



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:54 AM BST

PDB ID : 6OZP
Title : Crystal structure of Mus musculus (Mm) Endonuclease V in complex with a 23mer RNA oligo containing an inosine after a 180 min soak in 10 mM Mn²⁺
Authors : Samara, N.L.; Yang, W.
Deposited on : 2019-05-15
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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

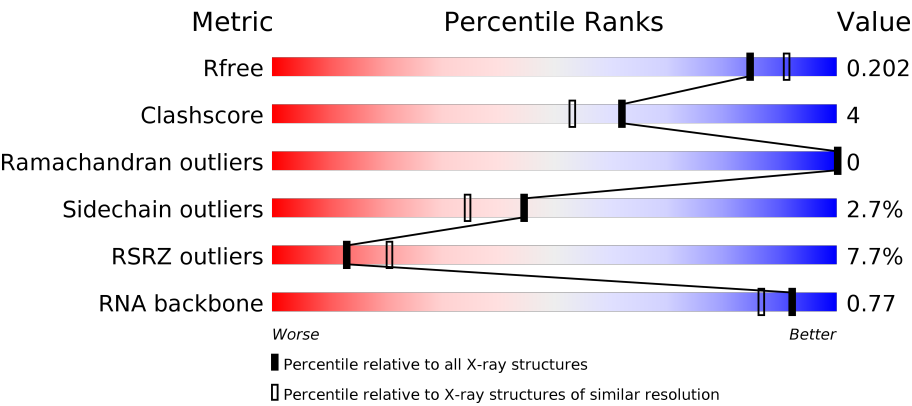
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)
RNA backbone	3102	1124 (2.50-1.42)

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 ≥ 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	245	<div><div>6%</div><div><div></div><div>88%</div><div>10%</div><div>.</div></div></div>
1	B	245	<div><div>9%</div><div><div></div><div>88%</div><div>11%</div></div></div>
2	c	11	<div><div>18%</div><div><div></div><div>36%</div><div>64%</div></div></div>
2	d	11	<div><div>18%</div><div><div></div><div>36%</div><div>64%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	12	<div><div></div><div>83%</div><div>17%</div></div>
3	D	12	<div><div></div><div>92%</div><div>8%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4948 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 Endonuclease V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	8	0
			1919	1218	351	341	9			
1	B	244	Total	C	N	O	S	0	5	0
			1933	1227	355	343	8			

- Molecule 2 is DNA/RNA hybrid called DNA/RNA (5'-R(*CP*GP*GP*UP*AP*AP*CP*C P*C)-D(P*I)-R(P*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	c	4	Total	C	N	O	P	0	0	0
			83	38	15	26	4			
2	d	4	Total	C	N	O	P	0	0	0
			83	38	15	26	4			

- Molecule 3 is a RNA chain called RNA (5'-R(P*UP*AP*UP*GP*CP*AP*UP*GP*CP*AP *UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			253	113	41	87	12			
3	D	12	Total	C	N	O	P	0	0	0
			253	113	41	87	12			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Mn	0	1
			5	5		
4	A	3	Total	Mn	0	0
			3	3		

Continued on next page...

Continued from previous page...

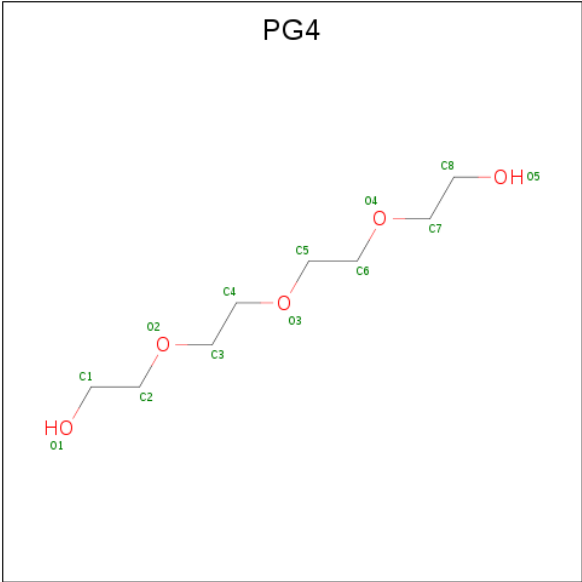
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mn	0	0
			2	2		
4	C	2	Total	Mn	0	0
			2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



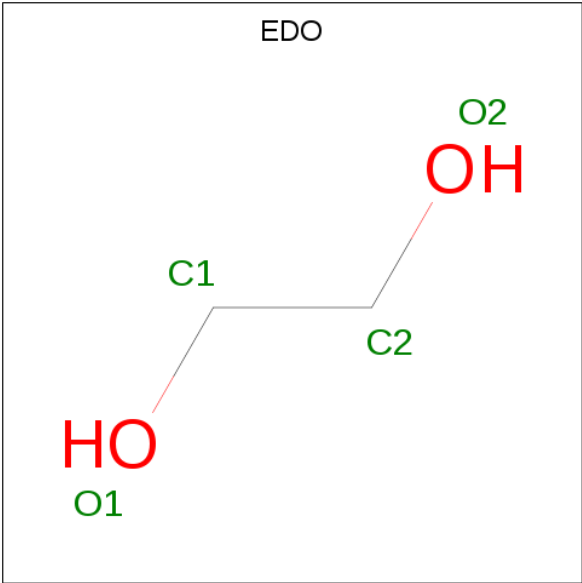
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



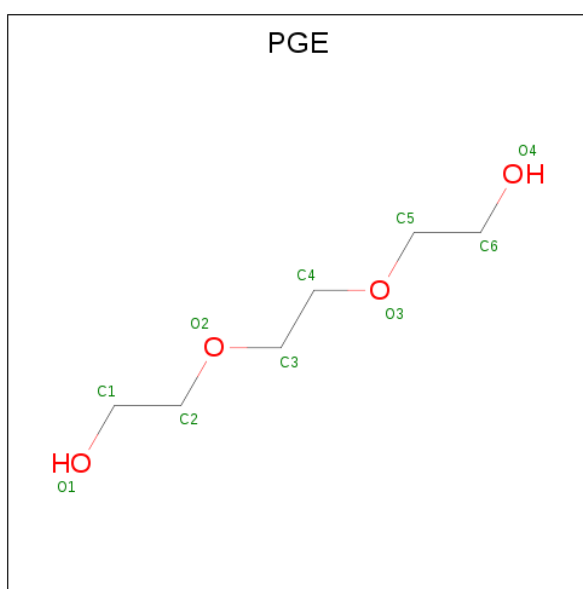
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	150	Total	O	0	0
			150	150		
9	B	108	Total	O	0	0
			108	108		

Continued on next page...

