



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2025 – 12:47 PM JST

PDB ID : 9JAW / pdb\_00009jaw  
Title : Crystal structure of NAD-dependent methanol dehydrogenases 2 from *Bacillus methanolicus* MGA3  
Authors : Kong, X.D.; Ma, B.D.  
Deposited on : 2024-08-25  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1



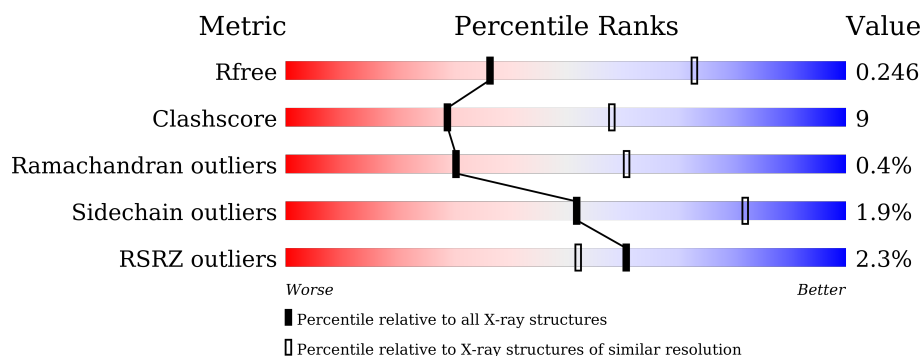
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	 84% 12% ..
1	B	393	 81% 16% ..
1	C	393	 82% 16% .
1	D	393	 5% 79% 18% ..
1	E	393	 75% 22% ..
1	F	393	 83% 14% ..

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Mol	Chain	Length	Quality of chain
1	G	393	<div><div>%</div><div><div></div><div>72%</div><div>24%</div><div>..</div></div></div>
1	H	393	<div><div>6%</div><div><div></div><div>72%</div><div>25%</div><div>..</div></div></div>
1	I	393	<div><div>4%</div><div><div></div><div>74%</div><div>23%</div><div>..</div></div></div>
1	J	393	<div><div>5%</div><div><div></div><div>79%</div><div>18%</div><div>..</div></div></div>



## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28512 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 NAD-dependent methanol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2847	1802	481	550	14			
1	B	384	Total	C	N	O	S	0	0	0
			2847	1802	481	550	14			
1	C	384	Total	C	N	O	S	0	0	0
			2847	1802	481	550	14			
1	D	384	Total	C	N	O	S	0	0	0
			2847	1802	481	550	14			
1	E	384	Total	C	N	O	S	0	0	0
			2847	1802	481	550	14			
1	F	384	Total	C	N	O	S	0	0	0
			2847	1802	481	550	14			
1	G	384	Total	C	N	O	S	0	0	0
			2847	1802	481	550	14			
1	H	384	Total	C	N	O	S	0	0	0
			2847	1802	481	550	14			
1	I	384	Total	C	N	O	S	0	0	0
			2847	1802	481	550	14			
1	J	384	Total	C	N	O	S	0	0	0
			2847	1802	481	550	14			

