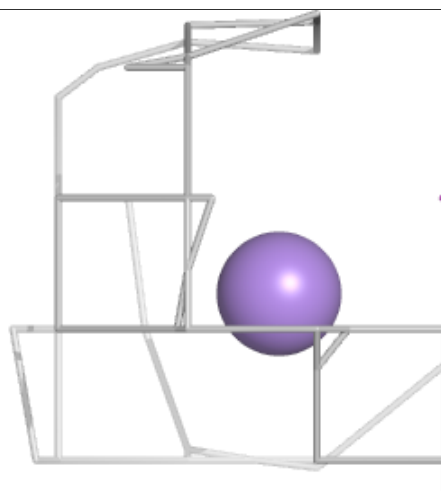
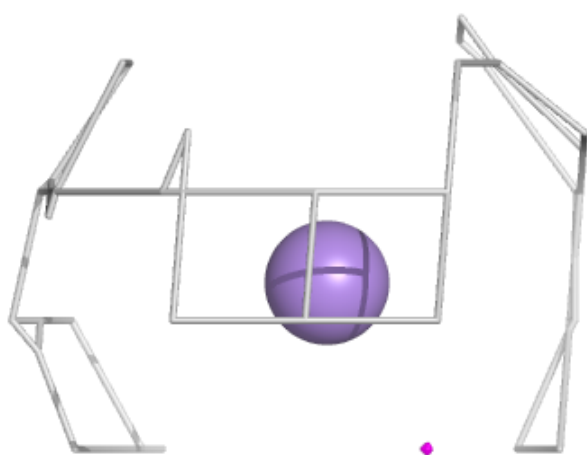
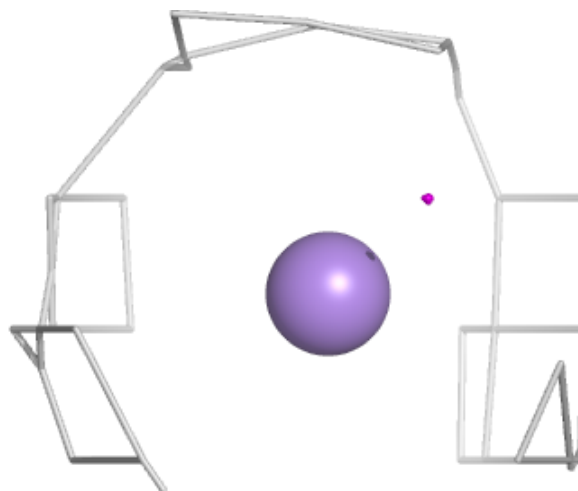
**Electron density around MN K 401:**

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



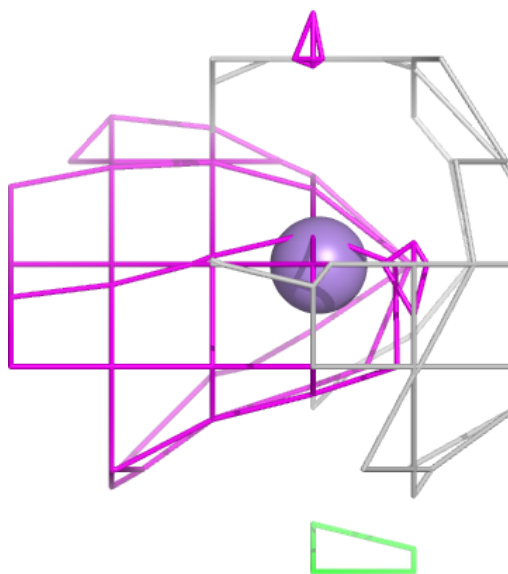
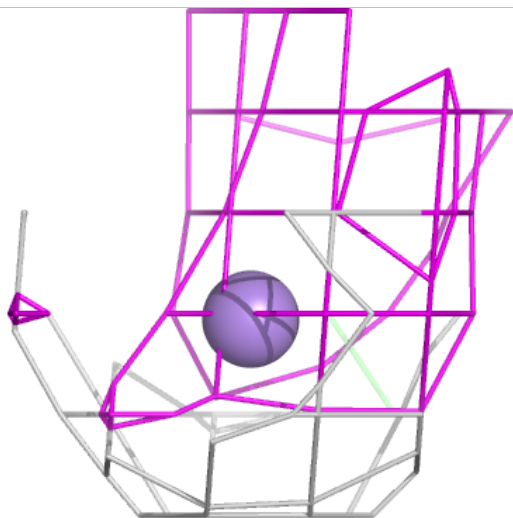
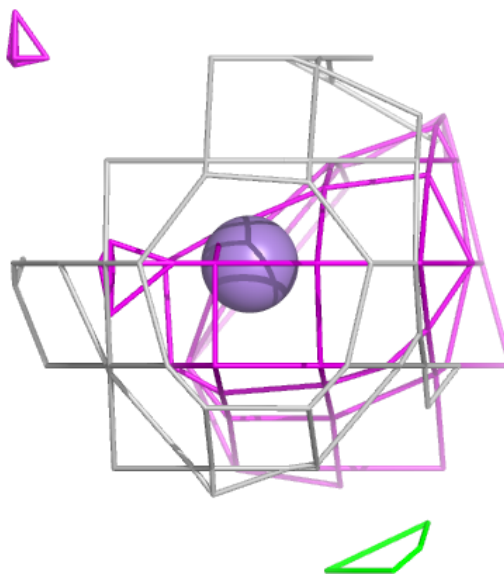
**Electron density around MN G 401:**

$2mF_o-DF_c$  (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:**

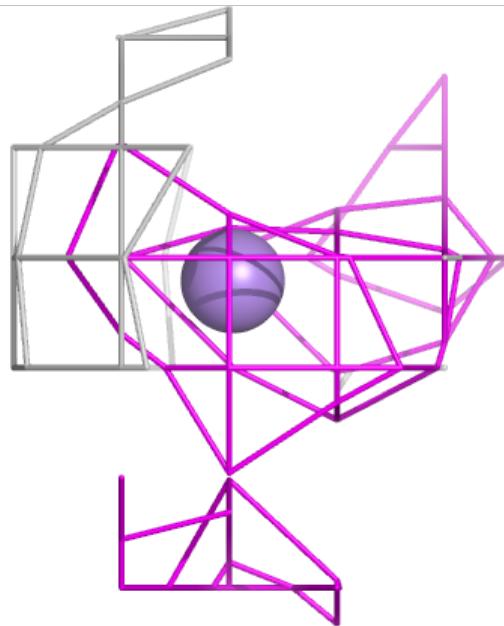
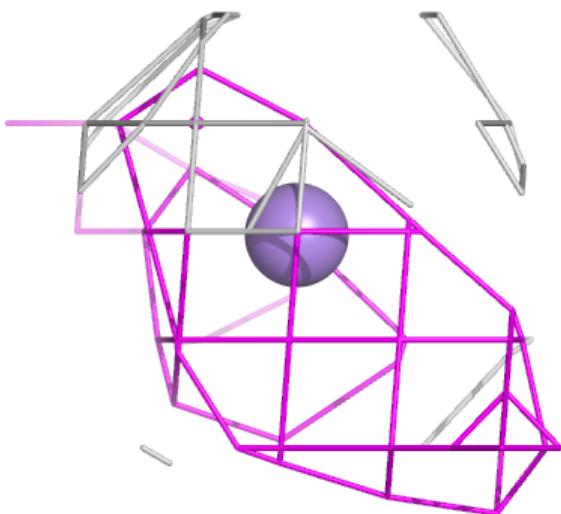
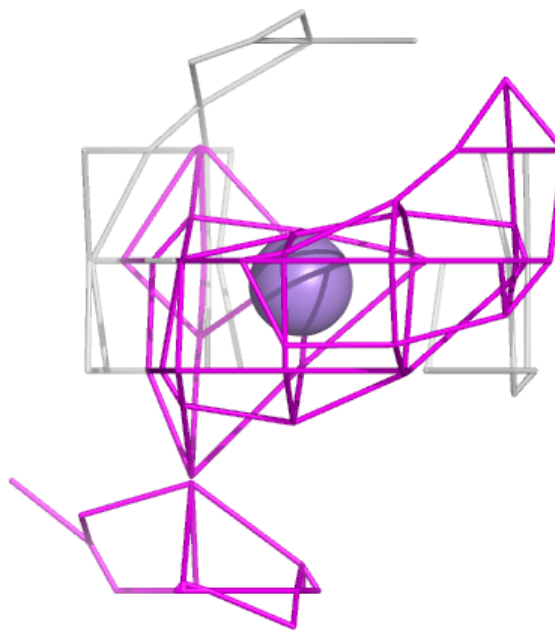
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN I 401:**

