



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:37 AM BST

PDB ID : 6VSS  
Title : Arginase from *Medicago truncatula*  
Authors : Sekula, B.  
Deposited on : 2020-02-11  
Resolution : 1.93 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
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

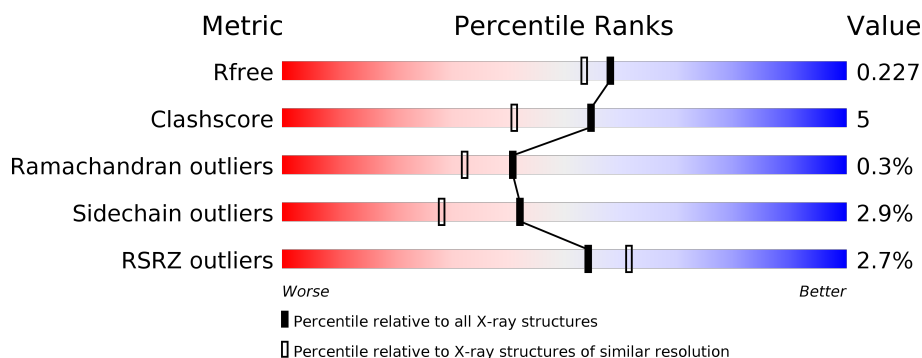
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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>%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 7%</div> </div> </div>
1	B	341	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>• 6%</div> </div> </div>
1	C	341	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 7%</div> </div> </div>
1	D	341	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 7%</div> </div> </div>
1	E	341	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>• 7%</div> </div> </div>
1	F	341	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15295 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	316	Total	C	N	O	S	0	0	0
			2441	1531	439	464	7			
1	B	319	Total	C	N	O	S	0	1	0
			2470	1547	445	471	7			
1	C	318	Total	C	N	O	S	0	0	0
			2455	1537	441	470	7			
1	D	318	Total	C	N	O	S	0	1	0
			2463	1542	444	470	7			
1	E	316	Total	C	N	O	S	0	1	0
			2449	1535	442	465	7			
1	F	318	Total	C	N	O	S	0	0	0
			2455	1537	441	470	7			

There are 18 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	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	D	2	Total Mn 2 2	0	0
2	E	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0
2	F	2	Total Mn 2 2	0	0

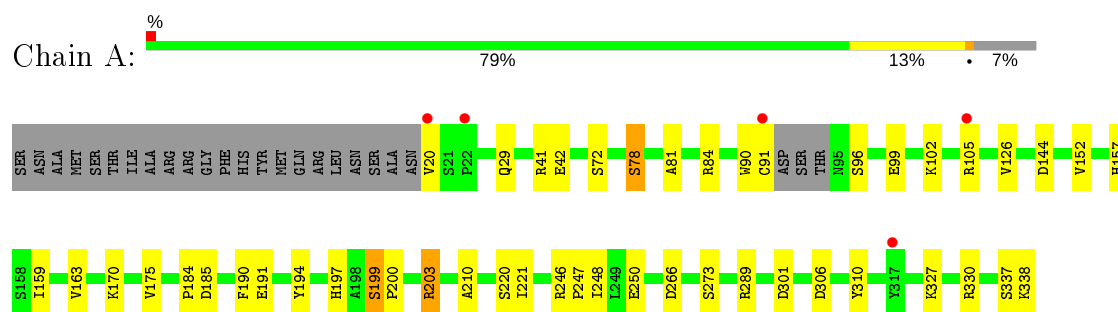
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	104	Total O 105 105	0	1
3	B	91	Total O 92 92	0	1
3	C	78	Total O 78 78	0	0
3	D	78	Total O 78 78	0	0
3	E	95	Total O 96 96	0	1
3	F	101	Total O 101 101	0	0

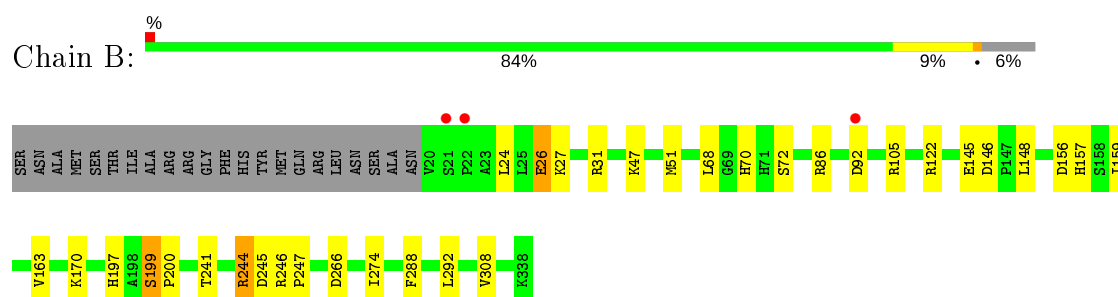
### 3 Residue-property plots [i](#)

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.

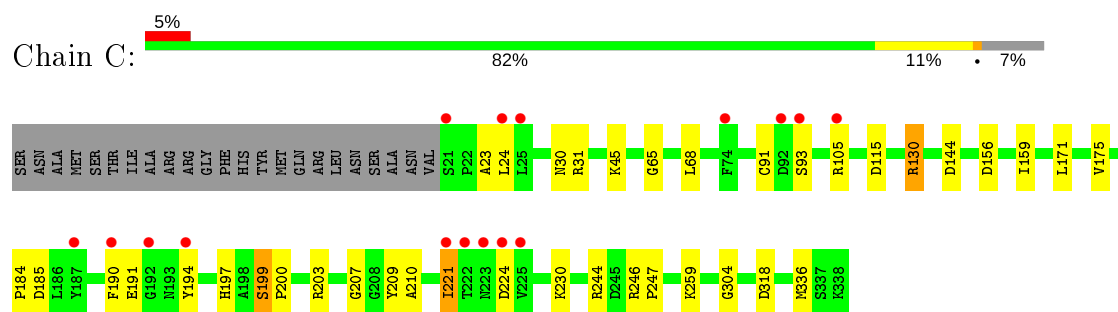
- Molecule 1: Arginase



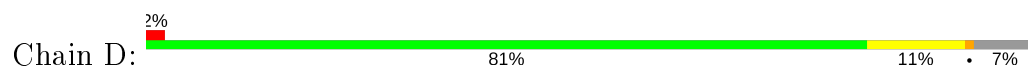
- Molecule 1: Arginase

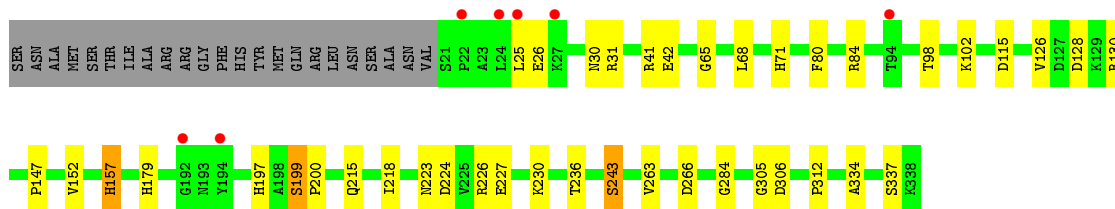


- Molecule 1: Arginase

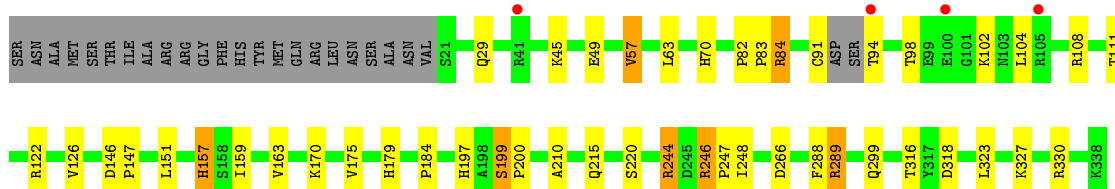
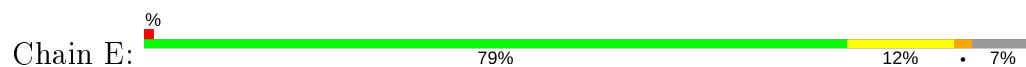