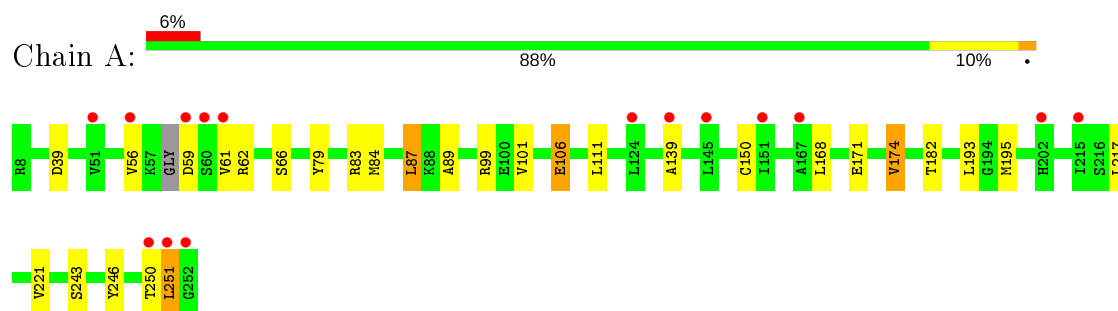
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	c	8	Total 8	O 8	0	0
9	C	23	Total 23	O 23	0	0
9	d	2	Total 2	O 2	0	0
9	D	29	Total 29	O 29	0	0

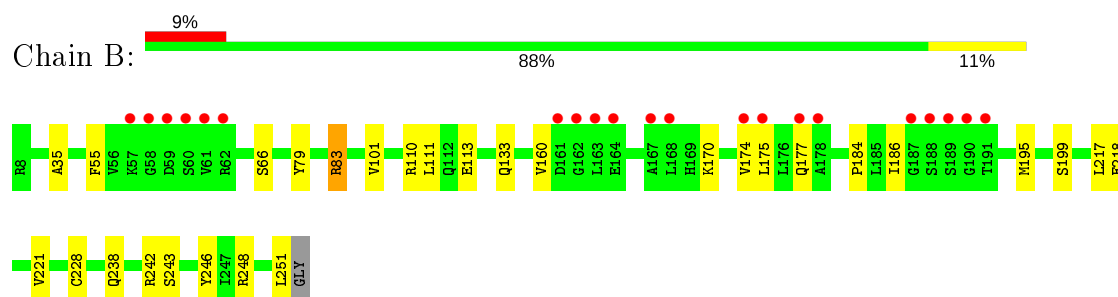
3 Residue-property plots [i](#)

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.

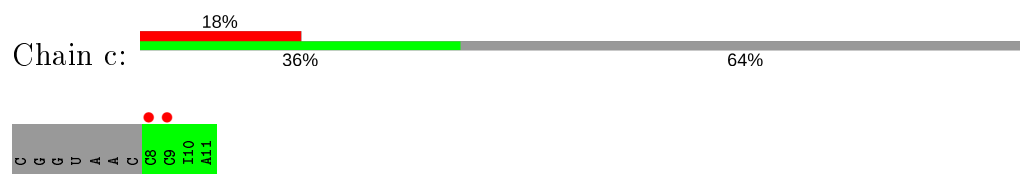
- Molecule 1: Endonuclease V



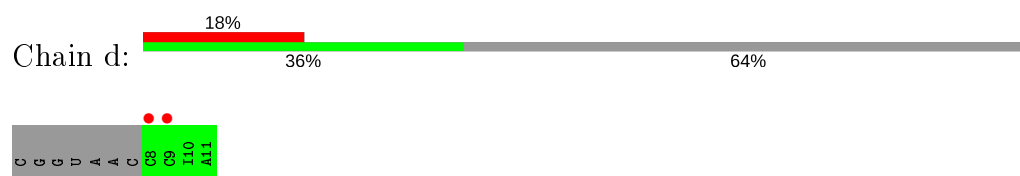
- Molecule 1: Endonuclease V



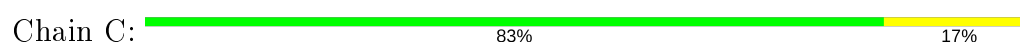
- Molecule 2: DNA/RNA (5'-R(*CP*GP*GP*UP*AP*AP*CP*CP*C)-D(P*I)-R(P*A)-3')



- Molecule 2: DNA/RNA (5'-R(*CP*GP*GP*UP*AP*AP*CP*CP*C)-D(P*I)-R(P*A)-3')



- Molecule 3: RNA (5'-R(P*UP*AP*UP*GP*CP*AP*UP*GP*CP*AP*UP*U)-3')





- Molecule 3: RNA (5'-R(P*UP*AP*UP*GP*CP*AP*UP*GP*CP*AP*UP*U)-3')

Chain D:  92% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.03Å 73.01Å 155.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.48 – 1.96 38.94 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.1 (36.48-1.96) 94.2 (38.94-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.175 , 0.201 0.175 , 0.202	Depositor DCC
R_{free} test set	2852 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.680	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4948	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2270e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: GOL, PG4, PGE, EDO, 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	0.39	0/1973	0.59	0/2674
1	B	0.38	0/1985	0.54	0/2684
2	c	0.52	0/67	0.88	0/99
2	d	0.34	0/67	0.75	0/99
3	C	0.84	1/281 (0.4%)	0.87	0/433
3	D	0.86	1/281 (0.4%)	0.89	0/433
All	All	0.47	2/4654 (0.0%)	0.62	0/6422

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	12	U	OP3-P	-12.30	1.46	1.61
3	C	12	U	OP3-P	-11.90	1.46	1.61

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	1919	0	1957	19	0
1	B	1933	0	2001	19	0
2	c	83	0	43	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	83	0	43	0	0
3	C	253	0	128	2	0
3	D	253	0	128	1	0
4	A	3	0	0	0	0
4	B	5	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	12	0	16	1	0
6	A	13	0	18	0	0
6	B	13	0	18	1	0
7	A	12	0	18	0	0
7	B	12	0	18	0	0
8	A	20	0	28	0	0
8	B	10	0	14	0	0
9	A	150	0	0	1	0
9	B	108	0	0	1	0
9	C	23	0	0	0	0
9	D	29	0	0	0	0
9	c	8	0	0	0	0
9	d	2	0	0	0	0
All	All	4948	0	4430	38	0

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

All (38) 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:A:89:ALA:O	1:A:99[A]:ARG:NH1	2.21	0.74
1:A:195:MET:HG3	1:A:221[A]:VAL:HG21	1.73	0.71
1:B:238:GLN:OE1	1:B:242[A]:ARG:NH1	2.27	0.67
1:B:195:MET:HG3	1:B:221:VAL:HG21	1.76	0.67
1:A:39:ASP:OD2	5:A:305:GOL:H12	1.98	0.62
1:B:83:ARG:HD2	1:B:110:ARG:HH11	1.65	0.62
1:A:83:ARG:HH12	1:A:106:GLU:HG2	1.67	0.60
1:A:56:VAL:HG23	1:A:59:ASP:HB3	1.84	0.59
1:B:199:SER:HB2	1:B:228:CYS:SG	2.45	0.57
1:A:84:MET:HG2	1:A:246:TYR:HE2	1.69	0.57
1:B:133:GLN:HA	1:B:160:VAL:HG21	1.86	0.57
1:A:195:MET:HG3	1:A:221[B]:VAL:HG11	1.88	0.56
1:B:83:ARG:HD2	1:B:110:ARG:NH1	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:HG21	1:A:221[A]:VAL:HG11	1.92	0.51
1:B:35:ALA:HA	6:B:304:PG4:H81	1.94	0.50
1:B:248[A]:ARG:NH2	9:B:401:HOH:O	2.29	0.49
1:A:139:ALA:HB1	1:A:150[B]:CYS:SG	2.53	0.49
1:A:87:LEU:HD11	1:A:99[B]:ARG:HG3	1.95	0.49
1:B:248[A]:ARG:HD3	3:C:15:G:OP1	2.15	0.46
1:B:195:MET:HG2	1:B:217:LEU:HD21	1.96	0.46
1:B:55:PHE:CD1	3:D:12:U:H4'	2.50	0.46
1:A:83:ARG:NH1	1:A:106:GLU:HG2	2.28	0.46
1:A:87:LEU:HD11	1:A:99[A]:ARG:HG3	1.96	0.46
1:B:218:GLU:H	1:B:218:GLU:CD	2.19	0.45
1:B:66[A]:SER:OG	1:B:243:SER:HB3	2.17	0.45
1:A:250:THR:OG1	1:A:251:LEU:N	2.51	0.44
1:A:168:LEU:HD22	9:A:521:HOH:O	2.18	0.43
1:A:66[B]:SER:HB2	1:A:243:SER:HB3	2.01	0.43
1:A:79:TYR:CZ	1:A:111:LEU:HD13	2.55	0.42
1:A:56:VAL:HG22	1:A:62:ARG:O	2.19	0.42
1:B:170:LYS:O	1:B:174:VAL:HG23	2.20	0.42
1:B:248[A]:ARG:CZ	3:C:15:G:H5''	2.49	0.42
1:B:175:LEU:O	1:B:177:GLN:HG2	2.20	0.41
1:B:79:TYR:CZ	1:B:111:LEU:HD13	2.55	0.41
1:B:184:PRO:HB2	1:B:186:ILE:HD11	2.03	0.40
1:A:171:GLU:O	1:A:174:VAL:HG12	2.20	0.40
1:A:217:LEU:O	1:A:221[B]:VAL:HG13	2.22	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	248/245 (101%)	242 (98%)	6 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	247/245 (101%)	242 (98%)	5 (2%)	0	100	100
All	All	495/490 (101%)	484 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/210 (100%)	203 (97%)	7 (3%)	38	26
1	B	214/210 (102%)	210 (98%)	4 (2%)	57	50
All	All	424/420 (101%)	413 (97%)	11 (3%)	44	36