There are 230 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	THR	LYS	conflict	UNP I3E2P9
A	9	PHE	TYR	conflict	UNP I3E2P9
A	30	ASP	GLY	conflict	UNP I3E2P9
A	46	GLY	SER	conflict	UNP I3E2P9
A	54	SER	ALA	conflict	UNP I3E2P9
A	55	SER	GLY	conflict	UNP I3E2P9
A	59	ALA	GLU	conflict	UNP I3E2P9
A	65	SER	ALA	conflict	UNP I3E2P9
A	118	LYS	THR	conflict	UNP I3E2P9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	130	GLU	LYS	conflict	UNP I3E2P9
A	285	VAL	ILE	conflict	UNP I3E2P9
A	289	TYR	HIS	conflict	UNP I3E2P9
A	320	ASP	GLU	conflict	UNP I3E2P9
A	334	LYS	ARG	conflict	UNP I3E2P9
A	361	LYS	ASN	conflict	UNP I3E2P9
A	386	LEU	-	expression tag	UNP I3E2P9
A	387	GLU	-	expression tag	UNP I3E2P9
A	388	HIS	-	expression tag	UNP I3E2P9
A	389	HIS	-	expression tag	UNP I3E2P9
A	390	HIS	-	expression tag	UNP I3E2P9
A	391	HIS	-	expression tag	UNP I3E2P9
A	392	HIS	-	expression tag	UNP I3E2P9
A	393	HIS	-	expression tag	UNP I3E2P9
B	2	THR	LYS	conflict	UNP I3E2P9
B	9	PHE	TYR	conflict	UNP I3E2P9
B	30	ASP	GLY	conflict	UNP I3E2P9
B	46	GLY	SER	conflict	UNP I3E2P9
B	54	SER	ALA	conflict	UNP I3E2P9
B	55	SER	GLY	conflict	UNP I3E2P9
B	59	ALA	GLU	conflict	UNP I3E2P9
B	65	SER	ALA	conflict	UNP I3E2P9
B	118	LYS	THR	conflict	UNP I3E2P9
B	130	GLU	LYS	conflict	UNP I3E2P9
B	285	VAL	ILE	conflict	UNP I3E2P9
B	289	TYR	HIS	conflict	UNP I3E2P9
B	320	ASP	GLU	conflict	UNP I3E2P9
B	334	LYS	ARG	conflict	UNP I3E2P9
B	361	LYS	ASN	conflict	UNP I3E2P9
B	386	LEU	-	expression tag	UNP I3E2P9
B	387	GLU	-	expression tag	UNP I3E2P9
B	388	HIS	-	expression tag	UNP I3E2P9
B	389	HIS	-	expression tag	UNP I3E2P9
B	390	HIS	-	expression tag	UNP I3E2P9
B	391	HIS	-	expression tag	UNP I3E2P9
B	392	HIS	-	expression tag	UNP I3E2P9
B	393	HIS	-	expression tag	UNP I3E2P9
C	2	THR	LYS	conflict	UNP I3E2P9
C	9	PHE	TYR	conflict	UNP I3E2P9
C	30	ASP	GLY	conflict	UNP I3E2P9
C	46	GLY	SER	conflict	UNP I3E2P9
C	54	SER	ALA	conflict	UNP I3E2P9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	55	SER	GLY	conflict	UNP I3E2P9
C	59	ALA	GLU	conflict	UNP I3E2P9
C	65	SER	ALA	conflict	UNP I3E2P9
C	118	LYS	THR	conflict	UNP I3E2P9
C	130	GLU	LYS	conflict	UNP I3E2P9
C	285	VAL	ILE	conflict	UNP I3E2P9
C	289	TYR	HIS	conflict	UNP I3E2P9
C	320	ASP	GLU	conflict	UNP I3E2P9
C	334	LYS	ARG	conflict	UNP I3E2P9
C	361	LYS	ASN	conflict	UNP I3E2P9
C	386	LEU	-	expression tag	UNP I3E2P9
C	387	GLU	-	expression tag	UNP I3E2P9
C	388	HIS	-	expression tag	UNP I3E2P9
C	389	HIS	-	expression tag	UNP I3E2P9
C	390	HIS	-	expression tag	UNP I3E2P9
C	391	HIS	-	expression tag	UNP I3E2P9
C	392	HIS	-	expression tag	UNP I3E2P9
C	393	HIS	-	expression tag	UNP I3E2P9
D	2	THR	LYS	conflict	UNP I3E2P9
D	9	PHE	TYR	conflict	UNP I3E2P9
D	30	ASP	GLY	conflict	UNP I3E2P9
D	46	GLY	SER	conflict	UNP I3E2P9
D	54	SER	ALA	conflict	UNP I3E2P9
D	55	SER	GLY	conflict	UNP I3E2P9
D	59	ALA	GLU	conflict	UNP I3E2P9