- Molecule 1: Arginase

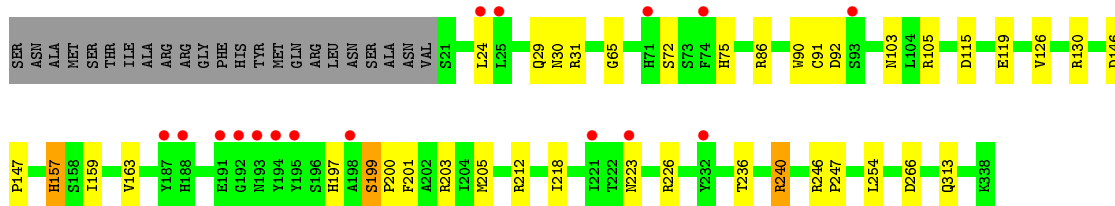
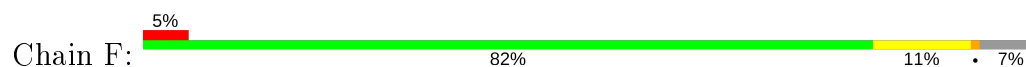




• Molecule 1: Arginase



• Molecule 1: Arginase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.33Å 142.91Å 90.05Å 90.00° 115.90° 90.00°	Depositor
Resolution (Å)	44.55 – 1.93 44.55 – 1.93	Depositor EDS
% Data completeness (in resolution range)	95.9 (44.55-1.93) 95.0 (44.55-1.93)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.182 , 0.218 0.191 , 0.227	Depositor DCC
$R_{free}$ test set	1040 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.240 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: 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	0.85	0/2485	0.97	0/3362
1	B	0.83	0/2518	0.97	0/3408
1	C	0.87	0/2500	0.98	0/3384
1	D	0.87	0/2511	0.98	0/3398
1	E	0.86	0/2496	1.00	0/3376
1	F	0.86	0/2500	1.00	0/3384
All	All	0.86	0/15010	0.98	0/20312

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	2441	0	2443	31	0
1	B	2470	0	2473	24	0
1	C	2455	0	2451	20	0
1	D	2463	0	2464	26	0
1	E	2449	0	2454	32	0
1	F	2455	0	2451	25	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	A	105	0	0	6	0
3	B	92	0	0	2	0
3	C	78	0	0	1	0
3	D	78	0	0	3	0
3	E	96	0	0	5	0
3	F	101	0	0	5	0
All	All	15295	0	14736	152	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 5.