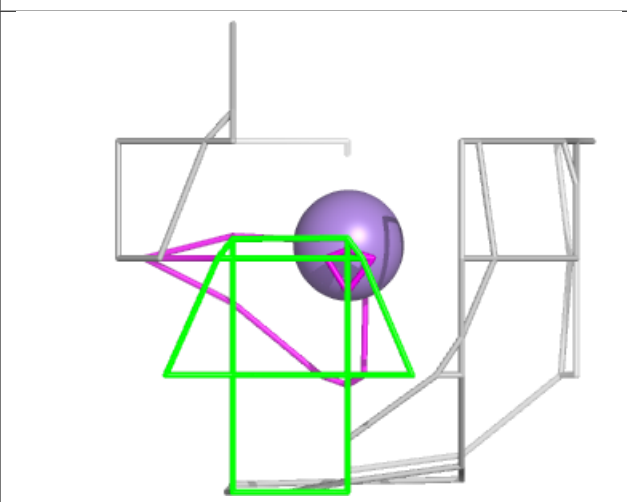
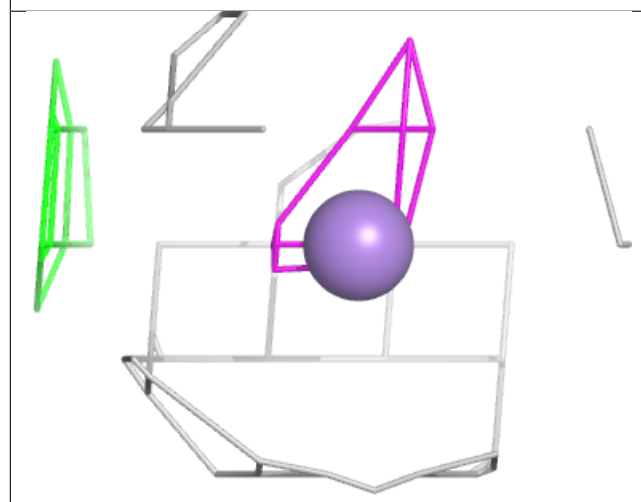
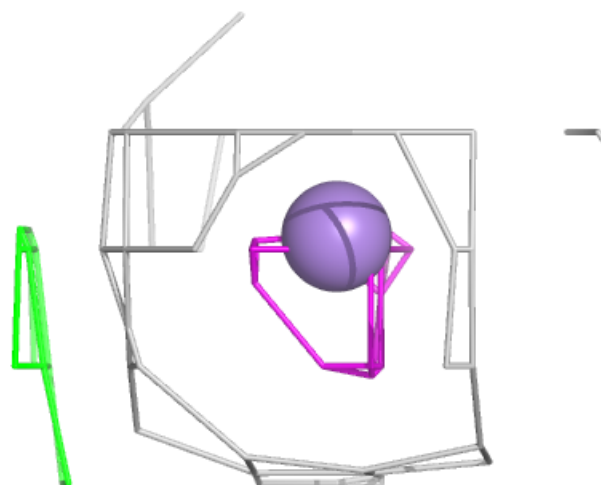
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





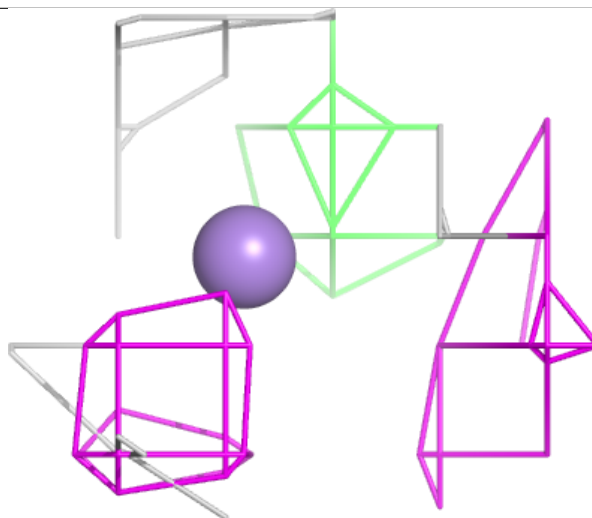
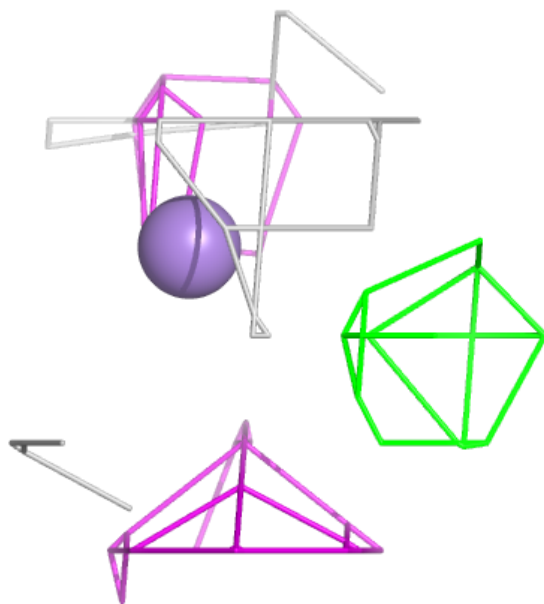
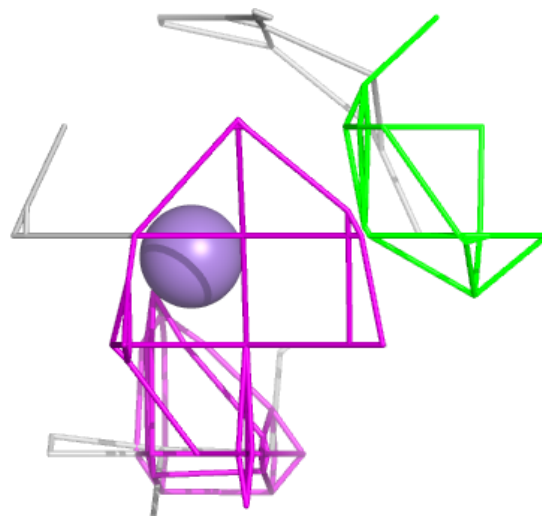
**Electron density around MN D 401:**

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



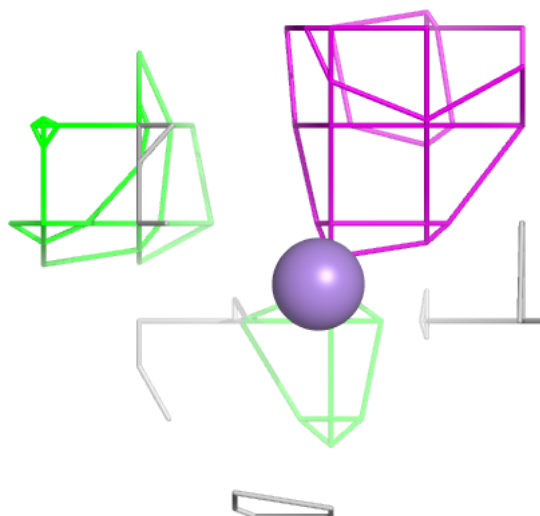
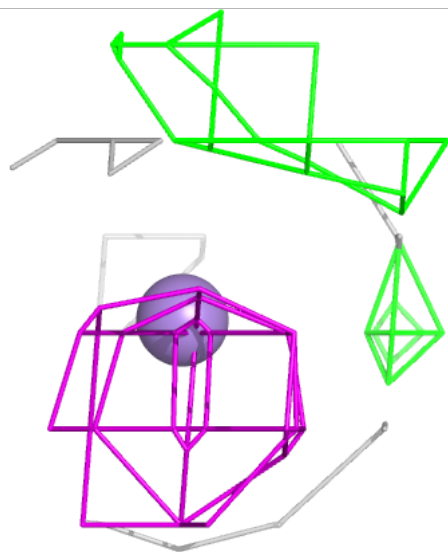
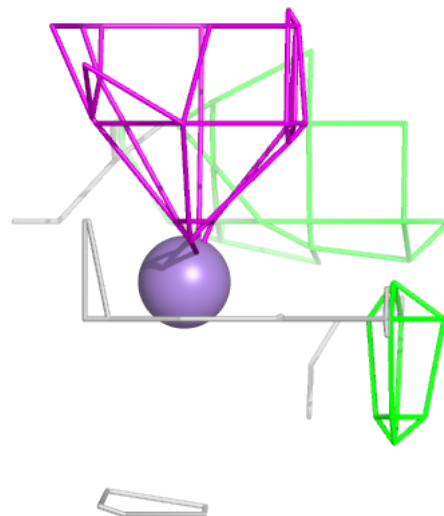
**Electron density around MN K 402:**