D	65	SER	ALA	conflict	UNP I3E2P9
D	118	LYS	THR	conflict	UNP I3E2P9
D	130	GLU	LYS	conflict	UNP I3E2P9
D	285	VAL	ILE	conflict	UNP I3E2P9
D	289	TYR	HIS	conflict	UNP I3E2P9
D	320	ASP	GLU	conflict	UNP I3E2P9
D	334	LYS	ARG	conflict	UNP I3E2P9
D	361	LYS	ASN	conflict	UNP I3E2P9
D	386	LEU	-	expression tag	UNP I3E2P9
D	387	GLU	-	expression tag	UNP I3E2P9
D	388	HIS	-	expression tag	UNP I3E2P9
D	389	HIS	-	expression tag	UNP I3E2P9
D	390	HIS	-	expression tag	UNP I3E2P9
D	391	HIS	-	expression tag	UNP I3E2P9
D	392	HIS	-	expression tag	UNP I3E2P9
D	393	HIS	-	expression tag	UNP I3E2P9
E	2	THR	LYS	conflict	UNP I3E2P9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	9	PHE	TYR	conflict	UNP I3E2P9
E	30	ASP	GLY	conflict	UNP I3E2P9
E	46	GLY	SER	conflict	UNP I3E2P9
E	54	SER	ALA	conflict	UNP I3E2P9
E	55	SER	GLY	conflict	UNP I3E2P9
E	59	ALA	GLU	conflict	UNP I3E2P9
E	65	SER	ALA	conflict	UNP I3E2P9
E	118	LYS	THR	conflict	UNP I3E2P9
E	130	GLU	LYS	conflict	UNP I3E2P9
E	285	VAL	ILE	conflict	UNP I3E2P9
E	289	TYR	HIS	conflict	UNP I3E2P9
E	320	ASP	GLU	conflict	UNP I3E2P9
E	334	LYS	ARG	conflict	UNP I3E2P9
E	361	LYS	ASN	conflict	UNP I3E2P9
E	386	LEU	-	expression tag	UNP I3E2P9
E	387	GLU	-	expression tag	UNP I3E2P9
E	388	HIS	-	expression tag	UNP I3E2P9
E	389	HIS	-	expression tag	UNP I3E2P9
E	390	HIS	-	expression tag	UNP I3E2P9
E	391	HIS	-	expression tag	UNP I3E2P9
E	392	HIS	-	expression tag	UNP I3E2P9
E	393	HIS	-	expression tag	UNP I3E2P9
F	2	THR	LYS	conflict	UNP I3E2P9
F	9	PHE	TYR	conflict	UNP I3E2P9
F	30	ASP	GLY	conflict	UNP I3E2P9
F	46	GLY	SER	conflict	UNP I3E2P9
F	54	SER	ALA	conflict	UNP I3E2P9
F	55	SER	GLY	conflict	UNP I3E2P9
F	59	ALA	GLU	conflict	UNP I3E2P9
F	65	SER	ALA	conflict	UNP I3E2P9
F	118	LYS	THR	conflict	UNP I3E2P9
F	130	GLU	LYS	conflict	UNP I3E2P9
F	285	VAL	ILE	conflict	UNP I3E2P9
F	289	TYR	HIS	conflict	UNP I3E2P9
F	320	ASP	GLU	conflict	UNP I3E2P9
F	334	LYS	ARG	conflict	UNP I3E2P9
F	361	LYS	ASN	conflict	UNP I3E2P9
F	386	LEU	-	expression tag	UNP I3E2P9
F	387	GLU	-	expression tag	UNP I3E2P9
F	388	HIS	-	expression tag	UNP I3E2P9
F	389	HIS	-	expression tag	UNP I3E2P9
F	390	HIS	-	expression tag	UNP I3E2P9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	391	HIS	-	expression tag	UNP I3E2P9
F	392	HIS	-	expression tag	UNP I3E2P9
F	393	HIS	-	expression tag	UNP I3E2P9
G	2	THR	LYS	conflict	UNP I3E2P9
G	9	PHE	TYR	conflict	UNP I3E2P9
G	30	ASP	GLY	conflict	UNP I3E2P9
G	46	GLY	SER	conflict	UNP I3E2P9
G	54	SER	ALA	conflict	UNP I3E2P9
G	55	SER	GLY	conflict	UNP I3E2P9
G	59	ALA	GLU	conflict	UNP I3E2P9
G	65	SER	ALA	conflict	UNP I3E2P9
G	118	LYS	THR	conflict	UNP I3E2P9
G	130	GLU	LYS	conflict	UNP I3E2P9
G	285	VAL	ILE	conflict	UNP I3E2P9
G	289	TYR	HIS	conflict	UNP I3E2P9
G	320	ASP	GLU	conflict	UNP I3E2P9
G	334	LYS	ARG	conflict	UNP I3E2P9
G	361	LYS	ASN	conflict	UNP I3E2P9