All (152) 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:F:240:ARG:HG3	1:F:240:ARG:HH11	1.27	0.99
1:E:299:GLN:HG3	3:E:590:HOH:O	1.65	0.94
1:B:26:GLU:HG2	1:B:27:LYS:N	1.91	0.84
1:C:190:PHE:CE2	1:C:191:GLU:OE2	2.38	0.76
1:F:240:ARG:CG	1:F:240:ARG:HH11	1.98	0.74
1:B:27:LYS:O	1:B:31:ARG:HG3	1.89	0.72
1:A:247:PRO:HD2	3:A:552:HOH:O	1.89	0.71
1:E:84[A]:ARG:HD2	3:E:501:HOH:O	1.92	0.68
1:E:288:PHE:HZ	1:E:327:LYS:HG2	1.59	0.68
1:C:30:ASN:OD1	1:C:130:ARG:NH2	2.27	0.66
1:B:24:LEU:HD11	1:E:49:GLU:HB3	1.77	0.65
1:A:246:ARG:O	1:A:250:GLU:HG3	2.00	0.62
1:D:65:GLY:HA3	1:D:115:ASP:OD1	2.01	0.60
1:D:30:ASN:OD1	1:D:130:ARG:NH2	2.35	0.60
1:E:289:ARG:HB2	3:E:569:HOH:O	2.00	0.60
1:F:199:SER:N	1:F:200:PRO:CD	2.64	0.59
1:E:84[A]:ARG:NH1	1:E:84[A]:ARG:HG3	2.17	0.59
1:A:81:ALA:HB2	1:A:310:TYR:O	2.03	0.58
1:D:84[B]:ARG:NE	3:D:501:HOH:O	2.26	0.57
1:F:90:TRP:HD1	3:F:595:HOH:O	1.87	0.56
1:E:70:HIS:CE1	1:E:122:ARG:HD3	2.40	0.56
1:C:199:SER:N	1:C:200:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:VAL:O	1:D:306:ASP:HA	2.07	0.55
1:E:84[A]:ARG:HH11	1:E:84[A]:ARG:CG	2.19	0.55
1:B:70:HIS:CE1	1:B:122:ARG:HD2	2.42	0.54
1:D:41:ARG:NH1	1:D:42:GLU:OE2	2.32	0.54
1:E:288:PHE:CZ	1:E:327:LYS:HG2	2.41	0.54
1:B:159:ILE:O	1:B:163:VAL:HG23	2.07	0.54
1:E:94:THR:HG21	1:E:323:LEU:HD11	1.89	0.54
1:A:96:SER:HB3	1:A:105:ARG:CZ	2.39	0.53
1:D:243:SER:HB2	3:D:513:HOH:O	2.07	0.53
1:F:86:ARG:NH1	3:F:503:HOH:O	2.42	0.53
1:A:301:ASP:OD1	1:A:338:LYS:NZ	2.41	0.52
1:C:207:GLY:HA3	1:C:209:TYR:CE2	2.45	0.52
1:A:29:GLN:HG2	1:A:126:VAL:HG23	1.92	0.52
1:C:194:TYR:CZ	1:C:203:ARG:HD3	2.45	0.52
1:E:244:ARG:HD3	3:E:592:HOH:O	2.09	0.52
1:A:96:SER:HB3	1:A:105:ARG:NH2	2.25	0.51
1:C:175:VAL:O	1:C:210:ALA:HA	2.09	0.51
1:B:86:ARG:NH1	3:B:502:HOH:O	2.41	0.51
1:E:82:PRO:HB2	1:E:83:PRO:HD3	1.92	0.51
1:A:20:VAL:HG13	1:A:20:VAL:O	2.11	0.51
1:E:316:THR:OG1	1:E:318:ASP:OD1	2.27	0.50
1:E:199:SER:N	1:E:200:PRO:CD	2.74	0.50
1:A:248:ILE:HG13	3:A:552:HOH:O	2.10	0.50
1:B:199:SER:N	1:B:200:PRO:CD	2.74	0.50
1:C:65:GLY:HA3	1:C:115:ASP:OD1	2.12	0.50
1:B:72:SER:HB3	3:B:552:HOH:O	2.13	0.49
1:F:199:SER:N	1:F:200:PRO:HD2	2.26	0.49
1:D:284:GLY:HA2	3:F:563:HOH:O	2.13	0.49
1:D:199:SER:N	1:D:200:PRO:CD	2.75	0.49
1:F:218:ILE:HG13	1:F:236:THR:HG23	1.95	0.49
1:D:224:ASP:O	1:D:227:GLU:HB2	2.12	0.48
1:E:84[A]:ARG:CG	1:E:84[A]:ARG:NH1	2.75	0.48
1:C:184:PRO:HG2	1:C:221:ILE:HD12	1.95	0.48
1:A:199:SER:N	1:A:200:PRO:CD	2.77	0.48
1:F:75:HIS:HE1	1:F:313:GLN:OE1	1.96	0.48
1:D:98:THR:HG21	1:D:334:ALA:HB2	1.94	0.48
1:F:91:CYS:SG	1:F:92:ASP:N	2.88	0.47
1:D:157:HIS:CE1	1:D:266:ASP:HB2	2.50	0.47
1:A:273:SER:HB3	1:B:274:ILE:HD13	1.97	0.47
1:B:145:GLU:O	1:B:148:LEU:HG	2.14	0.47
1:B:156:ASP:C	1:B:156:ASP:OD1	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:HIS:O	1:E:215:GLN:HA	2.15	0.47
1:F:159:ILE:O	1:F:163:VAL:HG23	2.15	0.46
1:B:199:SER:N	1:B:200:PRO:HD2	2.30	0.46
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.80	0.46
1:E:84[A]:ARG:HH11	1:E:84[A]:ARG:HG3	1.79	0.46
1:F:212:ARG:NH1	1:F:254:LEU:HD23	2.31	0.46
1:F:201:PHE:O	1:F:205:MET:HG2	2.15	0.46
1:D:80:PHE:HB2	1:D:312:PRO:HG2	1.97	0.46
1:A:190:PHE:CE1	1:A:191:GLU:HG3	2.50	0.46
1:A:221:ILE:O	1:A:221:ILE:HG23	2.16	0.46
1:D:218:ILE:HG13	1:D:236:THR:HG23	1.98	0.46
1:E:63:LEU:HA	1:E:151:LEU:O	2.16	0.46
1:C:199:SER:N	1:C:200:PRO:HD2	2.31	0.45
1:A:194:TYR:CZ	1:A:203:ARG:HD2	2.51	0.45
1:C:156:ASP:O	1:C:159:ILE:HG12	2.16	0.45
1:D:126:VAL:HG13	1:D:130:ARG:HG2	1.98	0.45
1:F:240:ARG:NH1	1:F:240:ARG:HG3	2.07	0.45
1:F:72:SER:HB3	3:F:561:HOH:O	2.15	0.45
1:B:68:LEU:C	1:B:68:LEU:HD23	2.37	0.45
1:E:104:LEU:HD11	1:E:330:ARG:NE	2.31	0.45
1:D:68:LEU:C	1:D:68:LEU:HD23	2.37	0.45
1:F:24:LEU:O	1:F:24:LEU:HD12	2.16	0.45
1:A:157:HIS:CE1	1:A:266:ASP:HB2	2.52	0.45
1:A:327:LYS:NZ	3:A:501:HOH:O	2.28	0.45
1:F:119:GLU:HG3	3:F:585:HOH:O	2.16	0.45
1:B:246:ARG:N	1:B:247:PRO:CD	2.79	0.45
1:D:199:SER:N	1:D:200:PRO:HD2	2.31	0.45
1:A:84:ARG:NH1	1:D:84[B]:ARG:NH2	2.65	0.44
1:E:244:ARG:CD	3:E:592:HOH:O	2.66	0.44
1:A:78:SER:HB2	3:A:536:HOH:O	2.16	0.44
1:E:199:SER:H	1:E:200:PRO:CD	2.31	0.44
1:D:84[B]:ARG:NH2	3:D:501:HOH:O	2.48	0.44
1:E:98:THR:OG1	1:E:102:LYS:HB2	2.18	0.44
1:A:175:VAL:O	1:A:210:ALA:HA	2.18	0.44
1:D:25:LEU:O	1:D:26:GLU:C	2.55	0.43
1:C:23:ALA:O	1:C:24:LEU:C	2.56	0.43
1:F:157:HIS:CE1	1:F:266:ASP:HB2	2.53	0.43
1:A:102:LYS:NZ	1:A:337:SER:O	2.51	0.43
1:C:318:ASP:OD1	1:C:318:ASP:N	2.46	0.43
1:F:65:GLY:HA3	1:F:115:ASP:OD1	2.18	0.43
1:E:175:VAL:O	1:E:210:ALA:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:PRO:HD3	1:E:220:SER:O	2.18	0.43
1:C:185:ASP:HB3	1:C:200:PRO:HD2	2.00	0.43
1:C:246:ARG:HB2	1:C:247:PRO:HD3	2.01	0.43
1:A:246:ARG:N	1:A:247:PRO:CD	2.82	0.43
1:F:246:ARG:N	1:F:247:PRO:CD	2.82	0.43
1:A:96:SER:CB	1:A:105:ARG:NH1	2.82	0.43
1:A:184:PRO:HD3	1:A:220:SER:O	2.19	0.43
1:A:273:SER:CB	1:B:274:ILE:HD13	2.49	0.43
1:C:244:ARG:HD2	3:C:576:HOH:O	2.18	0.43
1:D:71:HIS:HE1	1:D:128:ASP:OD2	2.02	0.43
1:B:244:ARG:HG3	1:B:245:ASP:N	2.34	0.42
1:B:47:LYS:O	1:B:51:MET:HG2	2.19	0.42
1:F:223:ASN:HA	1:F:226:ARG:HG3	2.01	0.42
1:C:199:SER:H	1:C:200:PRO:CD	2.33	0.42
1:E:29:GLN:HG2	1:E:126:VAL:HG23	2.01	0.42
1:B:157:HIS:CE1	1:B:266:ASP:HB2	2.53	0.42
1:F:240:ARG:NH1	1:F:240:ARG:CG	2.66	0.42
1:C:68:LEU:C	1:C:68:LEU:HD23	2.39	0.42
1:E:288:PHE:HZ	1:E:327:LYS:CG	2.28	0.42
1:B:157:HIS:CG	1:B:308:VAL:HG21	2.55	0.42
1:D:263:VAL:O	1:D:305:GLY:HA2	2.20	0.42
1:A:159:ILE:O	1:A:163:VAL:HG23	2.20	0.42
1:A:91:CYS:SG	1:A:91:CYS:O	2.78	0.42
1:B:199:SER:O	1:B:200:PRO:C	2.58	0.42
1:E:246:ARG:CB	1:E:247:PRO:HD3	2.50	0.42
1:C:45:LYS:HE3	1:F:31:ARG:NH1	2.35	0.42
1:B:241:THR:O	1:B:244:ARG:HG2	2.20	0.41
1:A:330:ARG:NH1	3:A:501:HOH:O	2.52	0.41
1:A:185:ASP:HB3	1:A:200:PRO:HD2	2.02	0.41
1:A:72:SER:HB3	3:A:569:HOH:O	2.20	0.41
1:E:57:VAL:HG11	1:E:108:ARG:HG2	2.03	0.41
1:E:157:HIS:CE1	1:E:266:ASP:HB2	2.55	0.41
1:F:30:ASN:OD1	1:F:130:ARG:NH2	2.53	0.41
1:B:157:HIS:CD2	1:B:308:VAL:HG21	2.55	0.41
1:D:25:LEU:HA	1:D:25:LEU:HD23	1.93	0.41
1:F:29:GLN:HG2	1:F:126:VAL:HG22	2.03	0.41
1:C:171:LEU:O	1:C:259:LYS:HE3	2.21	0.41
1:A:152:VAL:O	1:A:306:ASP:HA	2.20	0.41
1:C:304:GLY:HA2	1:C:336:MET:SD	2.60	0.41
1:E:170:LYS:HE2	1:E:170:LYS:HB2	1.87	0.40
1:F:103:ASN:HD21	1:F:105:ARG:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:PHE:HE2	1:B:292:LEU:HD11	1.86	0.40
1:D:223:ASN:O	1:D:226:ARG:HB2	2.22	0.40
1:A:42:GLU:CD	1:D:31:ARG:HH21	2.25	0.40
1:D:102:LYS:NZ	1:D:337:SER:O	2.54	0.40
1:E:146:ASP:HA	1:E:147:PRO:HA	1.88	0.40
1:D:179:HIS:O	1:D:215:GLN:HA	2.21	0.40
1:E:159:ILE:O	1:E:163:VAL:HG23	2.21	0.40