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



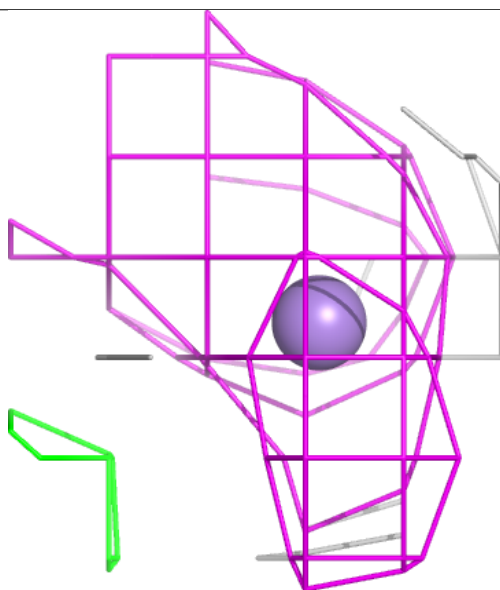
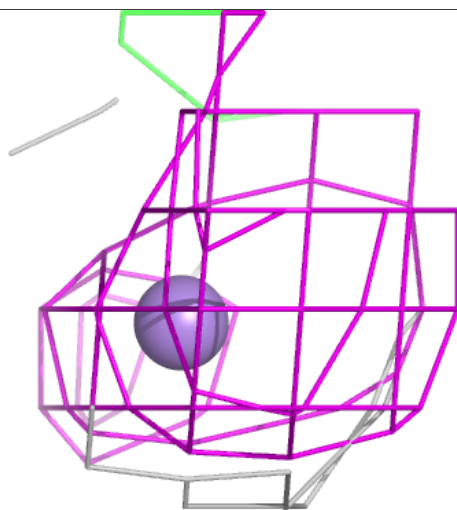
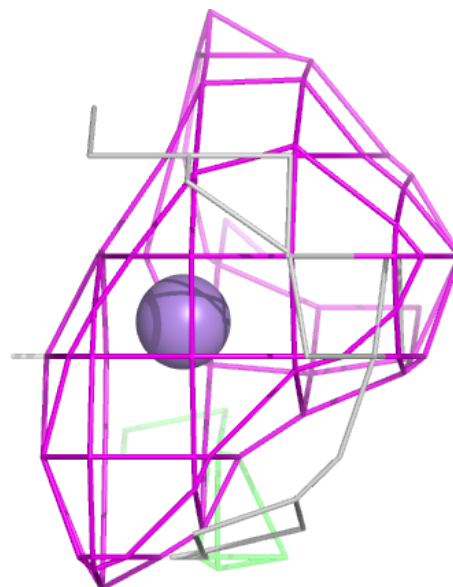
**Electron density around MN L 402:**

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



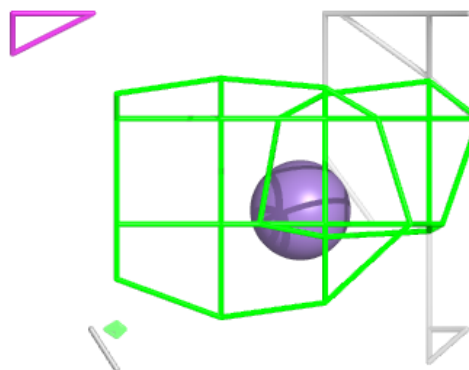
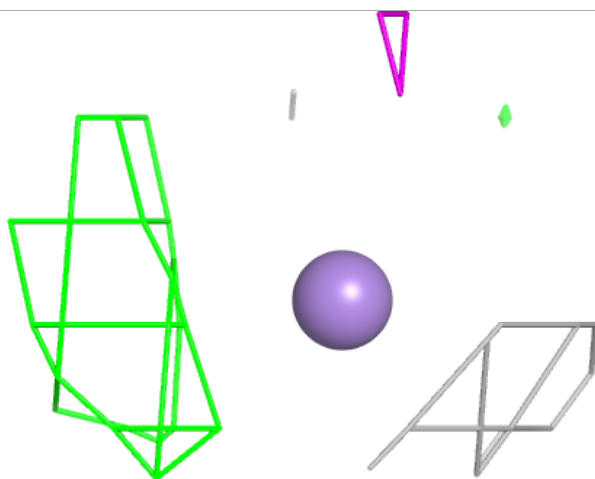
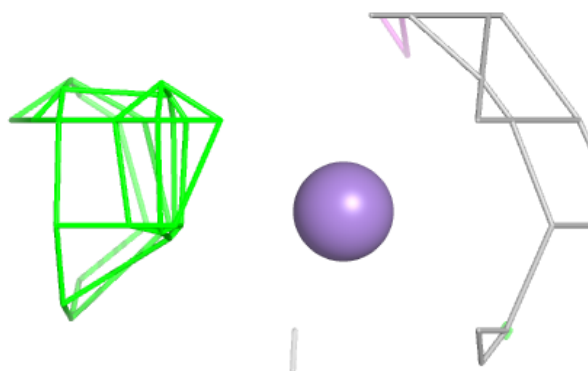
**Electron density around MN C 402:**

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



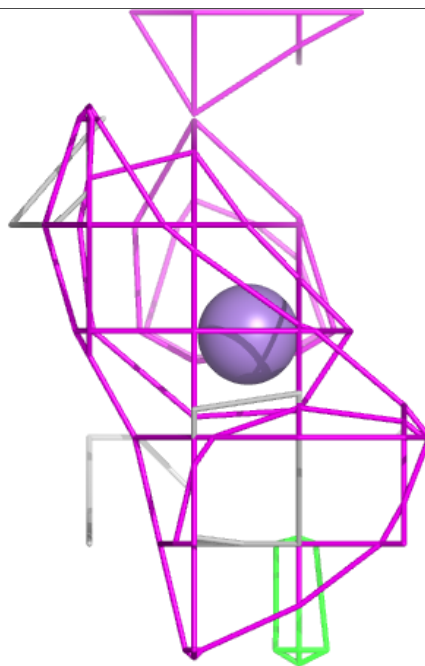
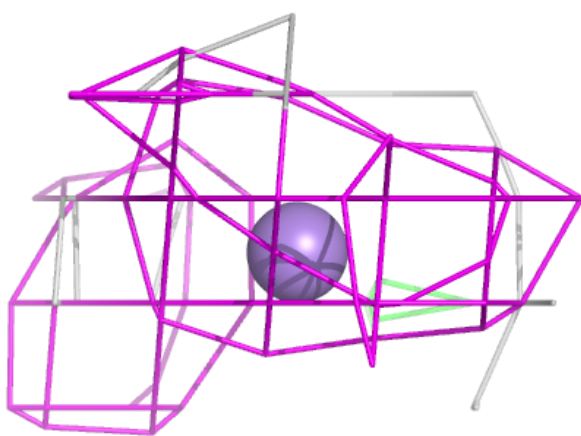
**Electron density around MN D 402:**