G	386	LEU	-	expression tag	UNP I3E2P9
G	387	GLU	-	expression tag	UNP I3E2P9
G	388	HIS	-	expression tag	UNP I3E2P9
G	389	HIS	-	expression tag	UNP I3E2P9
G	390	HIS	-	expression tag	UNP I3E2P9
G	391	HIS	-	expression tag	UNP I3E2P9
G	392	HIS	-	expression tag	UNP I3E2P9
G	393	HIS	-	expression tag	UNP I3E2P9
H	2	THR	LYS	conflict	UNP I3E2P9
H	9	PHE	TYR	conflict	UNP I3E2P9
H	30	ASP	GLY	conflict	UNP I3E2P9
H	46	GLY	SER	conflict	UNP I3E2P9
H	54	SER	ALA	conflict	UNP I3E2P9
H	55	SER	GLY	conflict	UNP I3E2P9
H	59	ALA	GLU	conflict	UNP I3E2P9
H	65	SER	ALA	conflict	UNP I3E2P9
H	118	LYS	THR	conflict	UNP I3E2P9
H	130	GLU	LYS	conflict	UNP I3E2P9
H	285	VAL	ILE	conflict	UNP I3E2P9
H	289	TYR	HIS	conflict	UNP I3E2P9
H	320	ASP	GLU	conflict	UNP I3E2P9
H	334	LYS	ARG	conflict	UNP I3E2P9
H	361	LYS	ASN	conflict	UNP I3E2P9
H	386	LEU	-	expression tag	UNP I3E2P9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	387	GLU	-	expression tag	UNP I3E2P9
H	388	HIS	-	expression tag	UNP I3E2P9
H	389	HIS	-	expression tag	UNP I3E2P9
H	390	HIS	-	expression tag	UNP I3E2P9
H	391	HIS	-	expression tag	UNP I3E2P9
H	392	HIS	-	expression tag	UNP I3E2P9
H	393	HIS	-	expression tag	UNP I3E2P9
I	2	THR	LYS	conflict	UNP I3E2P9
I	9	PHE	TYR	conflict	UNP I3E2P9
I	30	ASP	GLY	conflict	UNP I3E2P9
I	46	GLY	SER	conflict	UNP I3E2P9
I	54	SER	ALA	conflict	UNP I3E2P9
I	55	SER	GLY	conflict	UNP I3E2P9
I	59	ALA	GLU	conflict	UNP I3E2P9
I	65	SER	ALA	conflict	UNP I3E2P9
I	118	LYS	THR	conflict	UNP I3E2P9
I	130	GLU	LYS	conflict	UNP I3E2P9
I	285	VAL	ILE	conflict	UNP I3E2P9
I	289	TYR	HIS	conflict	UNP I3E2P9
I	320	ASP	GLU	conflict	UNP I3E2P9
I	334	LYS	ARG	conflict	UNP I3E2P9
I	361	LYS	ASN	conflict	UNP I3E2P9
I	386	LEU	-	expression tag	UNP I3E2P9
I	387	GLU	-	expression tag	UNP I3E2P9
I	388	HIS	-	expression tag	UNP I3E2P9
I	389	HIS	-	expression tag	UNP I3E2P9
I	390	HIS	-	expression tag	UNP I3E2P9
I	391	HIS	-	expression tag	UNP I3E2P9
I	392	HIS	-	expression tag	UNP I3E2P9
I	393	HIS	-	expression tag	UNP I3E2P9
J	2	THR	LYS	conflict	UNP I3E2P9
J	9	PHE	TYR	conflict	UNP I3E2P9
J	30	ASP	GLY	conflict	UNP I3E2P9
J	46	GLY	SER	conflict	UNP I3E2P9
J	54	SER	ALA	conflict	UNP I3E2P9
J	55	SER	GLY	conflict	UNP I3E2P9
J	59	ALA	GLU	conflict	UNP I3E2P9
J	65	SER	ALA	conflict	UNP I3E2P9
J	118	LYS	THR	conflict	UNP I3E2P9
J	130	GLU	LYS	conflict	UNP I3E2P9
J	285	VAL	ILE	conflict	UNP I3E2P9
J	289	TYR	HIS	conflict	UNP I3E2P9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	320	ASP	GLU	conflict	UNP I3E2P9
J	334	LYS	ARG	conflict	UNP I3E2P9
J	361	LYS	ASN	conflict	UNP I3E2P9
J	386	LEU	-	expression tag	UNP I3E2P9
J	387	GLU	-	expression tag	UNP I3E2P9
J	388	HIS	-	expression tag	UNP I3E2P9
J	389	HIS	-	expression tag	UNP I3E2P9
J	390	HIS	-	expression tag	UNP I3E2P9
J	391	HIS	-	expression tag	UNP I3E2P9
J	392	HIS	-	expression tag	UNP I3E2P9
J	393	HIS	-	expression tag	UNP I3E2P9