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	312/341 (92%)	302 (97%)	9 (3%)	1 (0%)	41	32
1	B	318/341 (93%)	301 (95%)	16 (5%)	1 (0%)	41	32
1	C	316/341 (93%)	298 (94%)	17 (5%)	1 (0%)	41	32
1	D	317/341 (93%)	304 (96%)	12 (4%)	1 (0%)	41	32
1	E	313/341 (92%)	305 (97%)	7 (2%)	1 (0%)	41	32
1	F	316/341 (93%)	302 (96%)	13 (4%)	1 (0%)	41	32
All	All	1892/2046 (92%)	1812 (96%)	74 (4%)	6 (0%)	41	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	199	SER
1	E	199	SER
1	A	199	SER
1	D	199	SER
1	B	199	SER
1	F	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	265/286 (93%)	256 (97%)	9 (3%)	37	22
1	B	269/286 (94%)	263 (98%)	6 (2%)	52	39
1	C	267/286 (93%)	257 (96%)	10 (4%)	34	19
1	D	268/286 (94%)	263 (98%)	5 (2%)	57	45
1	E	266/286 (93%)	254 (96%)	12 (4%)	27	12
1	F	267/286 (93%)	261 (98%)	6 (2%)	52	39
All	All	1602/1716 (93%)	1554 (97%)	48 (3%)	42	27

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	78	SER
1	A	90	TRP
1	A	99	GLU
1	A	144	ASP
1	A	170	LYS
1	A	197	HIS
1	A	203	ARG
1	A	289	ARG
1	B	26	GLU
1	B	92	ASP
1	B	146	ASP
1	B	170	LYS
1	B	197	HIS
1	B	244	ARG
1	C	31	ARG
1	C	91	CYS
1	C	93	SER
1	C	105	ARG
1	C	130	ARG
1	C	144	ASP
1	C	197	HIS

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Mol	Chain	Res	Type
1	C	221	ILE
1	C	224	ASP
1	C	230	LYS
1	D	147	PRO
1	D	157	HIS
1	D	197	HIS
1	D	230	LYS
1	D	243	SER
1	E	45	LYS
1	E	57	VAL
1	E	84[A]	ARG
1	E	84[B]	ARG
1	E	91	CYS
1	E	111	THR
1	E	157	HIS
1	E	197	HIS
1	E	244	ARG
1	E	246	ARG
1	E	248	ILE
1	E	289	ARG
1	F	146	ASP
1	F	147	PRO
1	F	157	HIS
1	F	197	HIS
1	F	203	ARG
1	F	240	ARG

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

Mol	Chain	Res	Type
1	E	70	HIS

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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.

## 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	316/341 (92%)	-0.23	5 (1%) 72 77	21, 33, 58, 99	0
1	B	319/341 (93%)	-0.28	3 (0%) 84 87	21, 35, 54, 71	0
1	C	318/341 (93%)	-0.08	16 (5%) 28 36	21, 33, 67, 87	0
1	D	318/341 (93%)	-0.23	7 (2%) 62 69	21, 34, 58, 79	0
1	E	316/341 (92%)	-0.31	4 (1%) 77 81	20, 34, 56, 81	0
1	F	318/341 (93%)	-0.04	16 (5%) 28 36	21, 32, 68, 88	0
All	All	1905/2046 (93%)	-0.20	51 (2%) 54 61	20, 34, 62, 99	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	VAL	7.1
1	D	25	LEU	6.6
1	F	74	PHE	5.1
1	C	24	LEU	5.1
1	C	74	PHE	5.1
1	F	221	ILE	5.1
1	F	223	ASN	4.6
1	C	221	ILE	4.5
1	D	24	LEU	4.3
1	F	192	GLY	4.2
1	C	194	TYR	3.9
1	B	92	ASP	3.8
1	C	223	ASN	3.7
1	C	187	TYR	3.6
1	C	92	ASP	3.4
1	C	93	SER	3.1
1	A	22	PRO	3.1
1	A	91	CYS	3.0
1	F	194	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	22	PRO	2.9
1	D	194	TYR	2.9
1	D	27	LYS	2.9
1	F	93	SER	2.8
1	E	94	THR	2.8
1	F	191	GLU	2.8
1	A	317	TYR	2.6
1	F	187	TYR	2.6
1	F	198	ALA	2.6
1	C	224	ASP	2.6
1	D	94	THR	2.6
1	F	24	LEU	2.5
1	D	22	PRO	2.5
1	C	222	THR	2.5
1	E	100	GLU	2.5
1	C	225	VAL	2.4
1	F	193	ASN	2.4
1	C	105	ARG	2.3
1	F	232	TYR	2.3
1	C	25	LEU	2.3
1	F	25	LEU	2.3
1	C	192	GLY	2.2
1	C	190	PHE	2.2
1	F	188	HIS	2.2
1	D	192	GLY	2.1
1	B	21	SER	2.1
1	A	105	ARG	2.1
1	F	195	TYR	2.1
1	F	71	HIS	2.0
1	E	41	ARG	2.0
1	E	105	ARG	2.0
1	C	21	SER	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 ⓘ

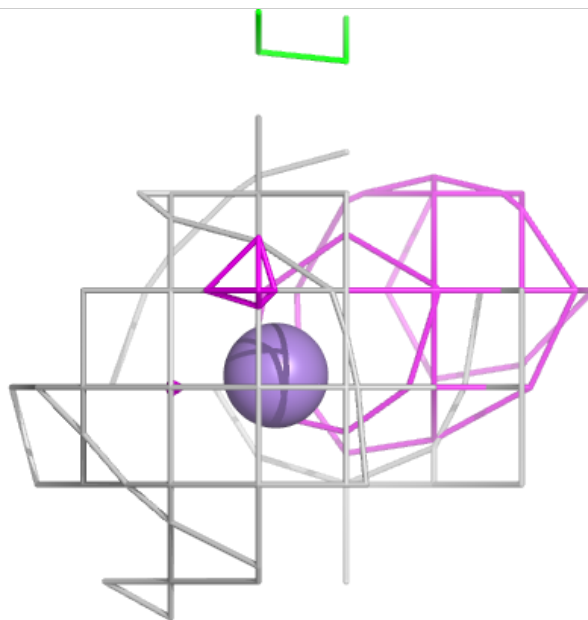
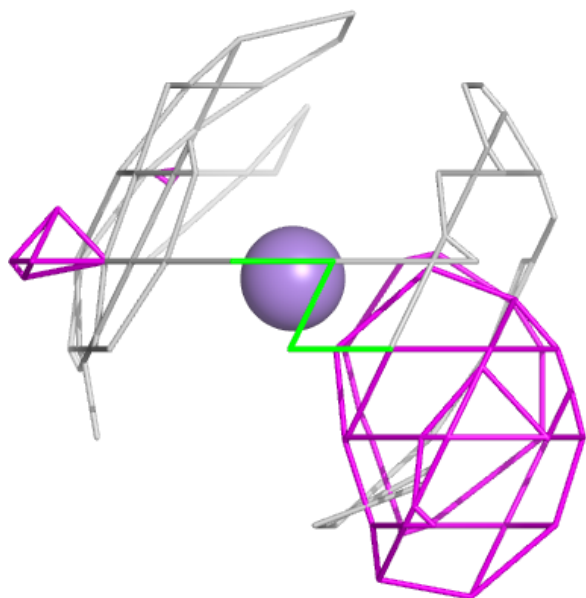
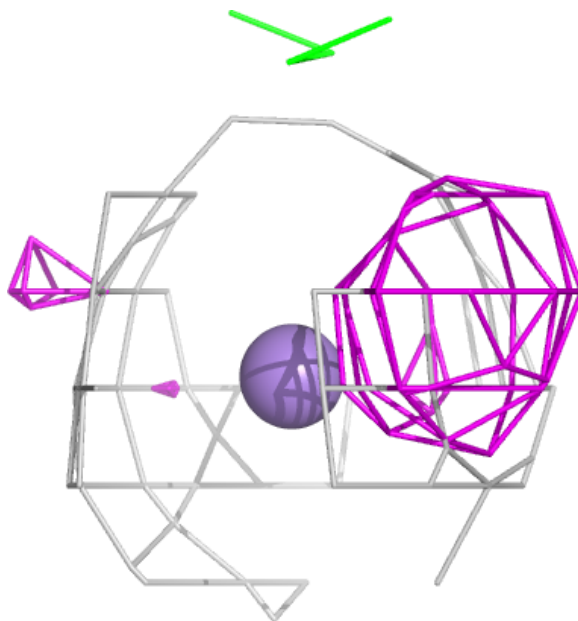
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	MN	C	402	1/1	0.98	0.04	37,37,37,37	0
2	MN	D	401	1/1	0.98	0.03	29,29,29,29	0
2	MN	C	401	1/1	0.98	0.04	33,33,33,33	0
2	MN	F	402	1/1	0.98	0.08	43,43,43,43	0
2	MN	B	402	1/1	0.99	0.06	34,34,34,34	0
2	MN	B	401	1/1	0.99	0.05	29,29,29,29	0
2	MN	D	402	1/1	0.99	0.04	36,36,36,36	0
2	MN	A	401	1/1	0.99	0.03	27,27,27,27	0
2	MN	F	401	1/1	0.99	0.03	33,33,33,33	0
2	MN	A	402	1/1	1.00	0.04	29,29,29,29	0
2	MN	E	402	1/1	1.00	0.07	27,27,27,27	0
2	MN	E	401	1/1	1.00	0.04	25,25,25,25	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.