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



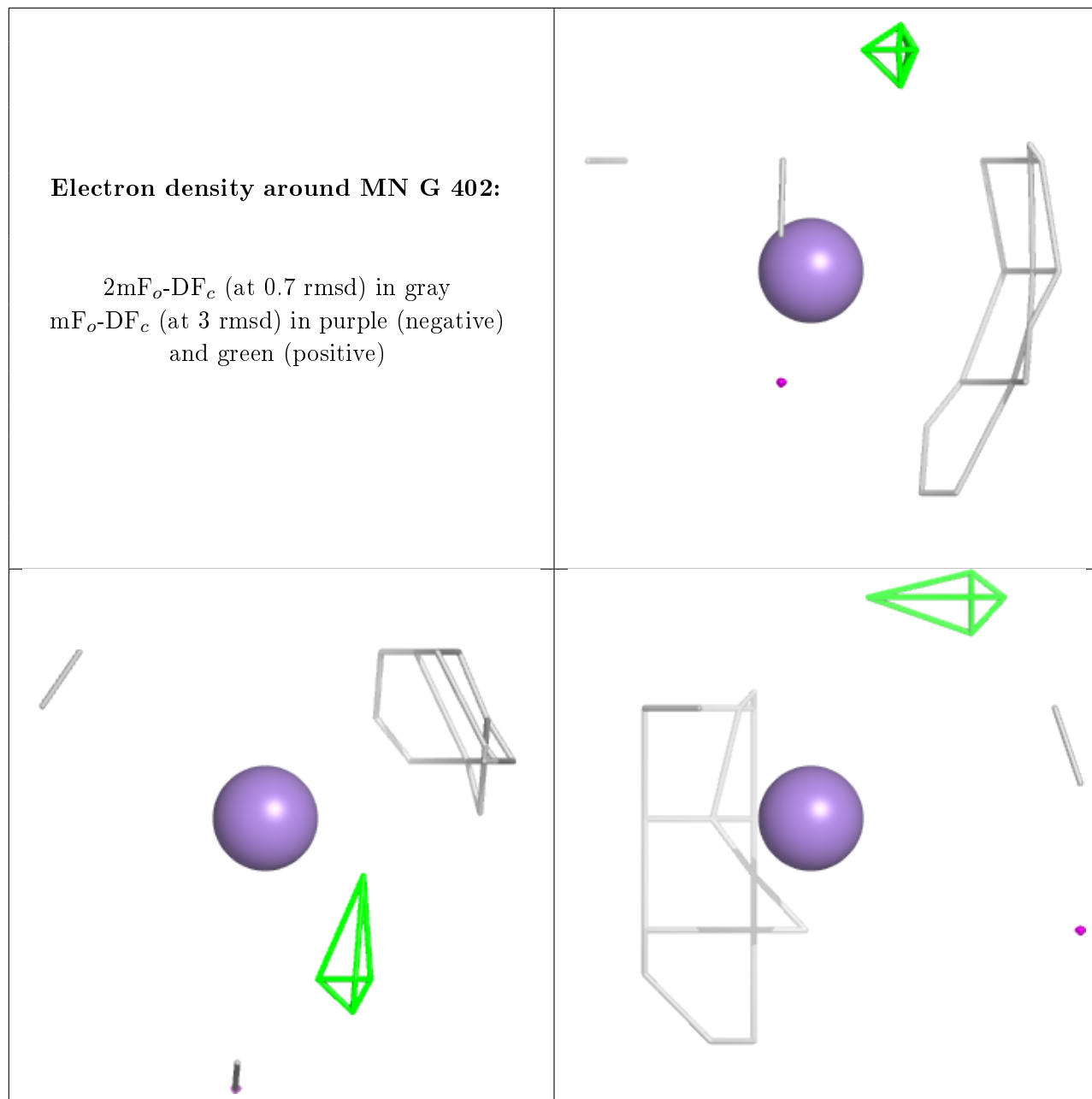
**Electron density around MN I 402:**

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



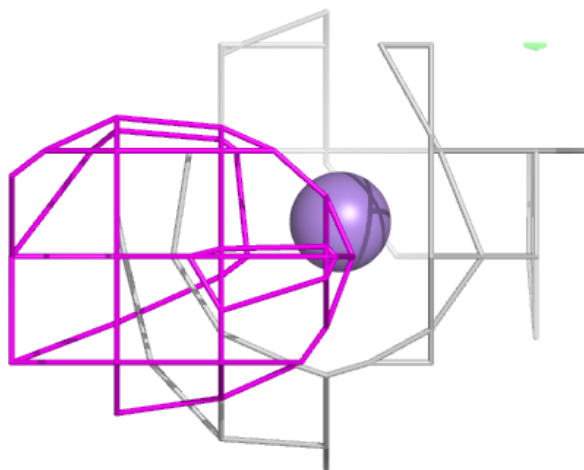
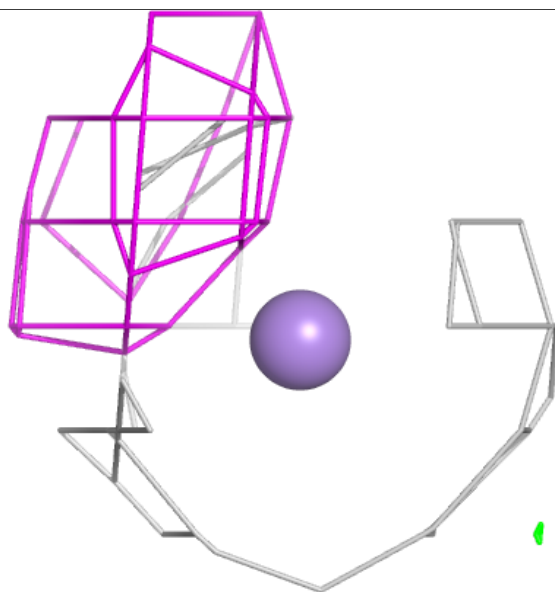
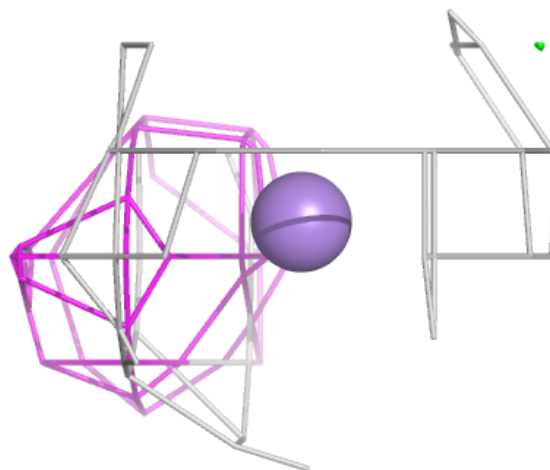
**Electron density around MN G 402:**

$2mF_o-DF_c$  (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:**

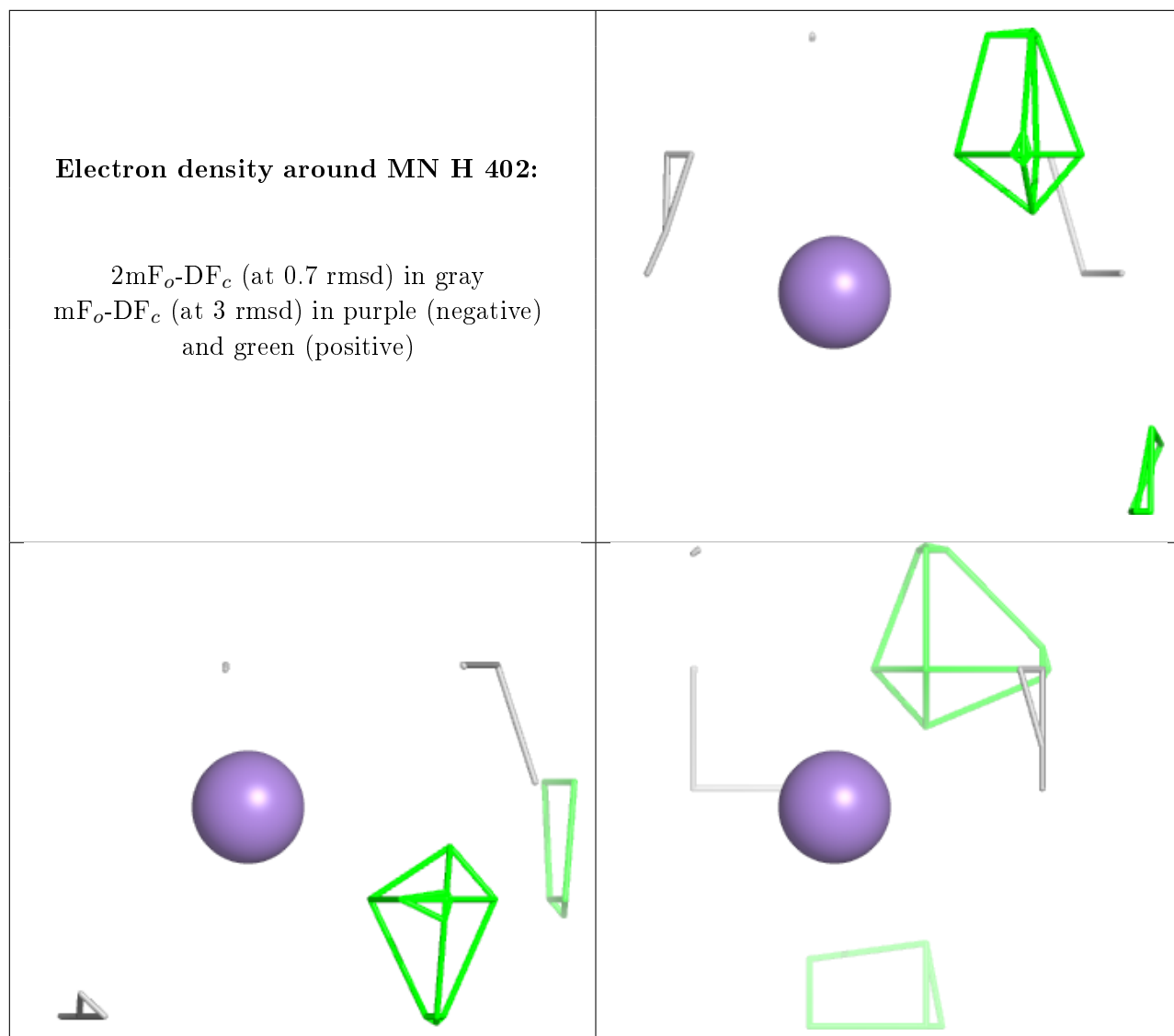
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