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	I	1	Total Mn 1 1	0	0
2	J	1	Total Mn 1 1	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0



- Molecule 4 is water.

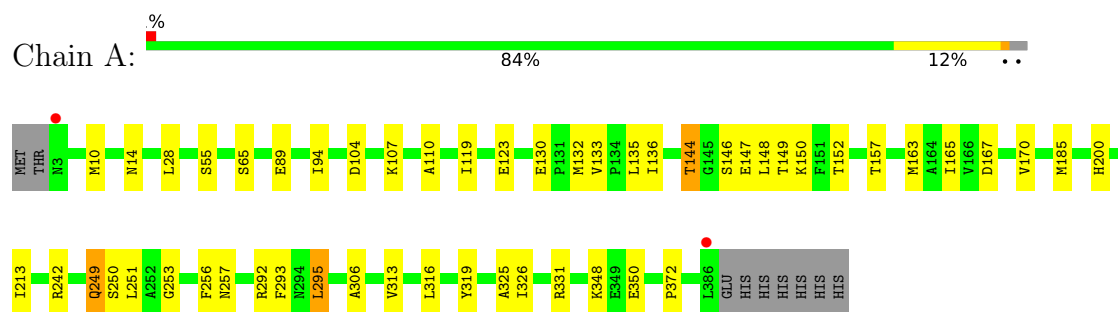
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	9	Total O 9 9	0	0
4	C	7	Total O 7 7	0	0
4	D	1	Total O 1 1	0	0
4	E	2	Total O 2 2	0	0
4	F	2	Total O 2 2	0	0
4	G	1	Total O 1 1	0	0
4	J	1	Total O 1 1	0	0



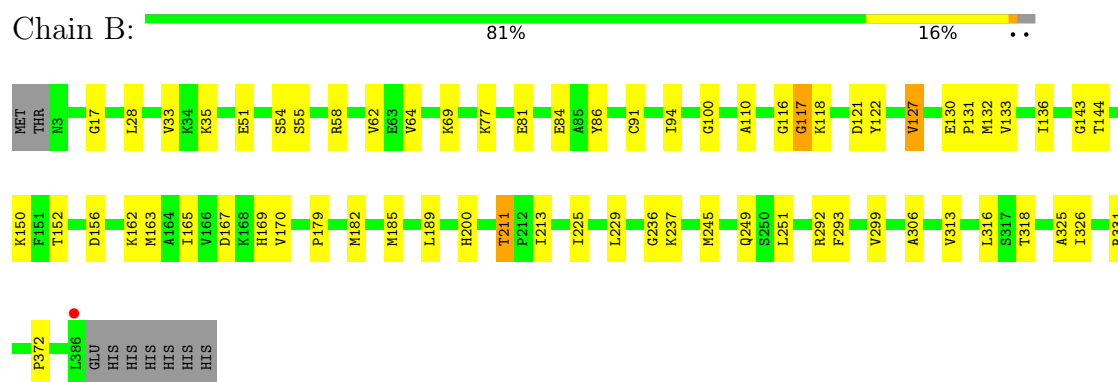
### 3 Residue-property plots [i](#)

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.

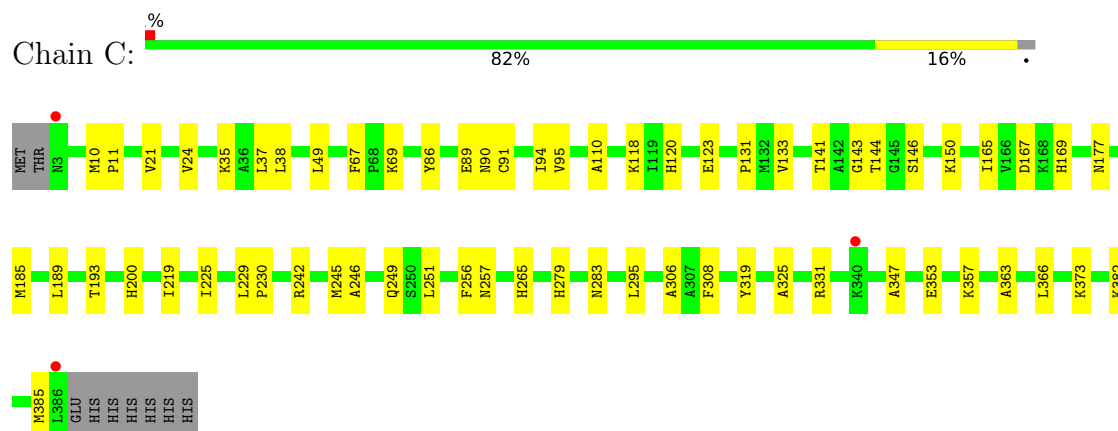
- Molecule 1: NAD-dependent methanol dehydrogenase