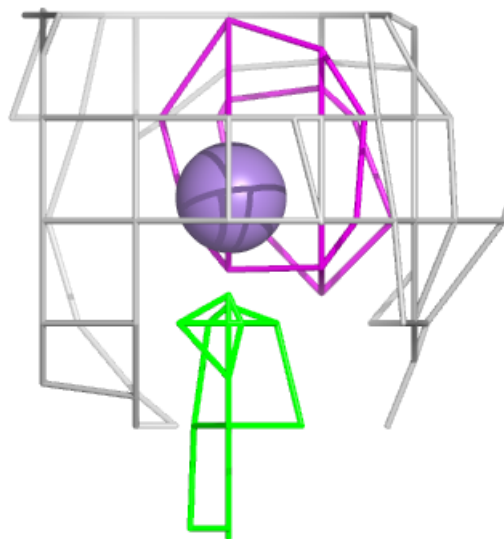
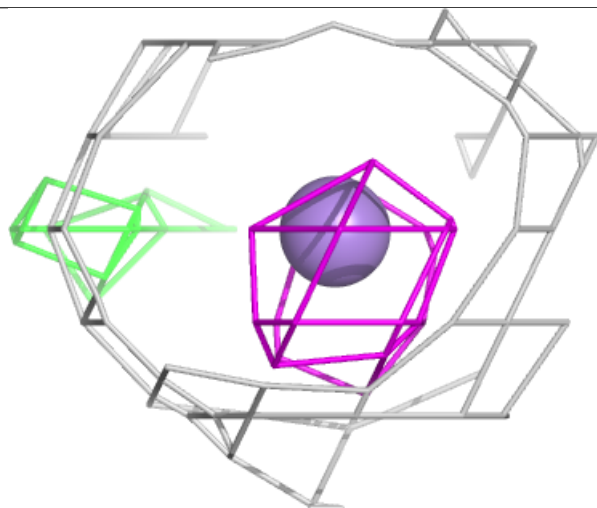
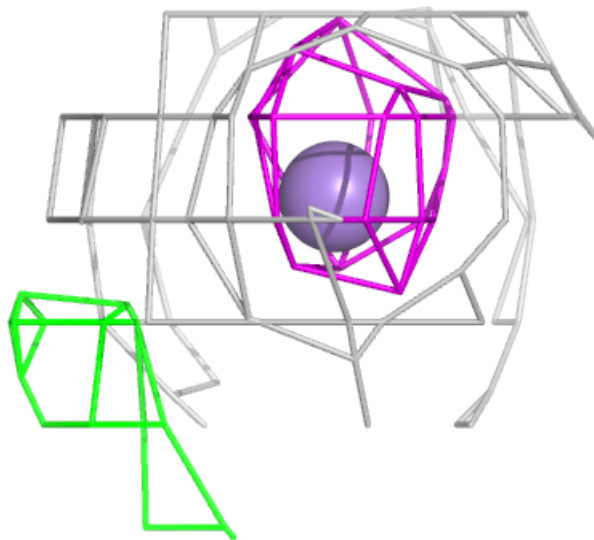
**Electron density around MN C 402:**

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



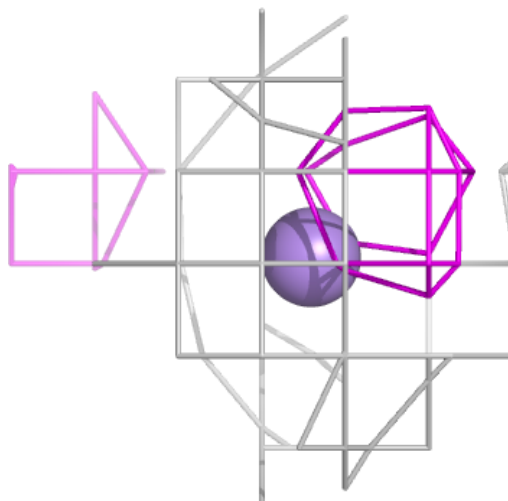
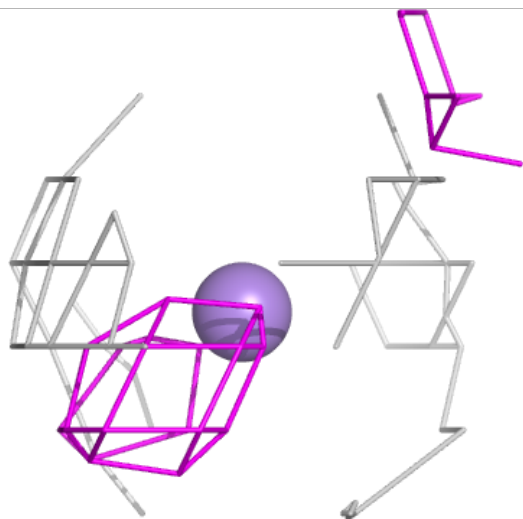
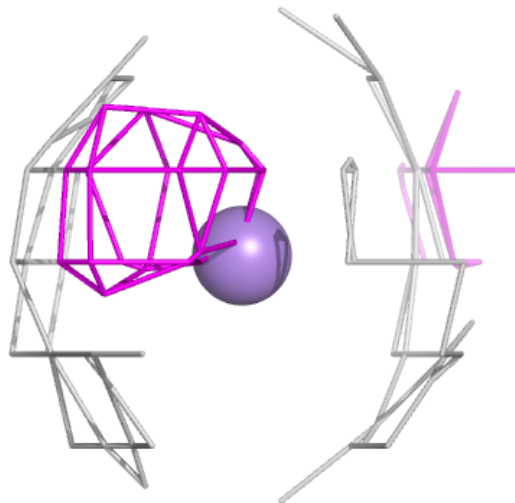
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and green (positive)