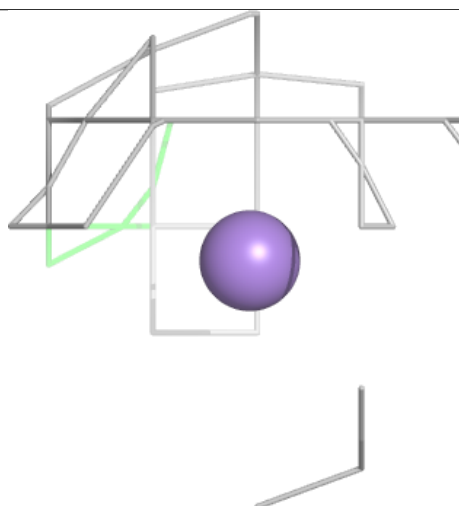
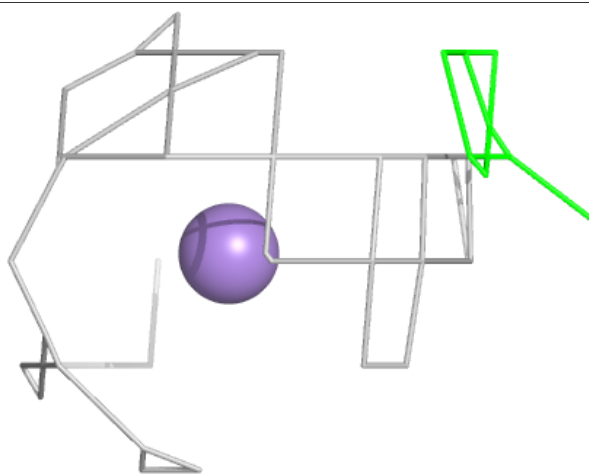
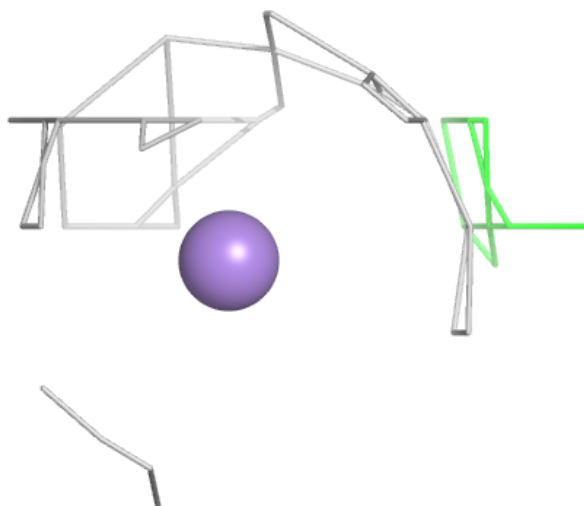
**Electron density around MN H 402:**

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



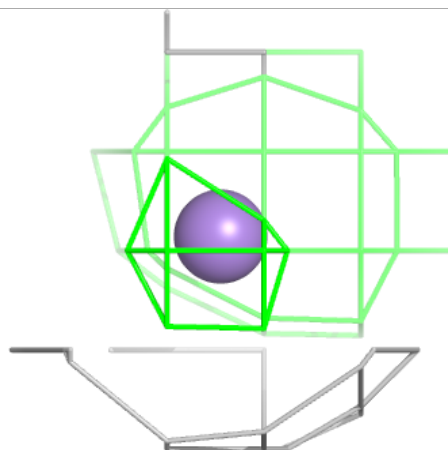
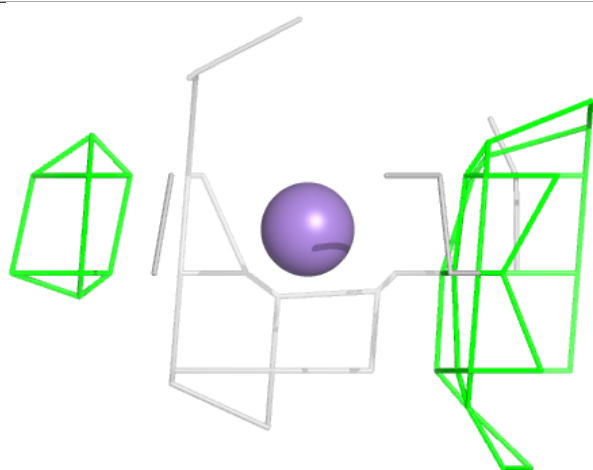
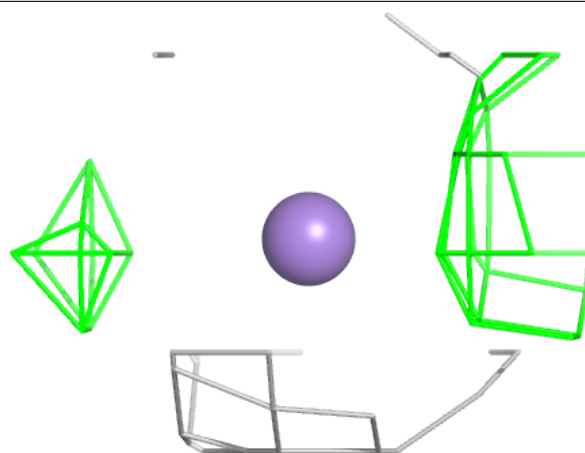
**Electron density around MN F 401:**

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



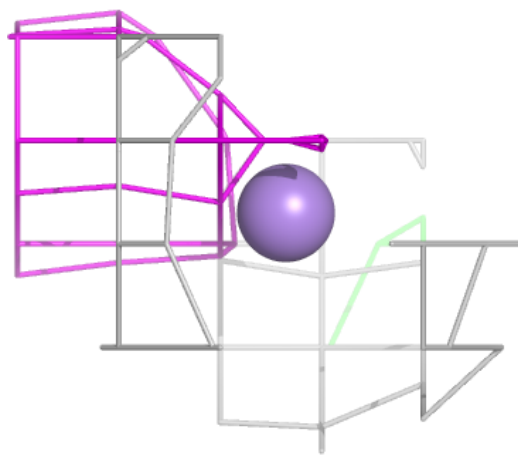
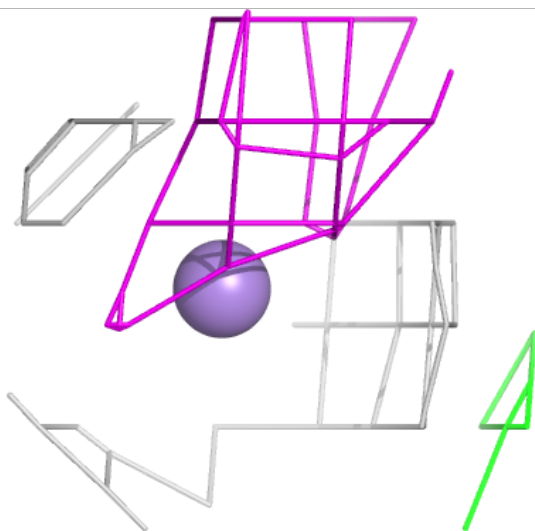
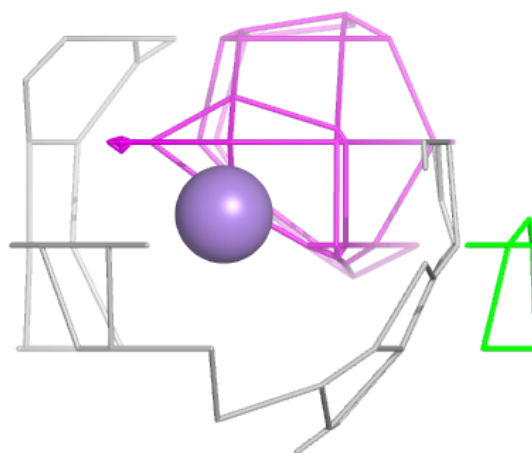
**Electron density around MN J 401:**