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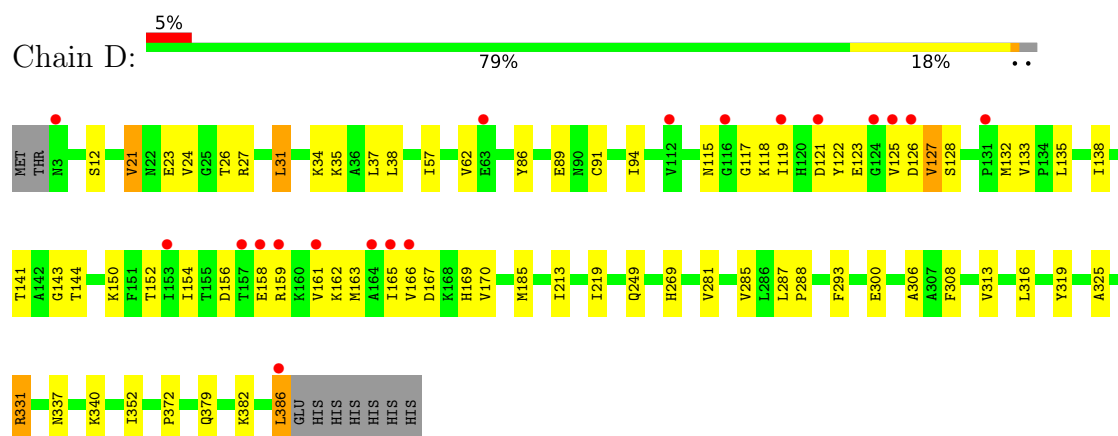


- Molecule 1: NAD-dependent methanol dehydrogenase





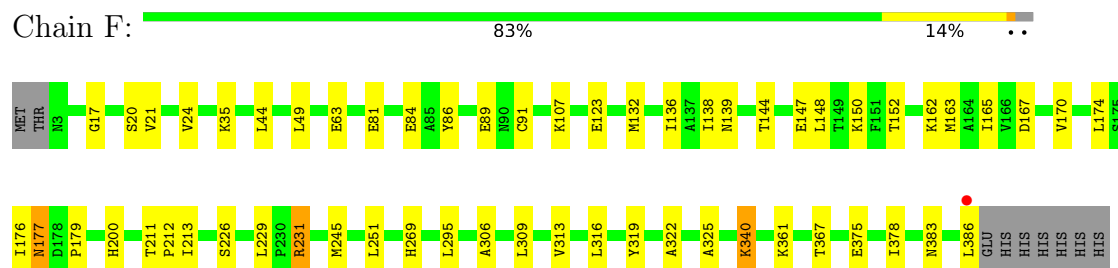
- Molecule 1: NAD-dependent methanol dehydrogenase



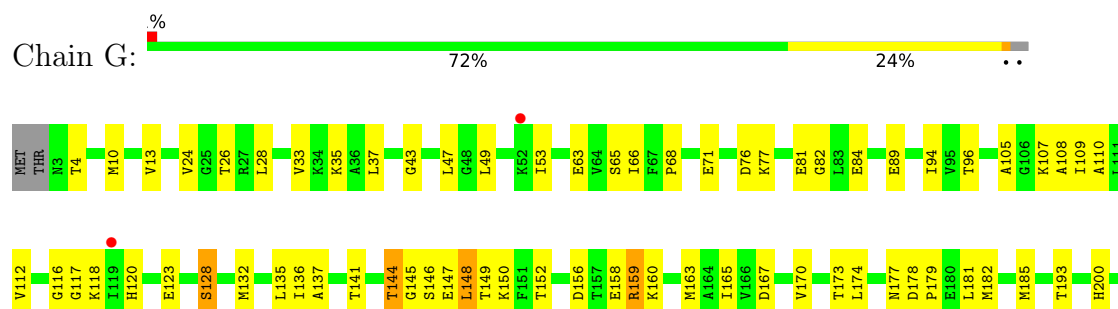
- Molecule 1: NAD-dependent methanol dehydrogenase



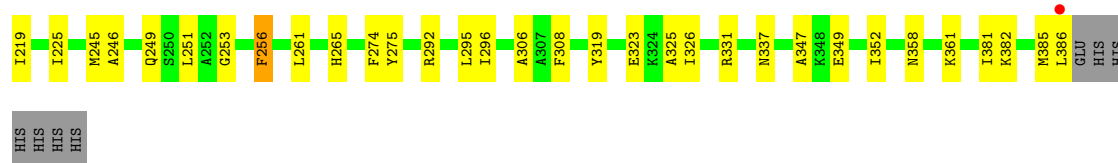
- Molecule 1: NAD-dependent methanol dehydrogenase