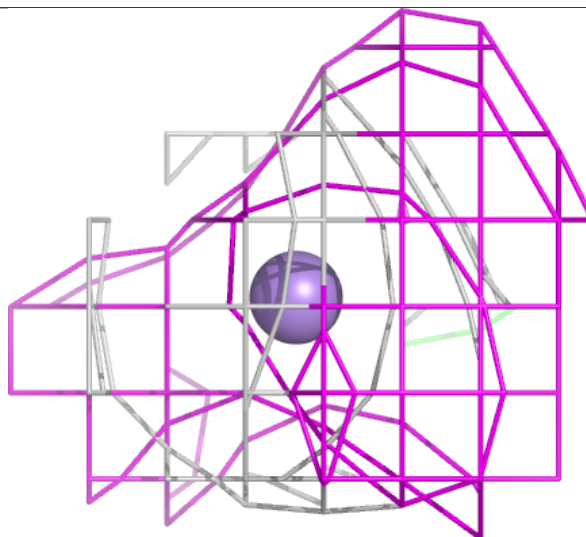
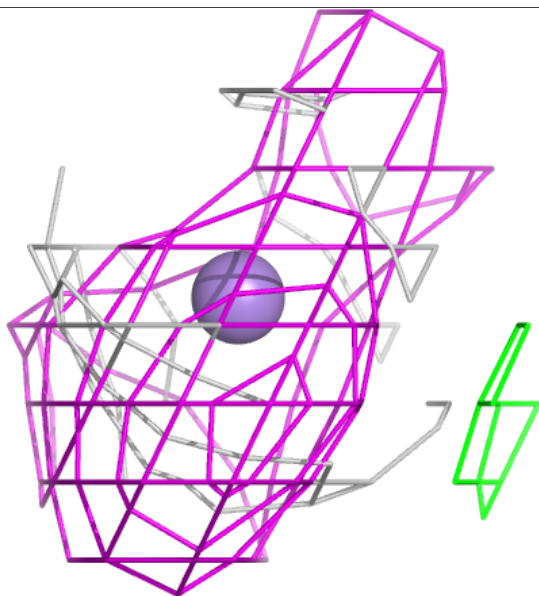
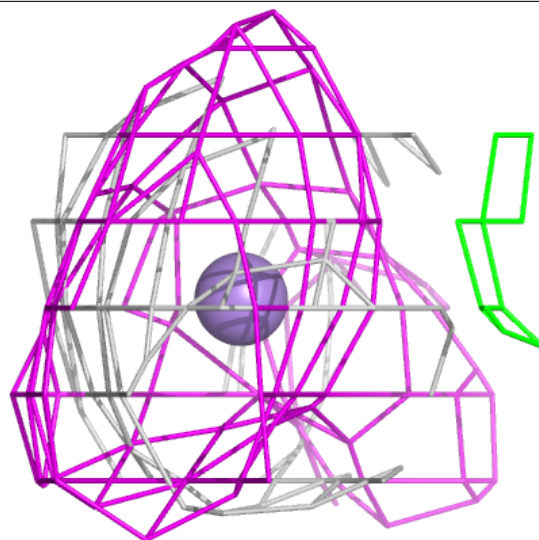
**Electron density around MN C 401:**

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



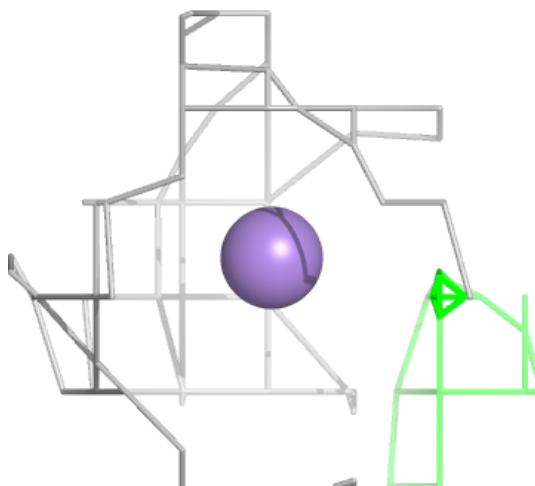
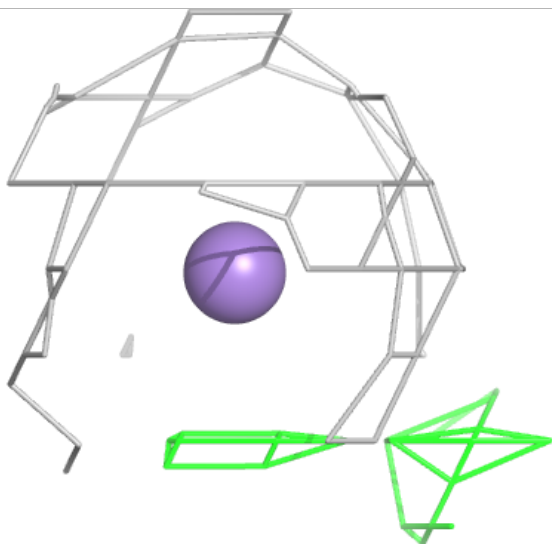
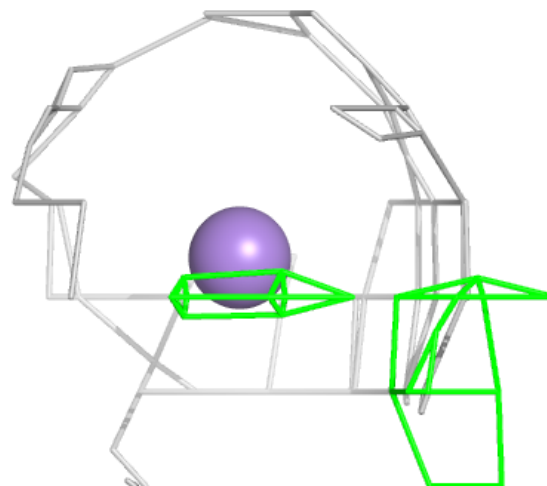
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and green (positive)



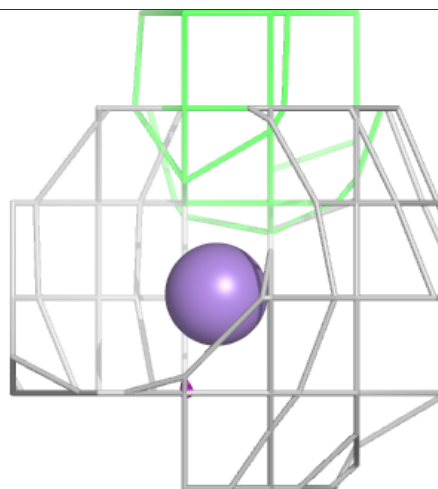
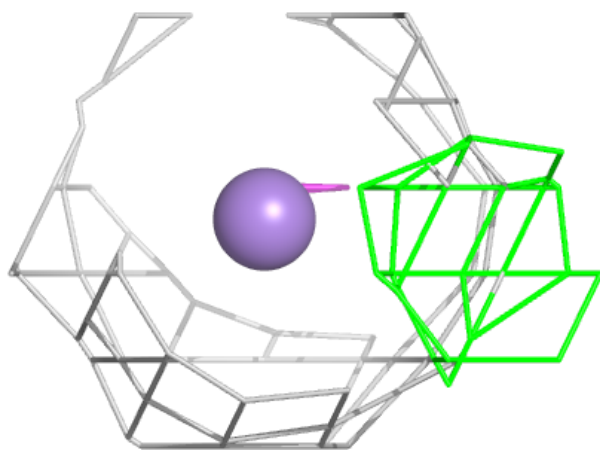
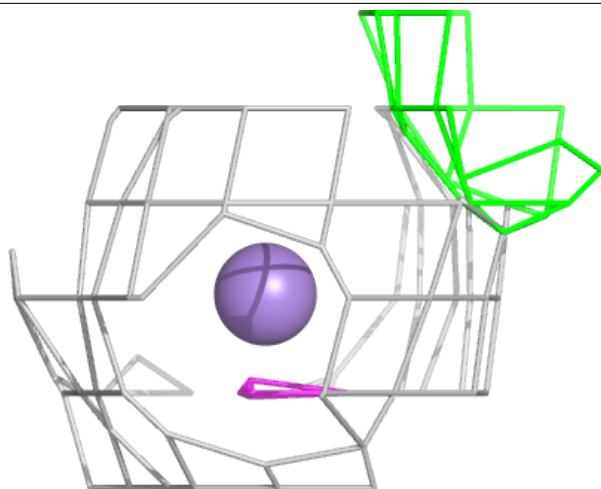
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and green (positive)