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	VAL
1	A	87	LEU
1	A	101	VAL
1	A	106	GLU
1	A	174	VAL
1	A	193	LEU
1	A	251	LEU
1	B	83	ARG
1	B	101	VAL
1	B	113	GLU
1	B	246	TYR

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	c	2/11 (18%)	0	0
2	d	2/11 (18%)	0	0
3	C	11/12 (91%)	0	0
3	D	11/12 (91%)	0	0
All	All	26/46 (56%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 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	$\# Z > 2$
7	EDO	A	308	-	3,3,3	0.45	0	2,2,2	0.36	0
8	PGE	A	310	-	9,9,9	0.31	0	8,8,8	0.31	0
7	EDO	B	307	-	3,3,3	0.45	0	2,2,2	0.34	0
7	EDO	B	306	-	3,3,3	0.45	0	2,2,2	0.54	0
6	PG4	A	306	-	12,12,12	0.52	0	11,11,11	0.27	0
8	PGE	B	308	-	9,9,9	0.31	0	8,8,8	0.32	0
5	GOL	A	304	-	5,5,5	0.39	0	5,5,5	0.27	0
7	EDO	B	305	-	3,3,3	0.49	0	2,2,2	0.29	0
7	EDO	A	309	-	3,3,3	0.43	0	2,2,2	0.43	0
8	PGE	A	311	-	9,9,9	0.33	0	8,8,8	0.26	0
7	EDO	A	307	-	3,3,3	0.49	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PG4	B	304	-	12,12,12	0.51	0	11,11,11	0.32	0
5	GOL	A	305	-	5,5,5	0.36	0	5,5,5	0.43	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
7	EDO	A	308	-	-	0/1/1/1	-
8	PGE	A	310	-	-	1/7/7/7	-
7	EDO	B	307	-	-	0/1/1/1	-
7	EDO	B	306	-	-	1/1/1/1	-
6	PG4	A	306	-	-	6/10/10/10	-
8	PGE	B	308	-	-	5/7/7/7	-
5	GOL	A	304	-	-	0/4/4/4	-
7	EDO	B	305	-	-	1/1/1/1	-
7	EDO	A	309	-	-	0/1/1/1	-
8	PGE	A	311	-	-	3/7/7/7	-
7	EDO	A	307	-	-	0/1/1/1	-
6	PG4	B	304	-	-	6/10/10/10	-
5	GOL	A	305	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	304	PG4	C1-C2-O2-C3
6	B	304	PG4	O2-C3-C4-O3
6	A	306	PG4	O4-C7-C8-O5
6	B	304	PG4	O4-C7-C8-O5
6	B	304	PG4	O3-C5-C6-O4
8	A	311	PGE	O1-C1-C2-O2
5	A	305	GOL	O1-C1-C2-C3
6	B	304	PG4	O1-C1-C2-O2
6	A	306	PG4	O3-C5-C6-O4
6	A	306	PG4	O2-C3-C4-O3
8	B	308	PGE	C3-C4-O3-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	311	PGE	C4-C3-O2-C2
8	A	310	PGE	C6-C5-O3-C4
5	A	305	GOL	O1-C1-C2-O2
6	A	306	PG4	C3-C4-O3-C5
6	A	306	PG4	C4-C3-O2-C2
8	B	308	PGE	C1-C2-O2-C3
8	A	311	PGE	O2-C3-C4-O3
7	B	305	EDO	O1-C1-C2-O2
8	B	308	PGE	O3-C5-C6-O4
8	B	308	PGE	O2-C3-C4-O3
6	B	304	PG4	C5-C6-O4-C7
7	B	306	EDO	O1-C1-C2-O2
6	A	306	PG4	C8-C7-O4-C6
8	B	308	PGE	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	304	PG4	1	0
5	A	305	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	244/245 (99%)	0.35	15 (6%) 21 29	17, 29, 60, 107	0
1	B	244/245 (99%)	0.36	21 (8%) 10 16	20, 35, 72, 95	0
2	c	3/11 (27%)	1.95	2 (66%) 0 0	29, 29, 67, 129	0
2	d	3/11 (27%)	2.00	2 (66%) 0 0	41, 41, 109, 136	0
3	C	12/12 (100%)	-0.47	0 100 100	31, 36, 60, 74	0
3	D	12/12 (100%)	-0.35	0 100 100	28, 40, 49, 66	0
All	All	518/536 (96%)	0.34	40 (7%) 13 21	17, 33, 70, 136	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	SER	8.5
1	A	251	LEU	7.4
1	B	59	ASP	5.6
1	B	61	VAL	4.6
1	A	61	VAL	4.4
2	c	8	C	4.2
1	B	175	LEU	4.2
1	A	59	ASP	4.2
1	A	252	GLY	4.0
1	B	177	GLN	3.9
1	B	168	LEU	3.9
2	d	8	C	3.9
1	B	188	SER	3.8
1	B	190	GLY	3.3
1	A	56	VAL	3.3
1	B	62	ARG	3.2
1	B	167	ALA	3.2
1	B	161	ASP	3.2
1	B	189	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	174	VAL	3.1
1	A	215	ILE	3.1
1	B	191	THR	3.0
1	B	163	LEU	2.9
1	B	58	GLY	2.7
1	A	167	ALA	2.7
2	d	9	C	2.5
1	A	124	LEU	2.3
1	B	164	GLU	2.3
1	A	51	VAL	2.3
1	A	139	ALA	2.3
1	A	250	THR	2.3
1	A	151	ILE	2.3
1	B	60	SER	2.3
1	B	178	ALA	2.2
1	A	202	HIS	2.2
1	B	187	GLY	2.2
1	B	162	GLY	2.1
1	B	57	LYS	2.1
1	A	145	LEU	2.0
2	c	9	C	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	309	4/4	0.56	0.31	129,131,132,132	0
7	EDO	B	305	4/4	0.77	0.16	63,64,67,68	0

Continued on next page...