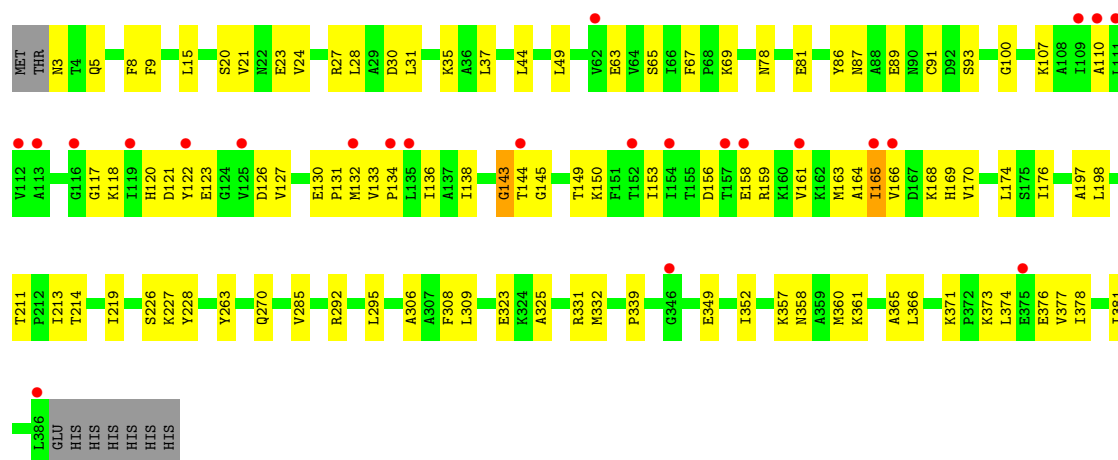
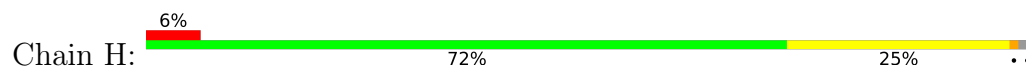
- Molecule 1: NAD-dependent methanol dehydrogenase



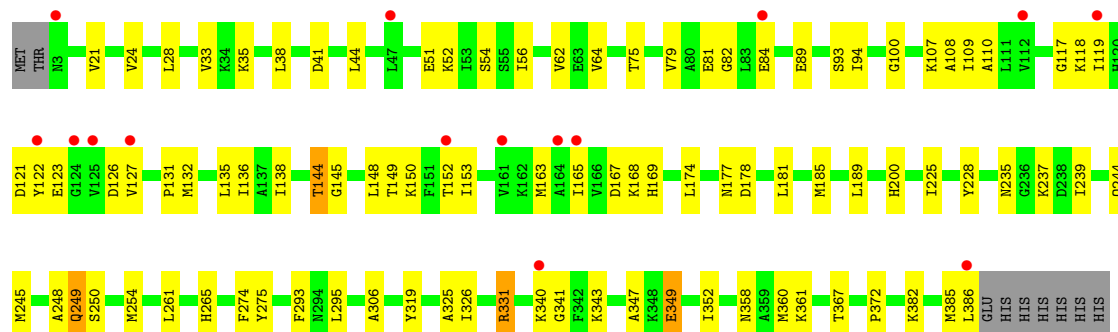
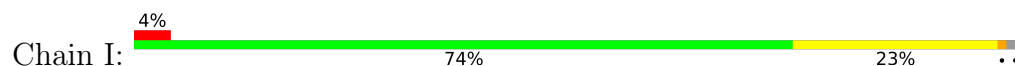




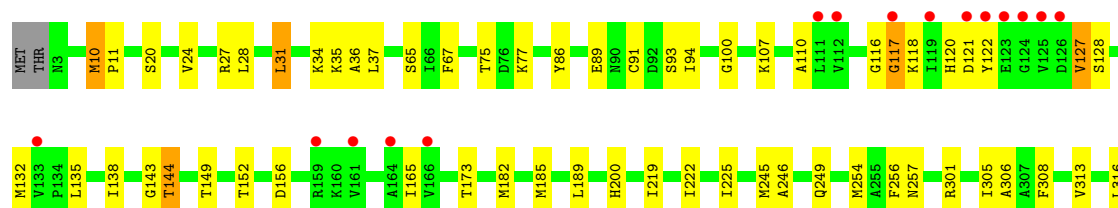
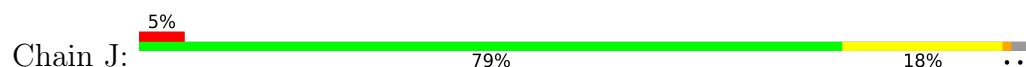
• Molecule 1: NAD-dependent methanol dehydrogenase