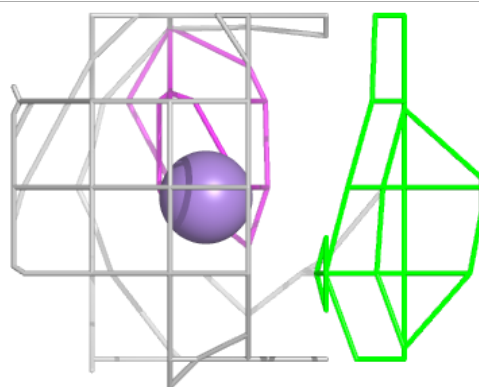
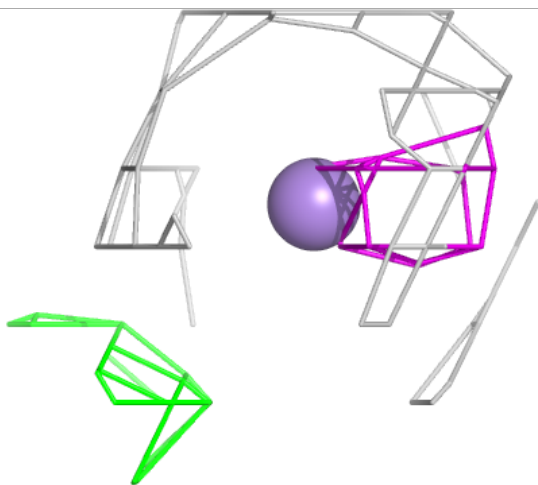
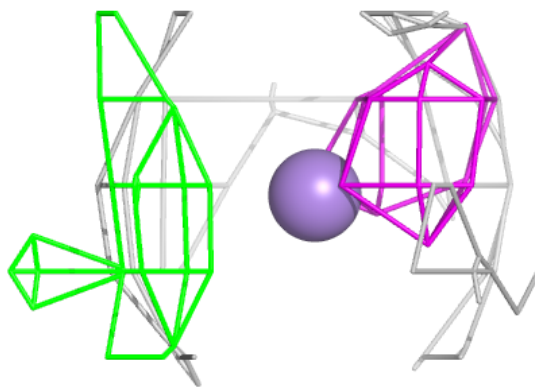
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and green (positive)



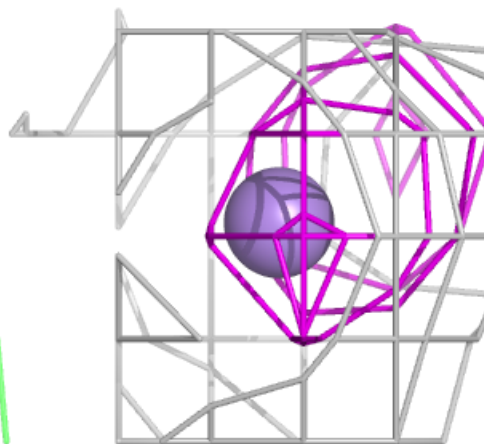
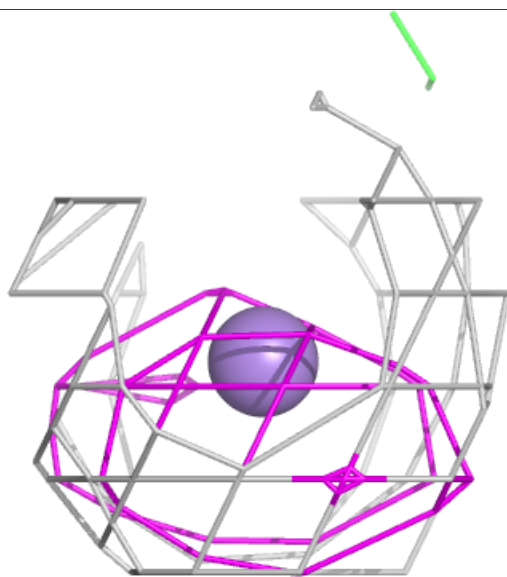
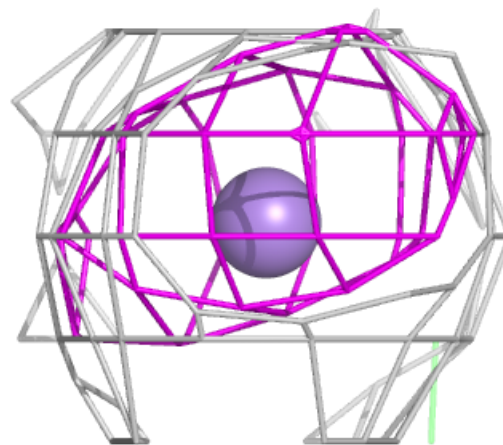
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and green (positive)



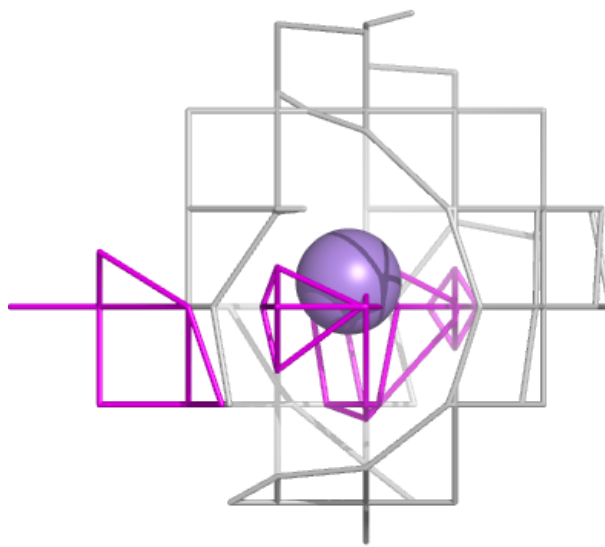
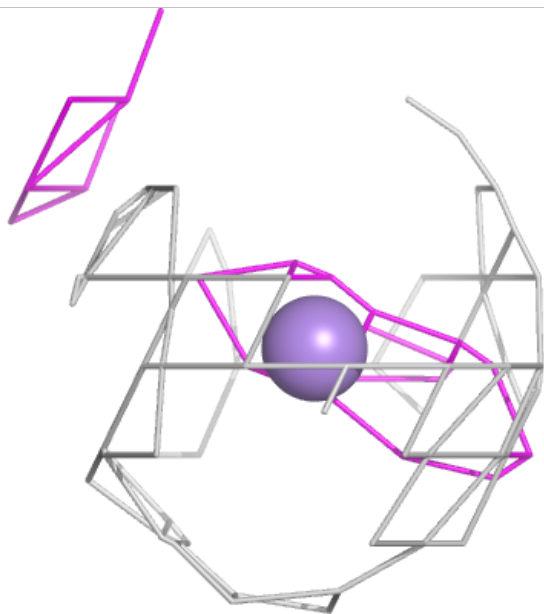
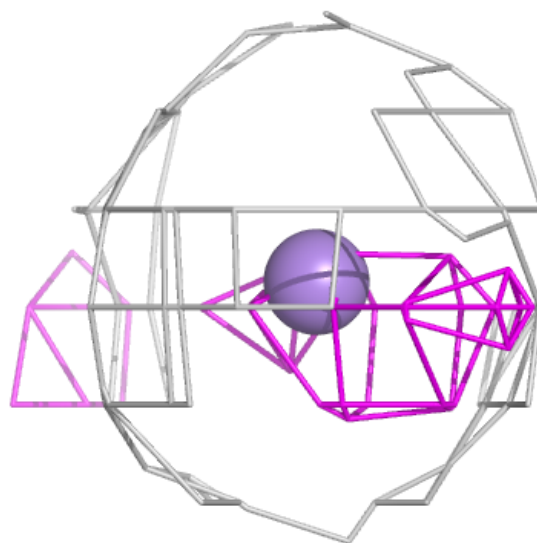
**Electron density around MN A 401:**

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and green (positive)