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



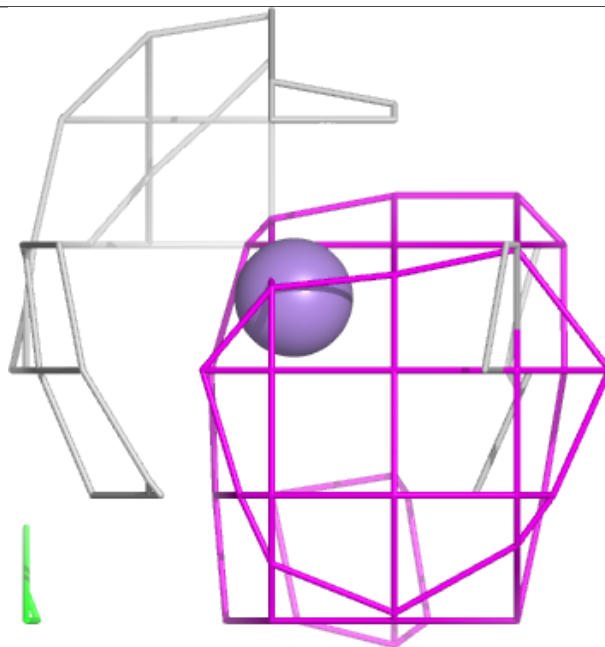
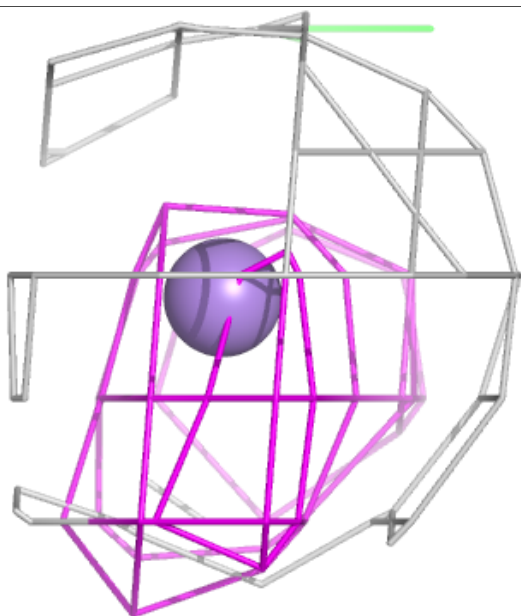
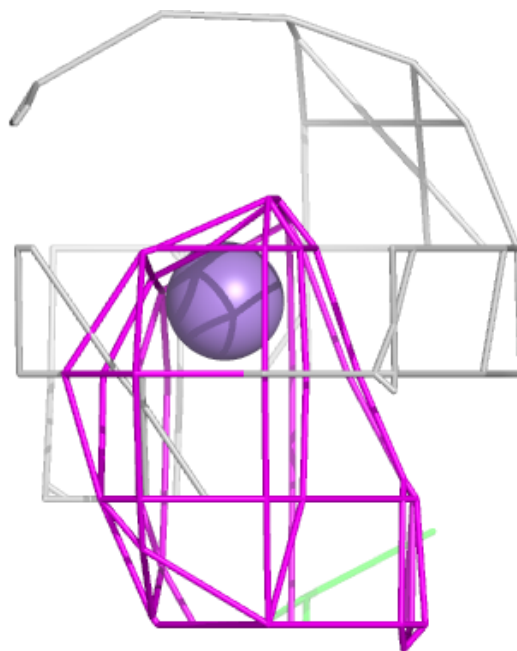
**Electron density around MN H 401:**

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



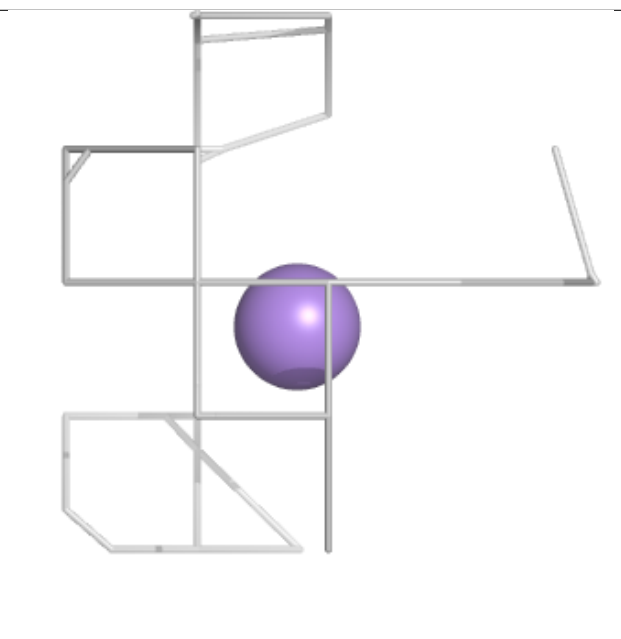
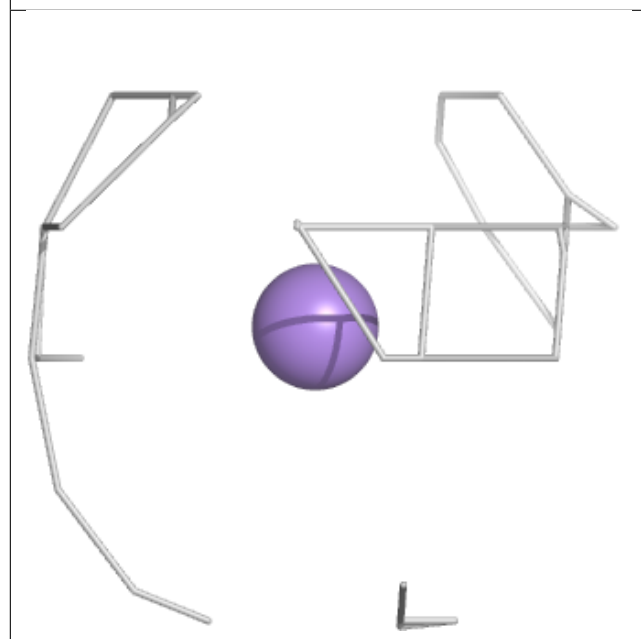
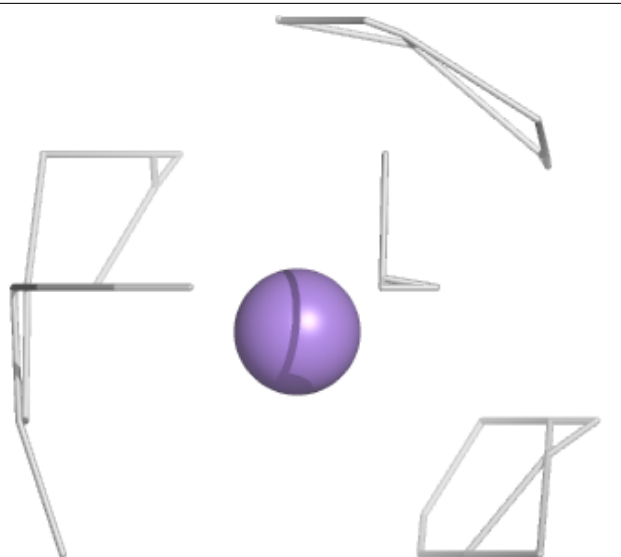
**Electron density around MN L 401:**