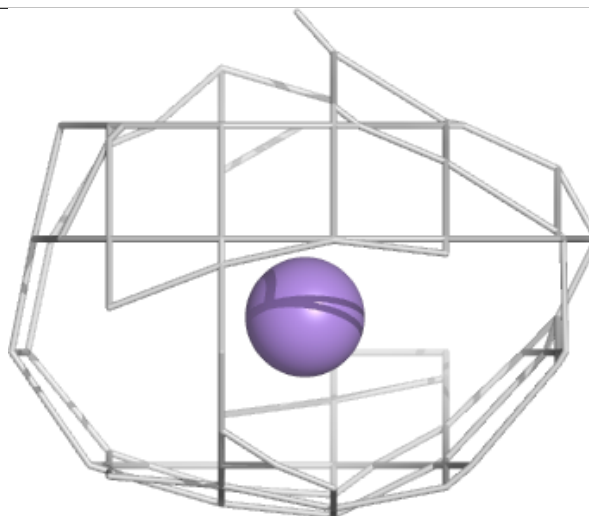
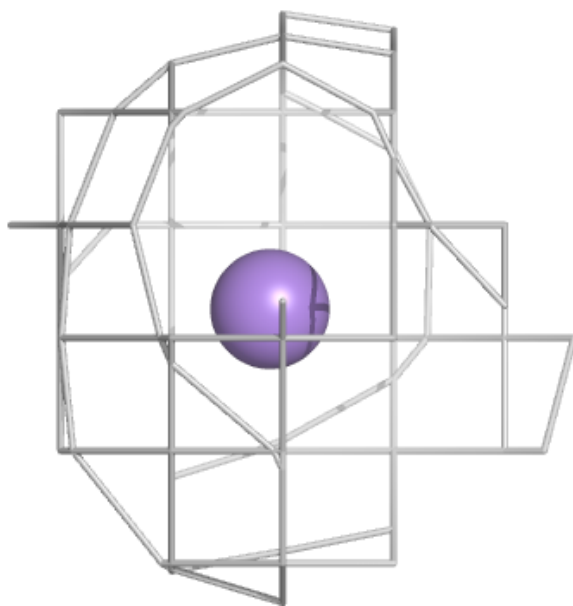
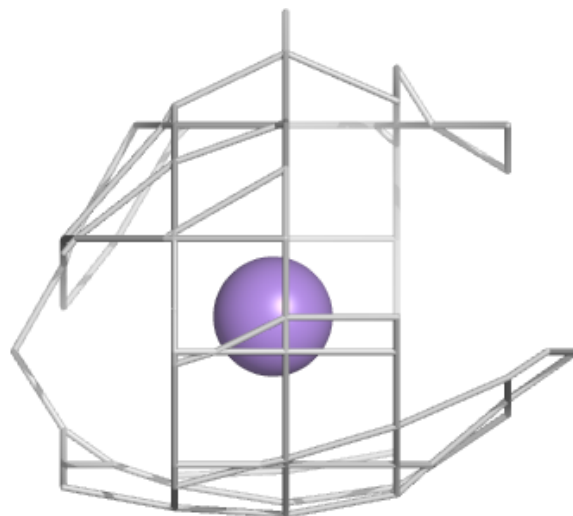
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	307	4/4	0.82	0.21	60,61,62,65	0
7	EDO	B	306	4/4	0.84	0.11	71,73,73,73	0
7	EDO	A	308	4/4	0.84	0.28	67,69,69,70	0
8	PGE	A	310	10/10	0.86	0.18	55,61,66,69	0
6	PG4	A	306	13/13	0.87	0.25	67,69,85,87	0
5	GOL	A	305	6/6	0.87	0.27	42,64,68,71	0
8	PGE	A	311	10/10	0.88	0.12	58,65,75,77	0
5	GOL	A	304	6/6	0.90	0.26	75,79,82,84	0
7	EDO	B	307	4/4	0.91	0.12	65,65,65,72	0
4	MN	B	303[A]	1/1	0.91	0.10	58,58,58,58	1
6	PG4	B	304	13/13	0.91	0.18	42,58,63,65	0
4	MN	B	303[B]	1/1	0.91	0.10	47,47,47,47	1
8	PGE	B	308	10/10	0.92	0.15	61,66,73,75	0
4	MN	A	303	1/1	0.95	0.12	59,59,59,59	1
4	MN	C	102	1/1	0.97	0.19	45,45,45,45	1
4	MN	D	102	1/1	0.97	0.05	45,45,45,45	1
4	MN	B	302	1/1	0.98	0.02	43,43,43,43	1
4	MN	D	101	1/1	0.99	0.06	32,32,32,32	0
4	MN	A	301	1/1	0.99	0.07	24,24,24,24	0
4	MN	B	301	1/1	0.99	0.07	26,26,26,26	0
4	MN	C	101	1/1	0.99	0.06	30,30,30,30	0
4	MN	A	302	1/1	1.00	0.08	23,23,23,23	0
4	MN	B	309	1/1	1.00	0.10	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.

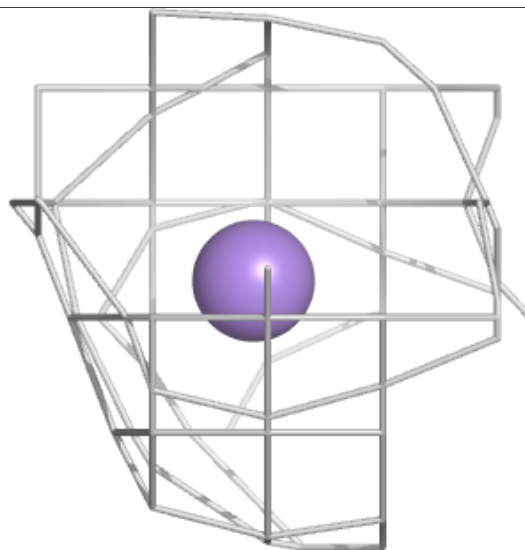
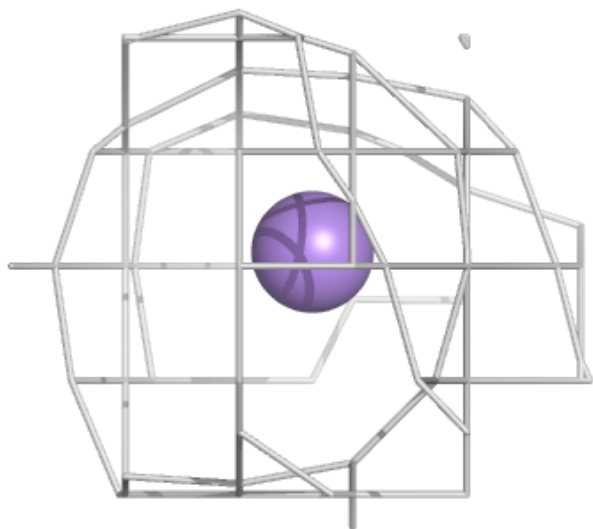
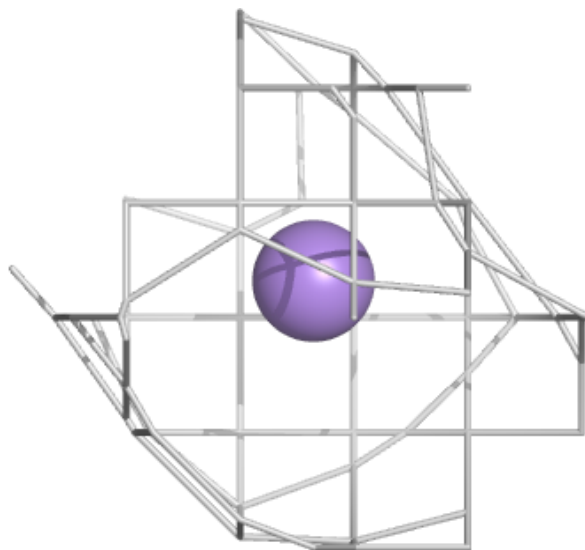
Electron density around MN B 303 (A):