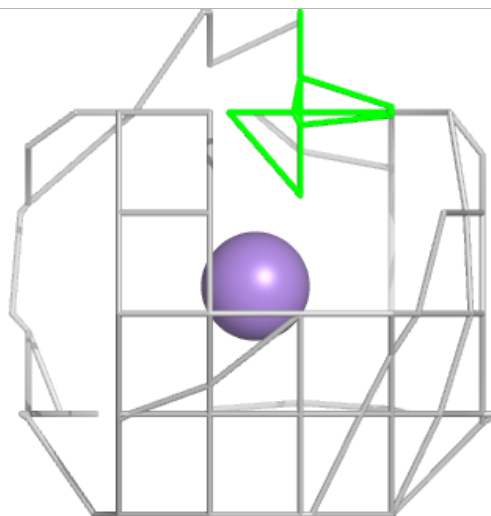
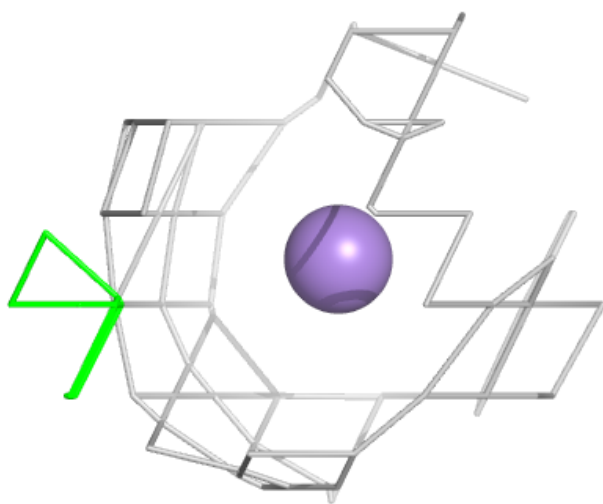
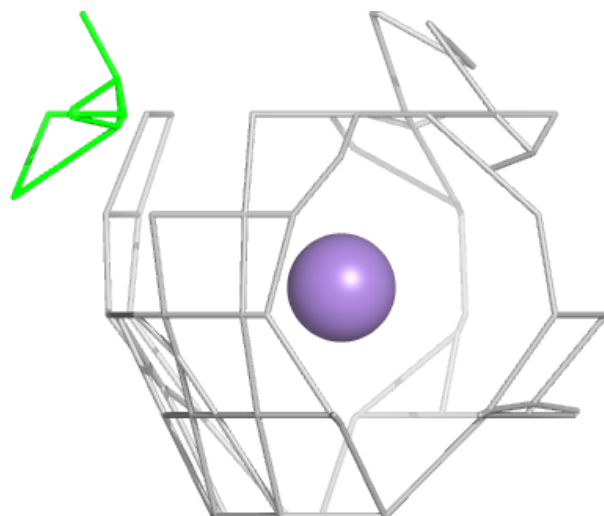
**Electron density around MN F 401:**

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and green (positive)



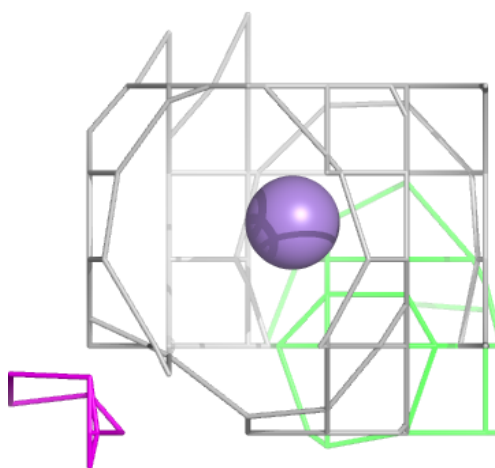
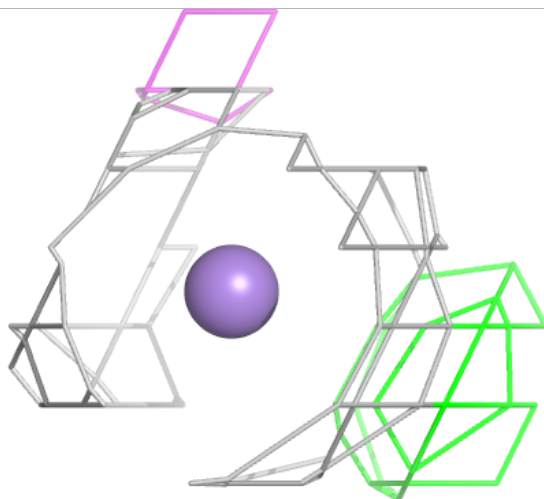
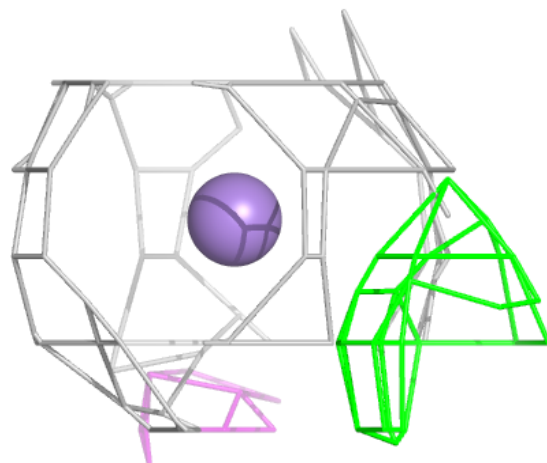
**Electron density around MN A 402:**

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



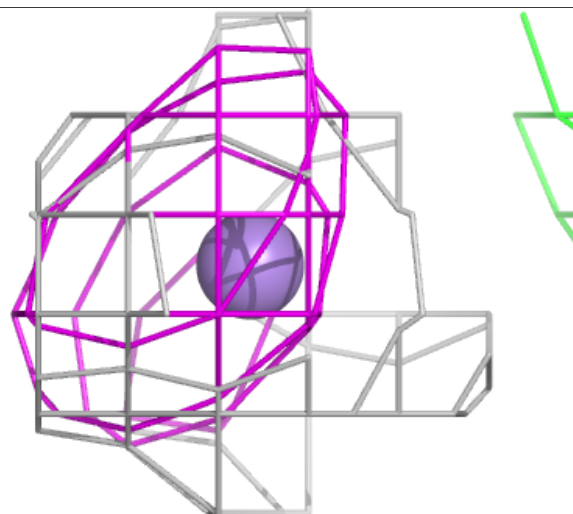
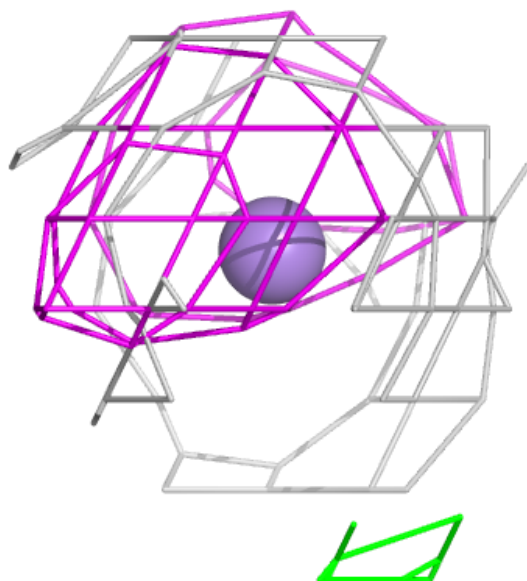
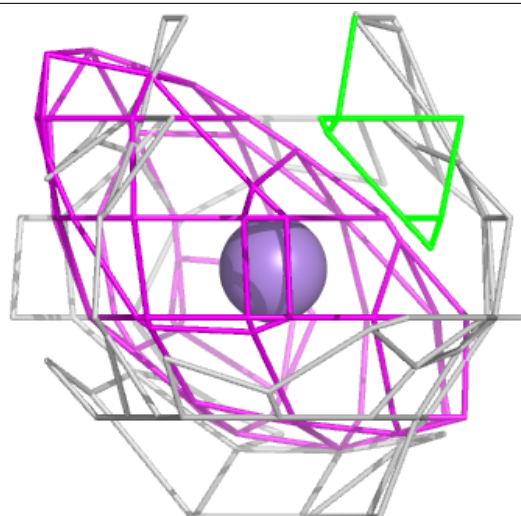
**Electron density around MN E 402:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.