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



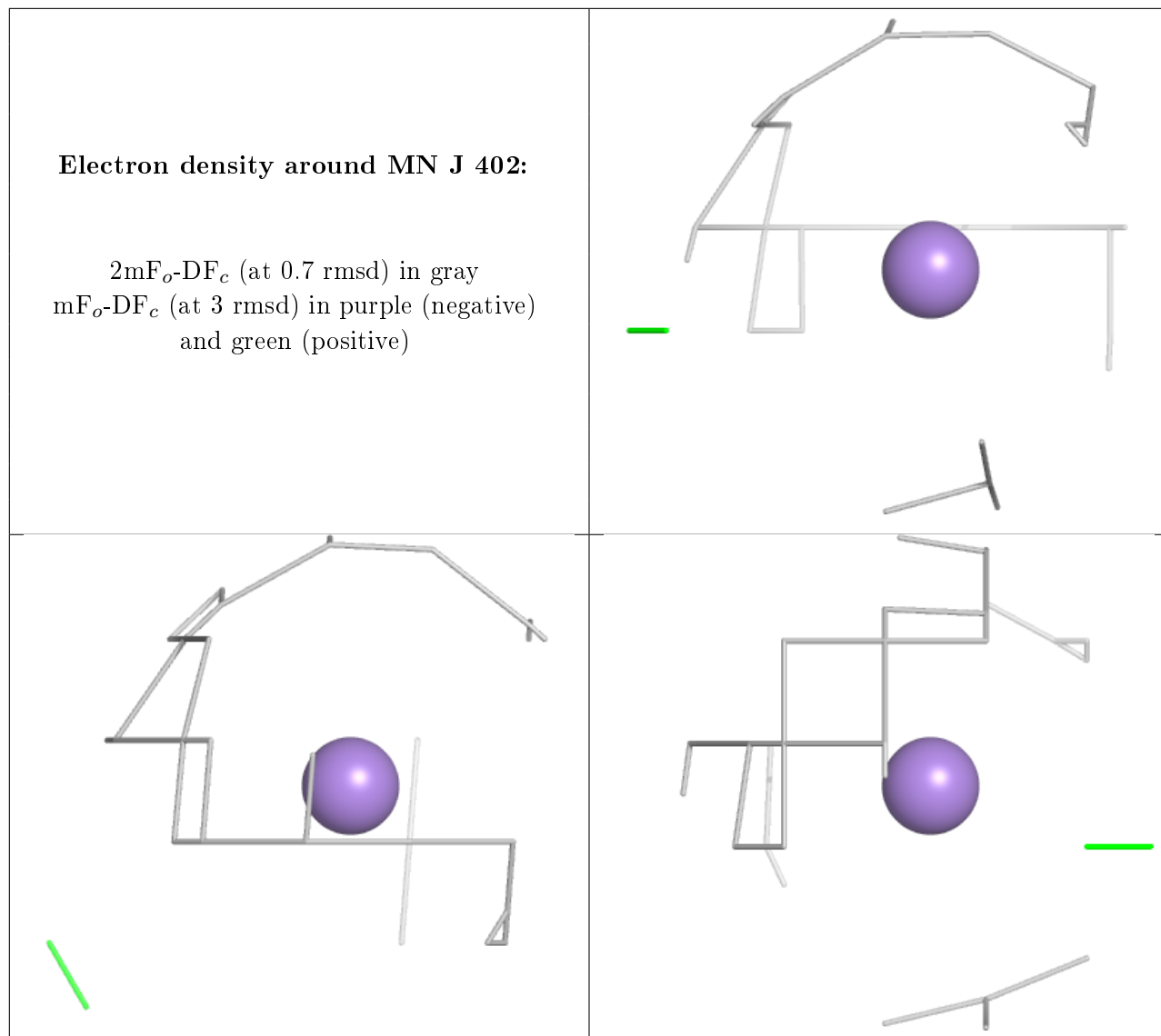
**Electron density around MN B 402:**

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



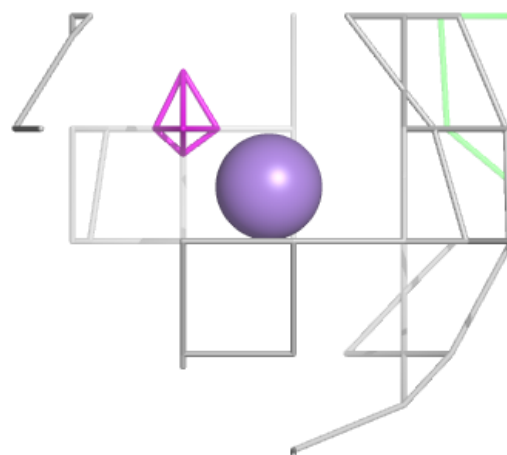
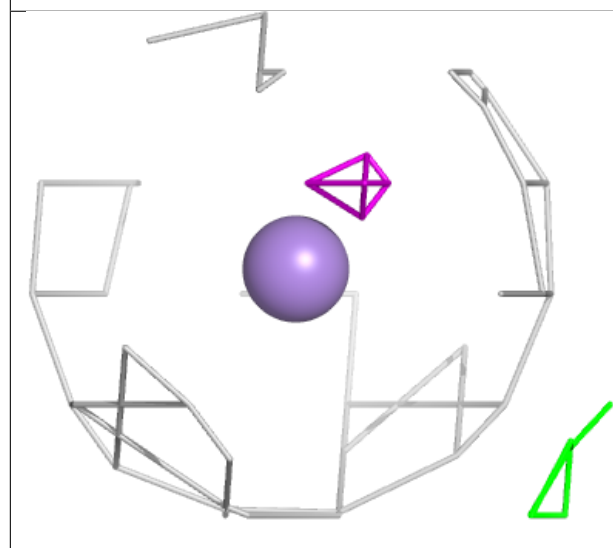
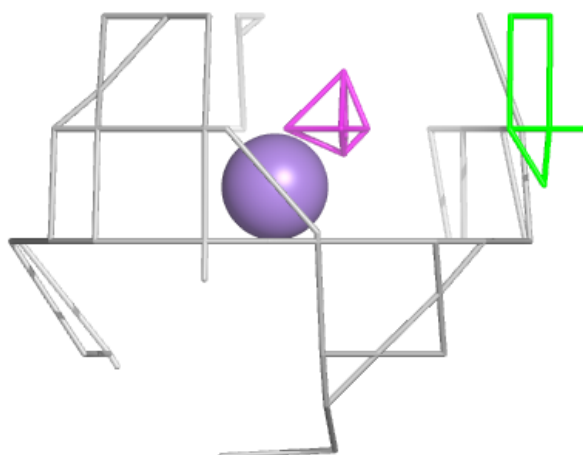
**Electron density around MN J 402:**

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



**Electron density around MN B 401:**

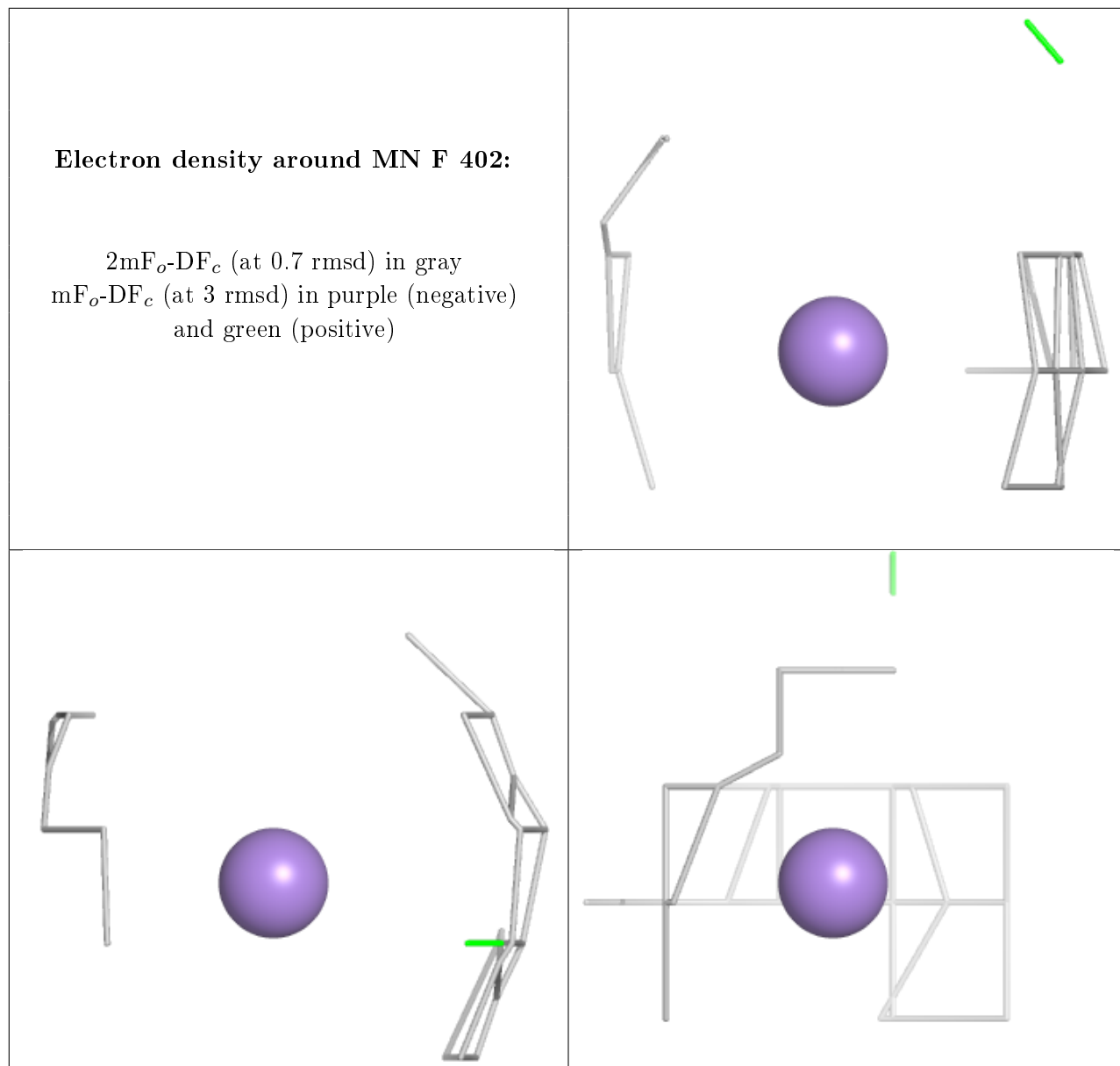
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





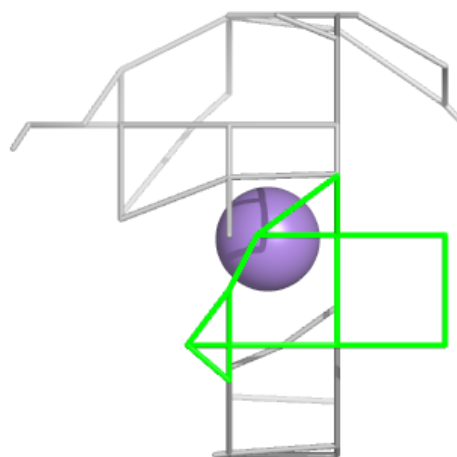
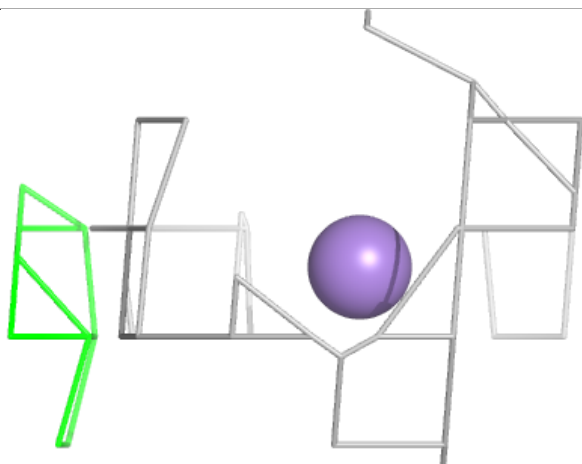
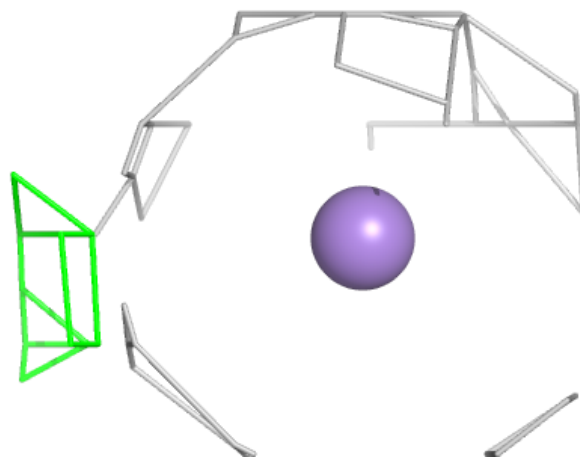
**Electron density around MN F 402:**