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



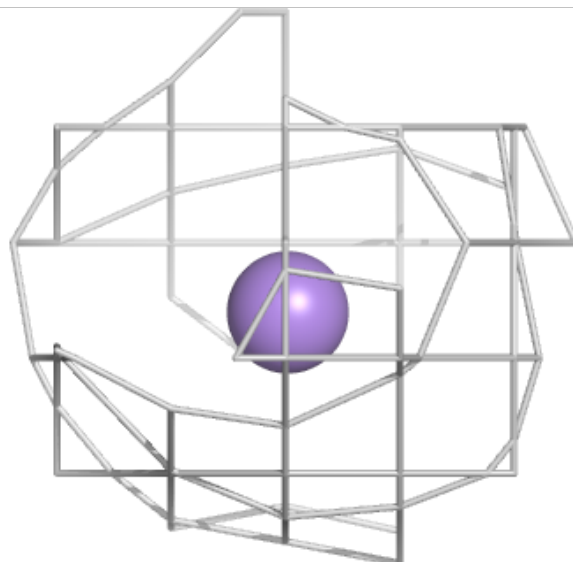
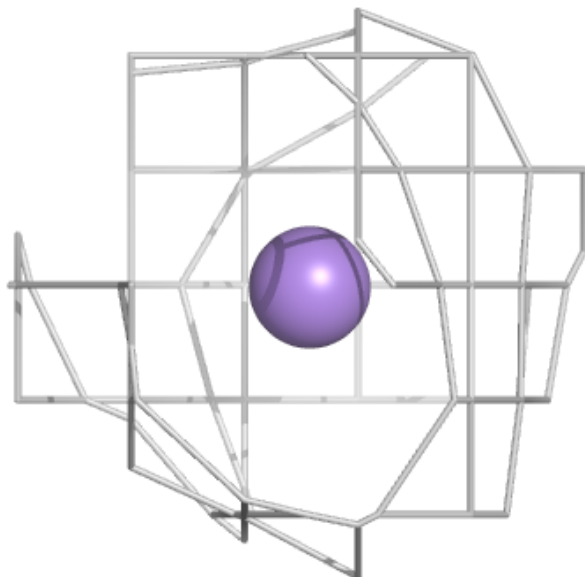
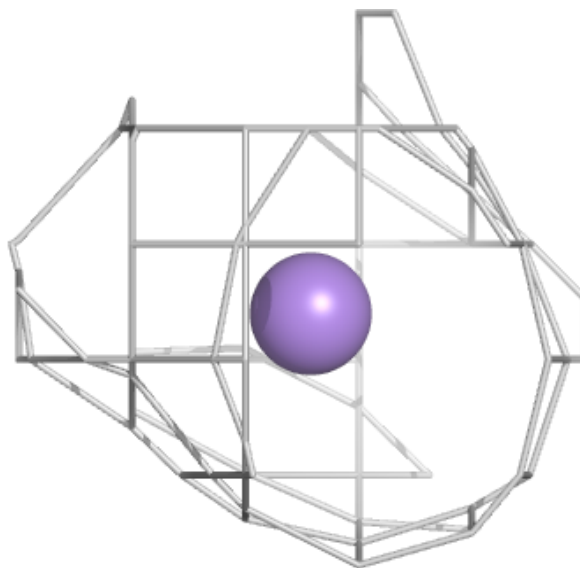
Electron density around MN B 303 (B):

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



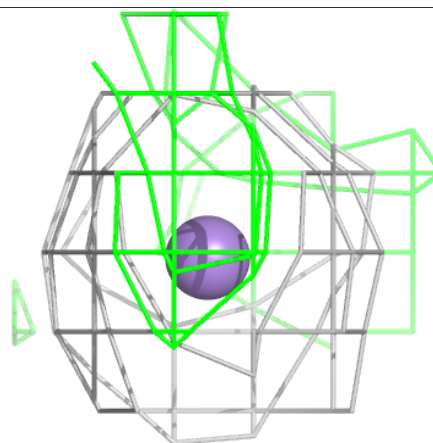
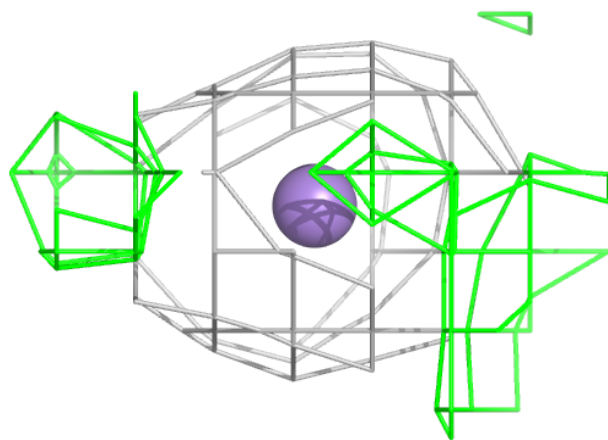
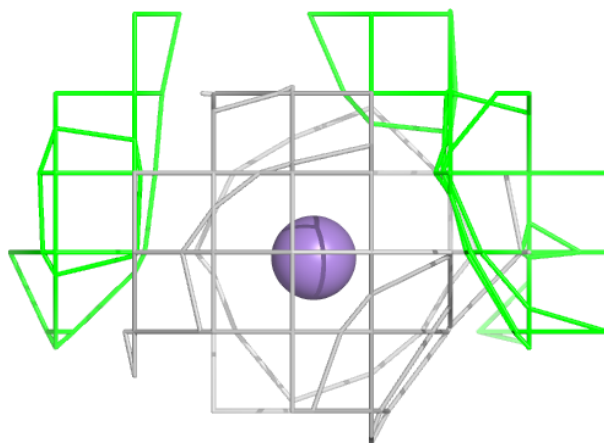
Electron density around MN A 303:

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



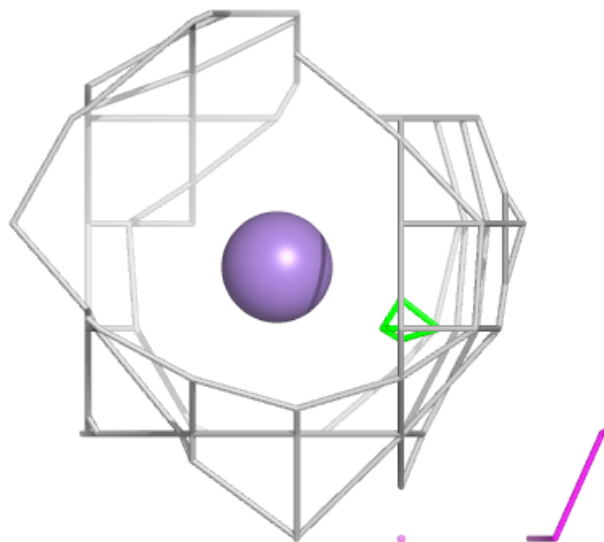
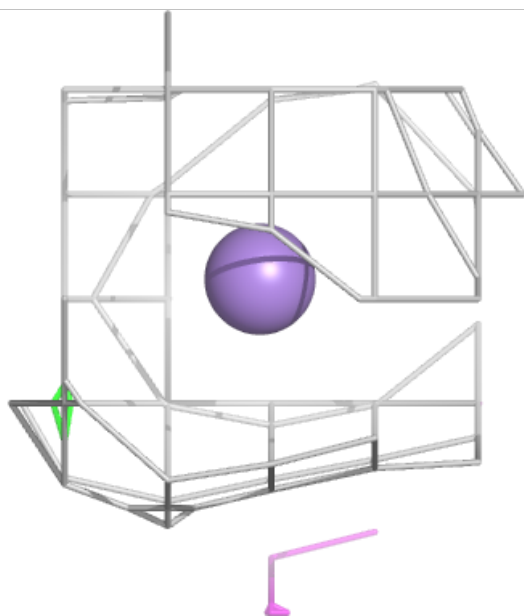
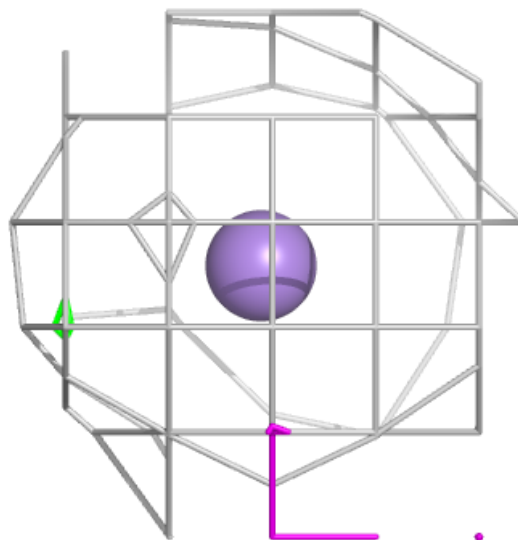
Electron density around MN C 102:

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



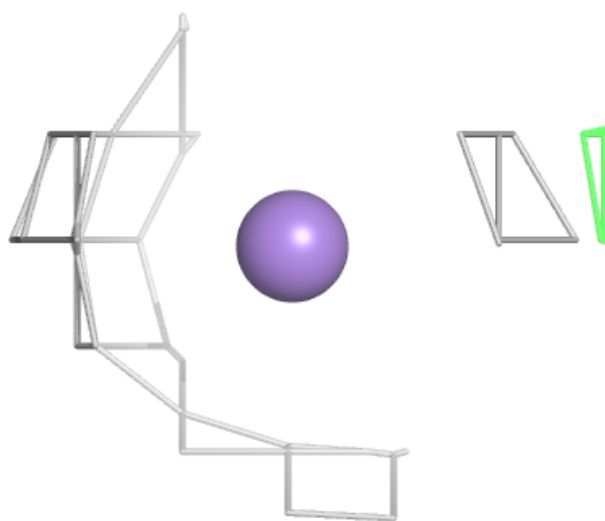
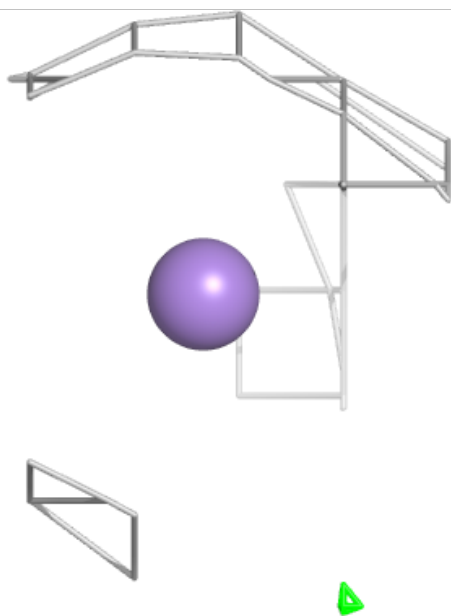
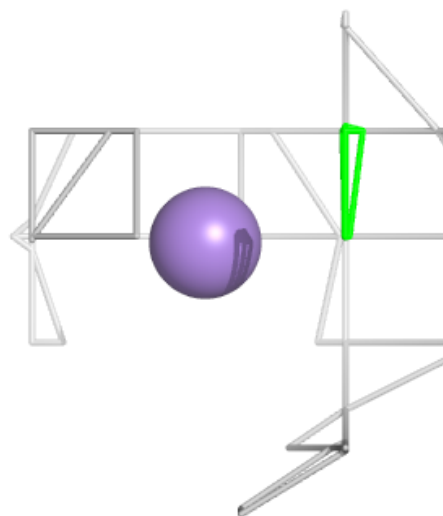
Electron density around MN D 102:

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



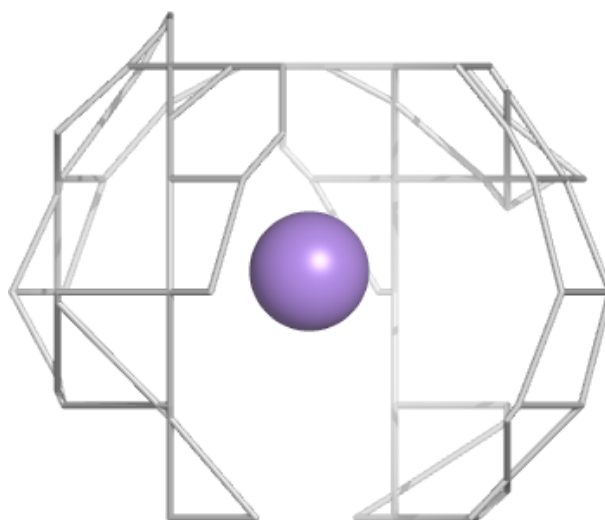
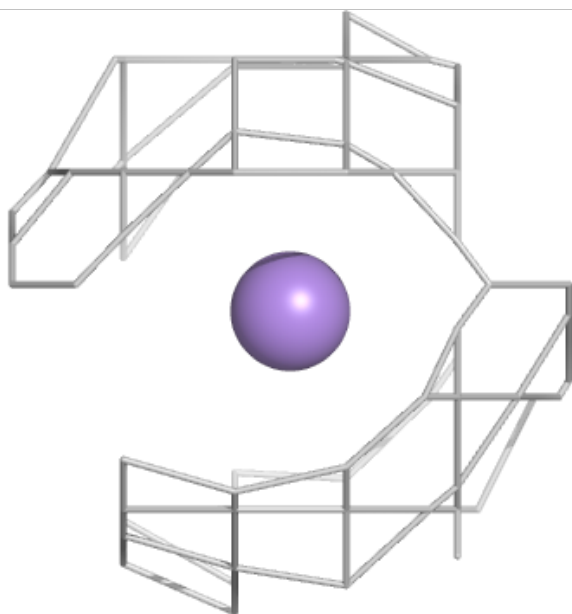
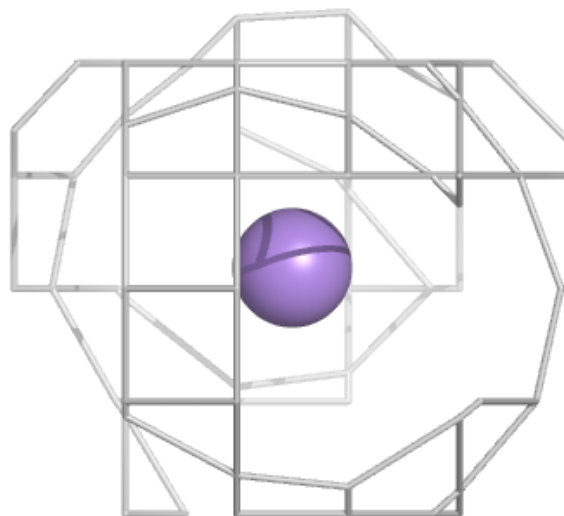
Electron density around MN B 302:

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



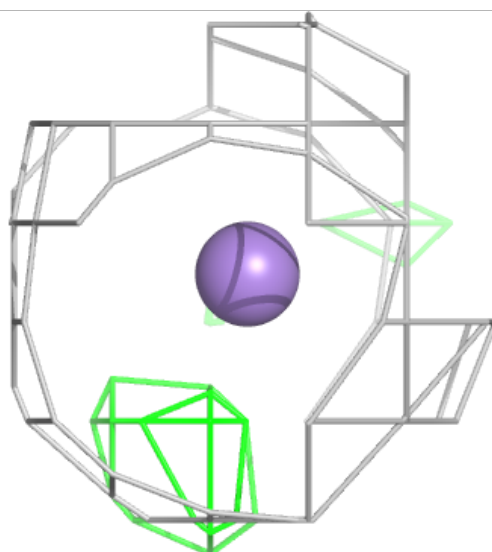
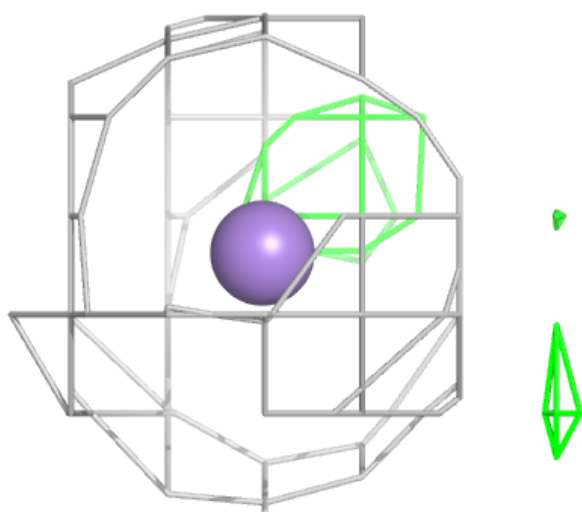
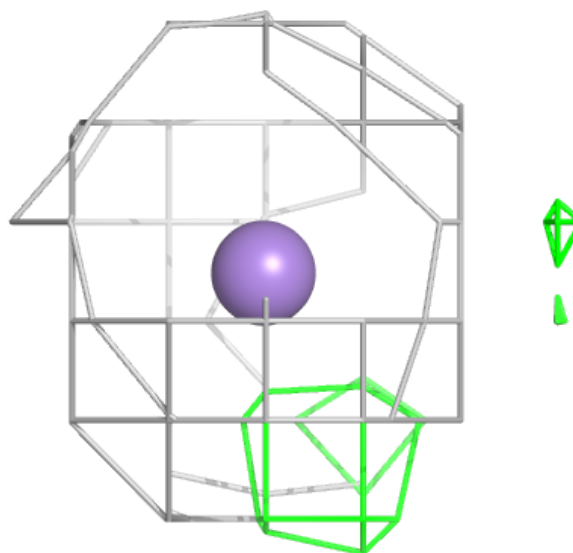
Electron density around MN D 101:

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



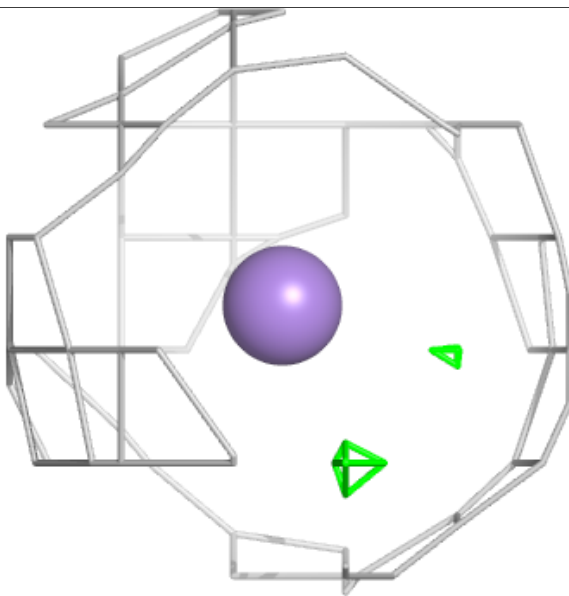
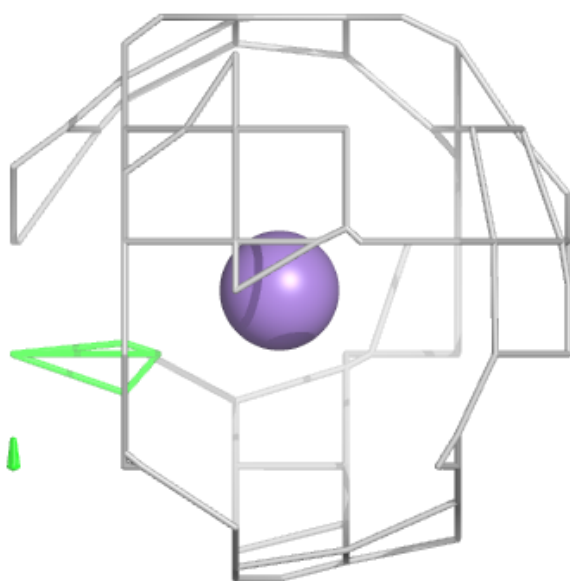
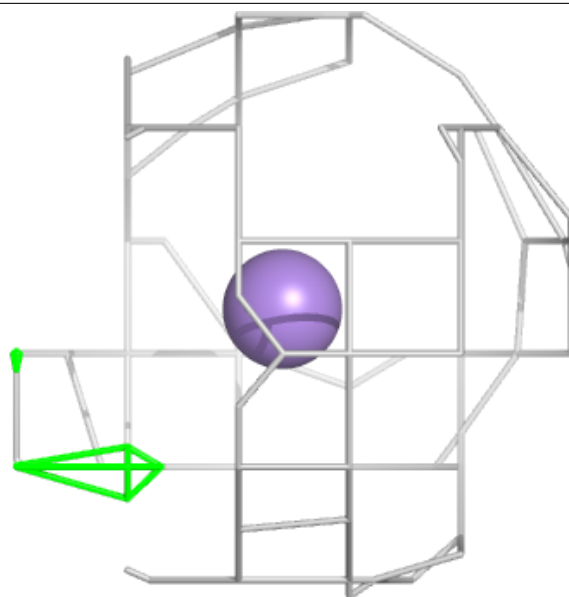
Electron density around MN A 301:

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



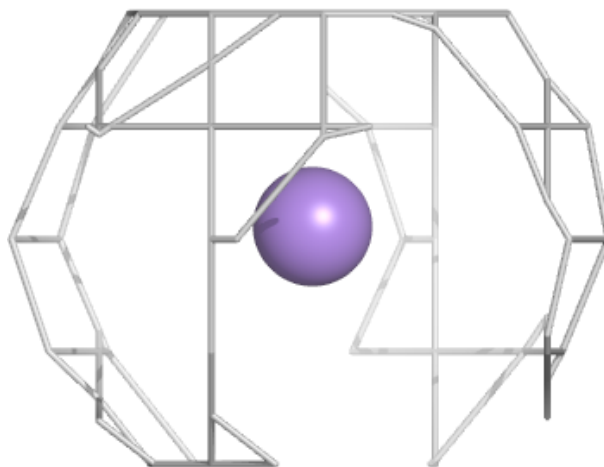
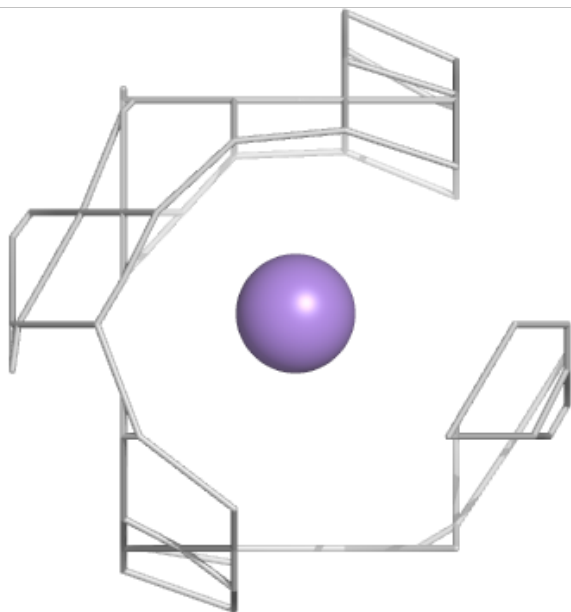
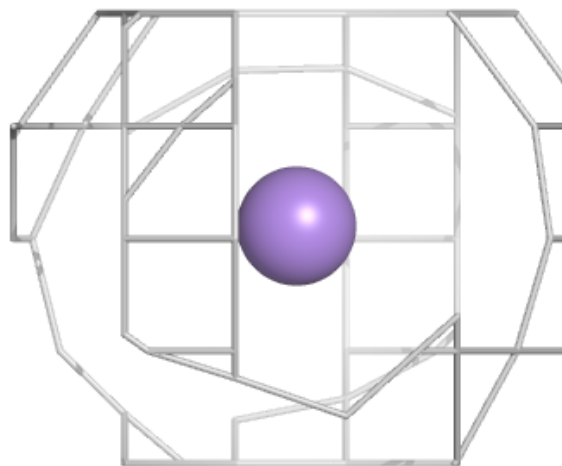
Electron density around MN B 301:

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



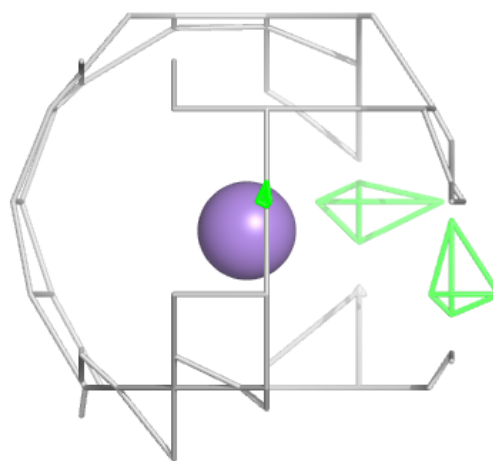
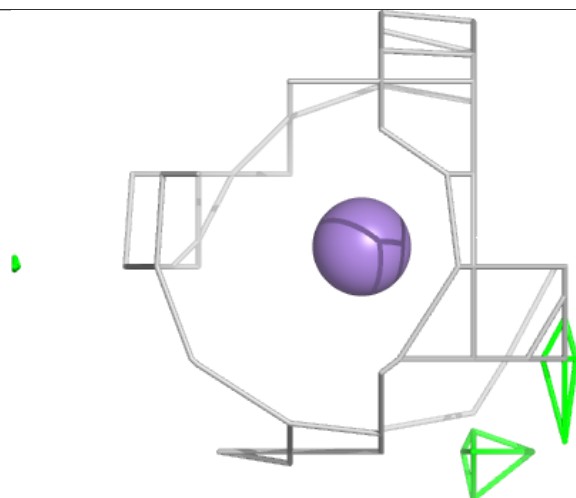
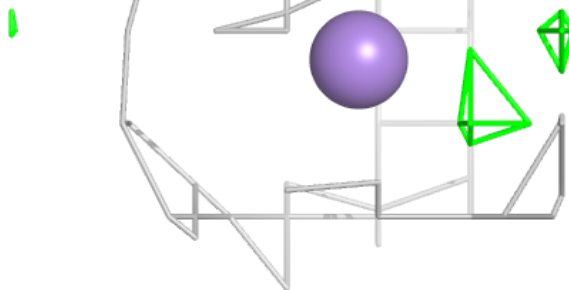
Electron density around MN C 101:

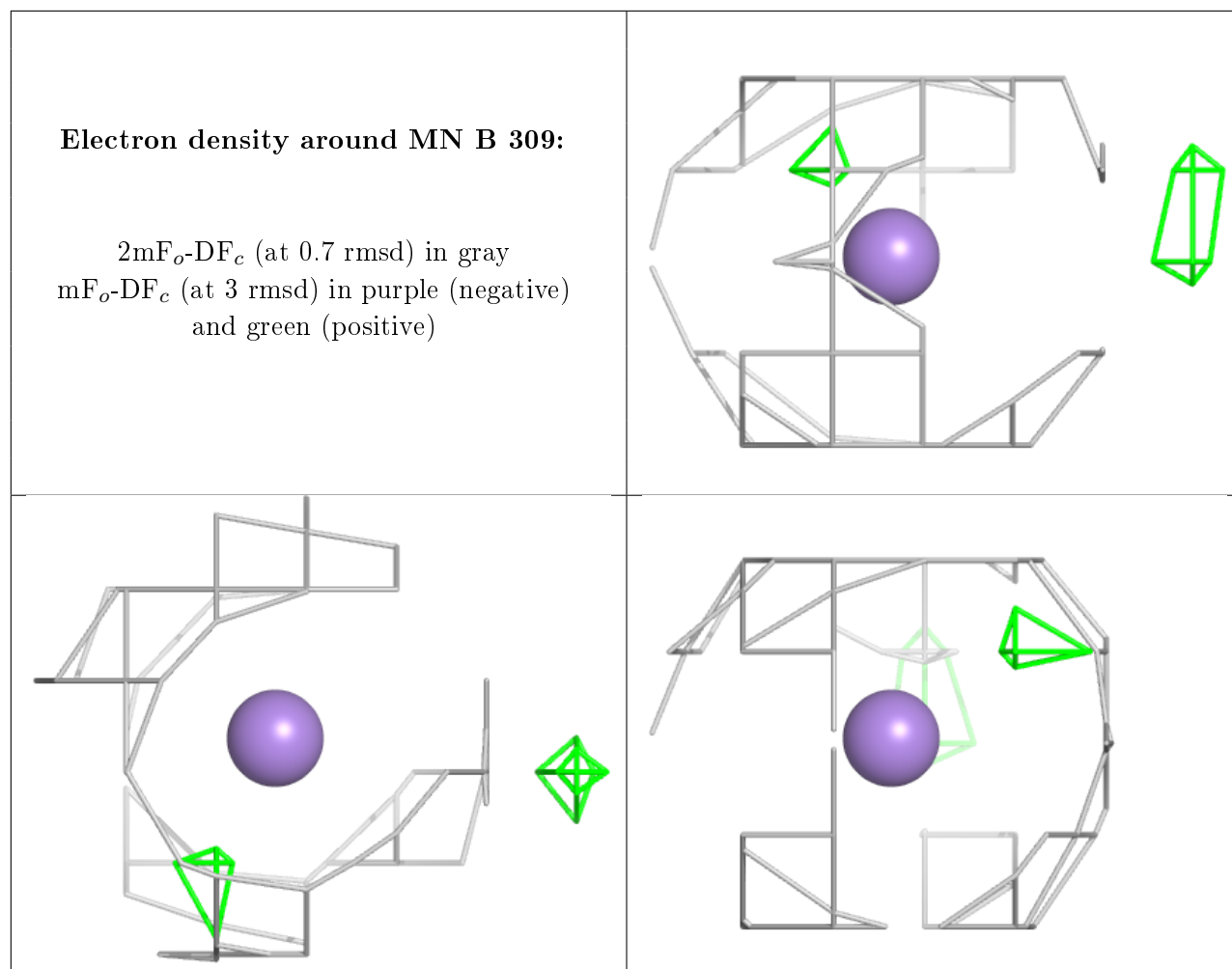
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN A 302:

$2mF_o-DF_c$ (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.