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



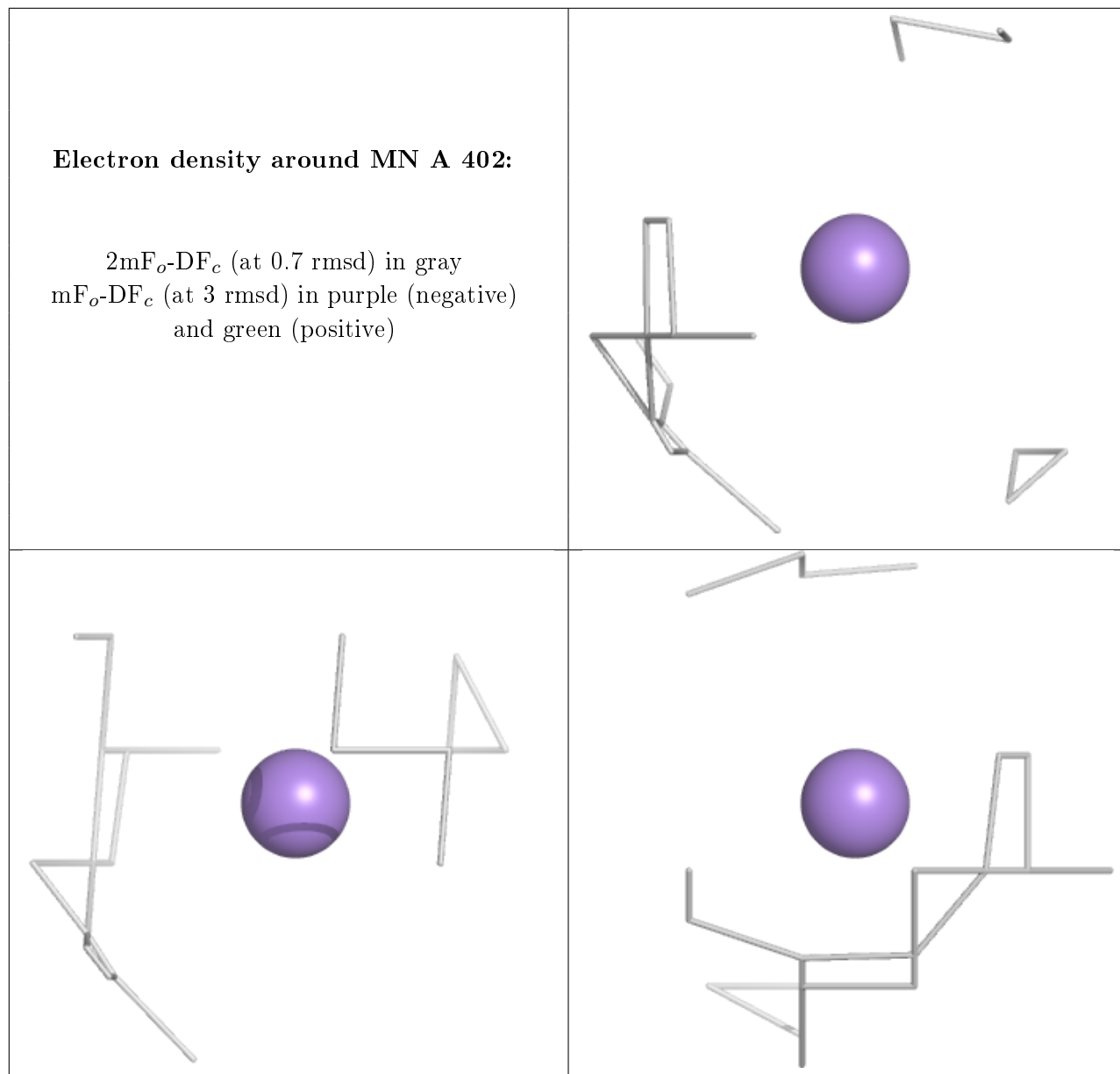
**Electron density around MN A 401:**

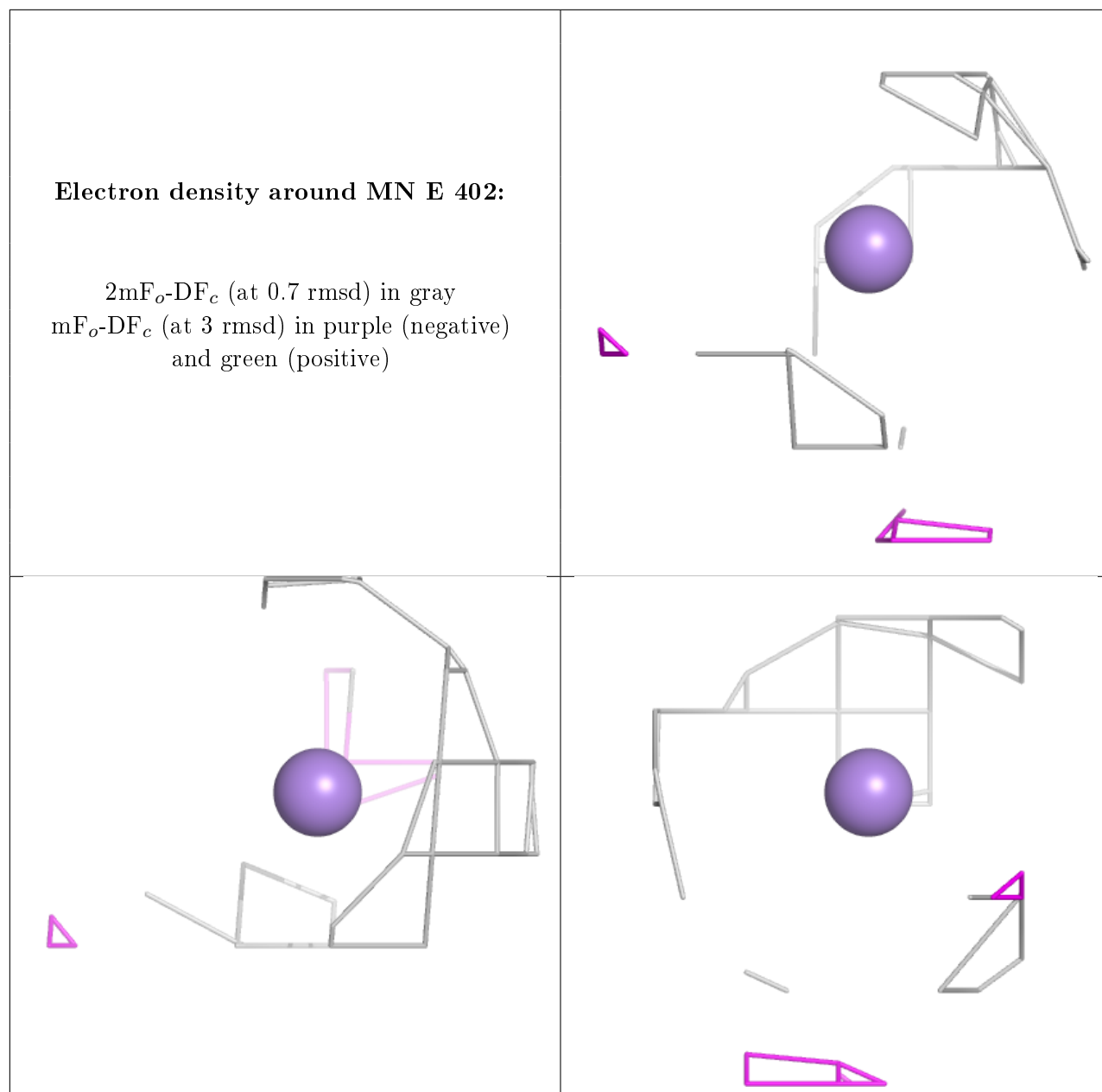
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.