• Molecule 1: NAD-dependent methanol dehydrogenase



• Molecule 1: NAD-dependent methanol dehydrogenase









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.33Å 203.53Å 254.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.21 – 2.80 39.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.21-2.80) 99.9 (39.21-2.80)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.200 , 0.246 0.200 , 0.246	Depositor DCC
$R_{free}$ test set	5442 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.38	0/2892	0.69	1/3920 (0.0%)
1	B	0.39	0/2892	0.73	3/3920 (0.1%)
1	C	0.39	0/2892	0.74	2/3920 (0.1%)
1	D	0.40	0/2892	0.83	3/3920 (0.1%)
1	E	0.38	0/2892	0.78	1/3920 (0.0%)
1	F	0.36	0/2892	0.71	2/3920 (0.1%)
1	G	0.39	0/2892	0.79	3/3920 (0.1%)
1	H	0.40	0/2892	0.78	1/3920 (0.0%)
1	I	0.39	0/2892	0.81	2/3920 (0.1%)
1	J	0.41	0/2892	0.84	3/3920 (0.1%)
All	All	0.39	0/28920	0.77	21/39200 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	2
1	F	0	1
1	G	0	2
1	I	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	231	ARG	CA-CB-CG	7.31	128.72	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	371	LYS	CB-CG-CD	6.30	125.79	111.30
1	B	77	LYS	CB-CG-CD	-6.26	96.89	111.30
1	I	349	GLU	N-CA-CB	-6.08	100.85	110.22
1	A	157	THR	OG1-CB-CG2	-5.83	97.64	109.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	GLU	Sidechain
1	E	159	ARG	Sidechain
1	E	349	GLU	Mainchain
1	F	231	ARG	Sidechain
1	G	24	VAL	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2847	0	2898	32	0
1	B	2847	0	2898	45	0
1	C	2847	0	2898	37	0
1	D	2847	0	2898	47	0
1	E	2847	0	2898	63	0
1	F	2847	0	2898	39	0
1	G	2847	0	2898	68	0
1	H	2847	0	2898	71	0
1	I	2847	0	2898	61	0
1	J	2847	0	2898	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	0	0	0
4	B	9	0	0	1	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	1	0
All	All	28512	0	28980	496	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 9.

The worst 5 of 496 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:122:TYR:HA	1:I:127:VAL:HG21	1.40	1.00
1:H:110:ALA:HB3	1:H:132:MET:HE3	1.47	0.97
1:C:144:THR:HG22	1:C:146:SER:H	1.30	0.95
1:F:211:THR:HG22	1:F:213:ILE:H	1.36	0.90
1:G:120:HIS:HA	1:G:163:MET:HE1	1.55	0.89

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	382/393 (97%)	373 (98%)	8 (2%)	1 (0%)	37 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	382/393 (97%)	372 (97%)	9 (2%)	1 (0%)	37	67
1	C	382/393 (97%)	370 (97%)	12 (3%)	0	100	100
1	D	382/393 (97%)	368 (96%)	12 (3%)	2 (0%)	25	56
1	E	382/393 (97%)	365 (96%)	16 (4%)	1 (0%)	37	67
1	F	382/393 (97%)	374 (98%)	8 (2%)	0	100	100
1	G	382/393 (97%)	370 (97%)	10 (3%)	2 (0%)	25	56
1	H	382/393 (97%)	368 (96%)	12 (3%)	2 (0%)	25	56
1	I	382/393 (97%)	370 (97%)	10 (3%)	2 (0%)	25	56
1	J	382/393 (97%)	370 (97%)	9 (2%)	3 (1%)	16	44
All	All	3820/3930 (97%)	3700 (97%)	106 (3%)	14 (0%)	30	61

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	117	GLY
1	D	117	GLY
1	E	117	GLY
1	G	117	GLY
1	G	144	THR

### 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	299/308 (97%)	295 (99%)	4 (1%)	65	88
1	B	299/308 (97%)	296 (99%)	3 (1%)	73	91
1	C	299/308 (97%)	295 (99%)	4 (1%)	65	88
1	D	299/308 (97%)	292 (98%)	7 (2%)	45	78
1	E	299/308 (97%)	293 (98%)	6 (2%)	50	81
1	F	299/308 (97%)	294 (98%)	5 (2%)	56	84
1	G	299/308 (97%)	290 (97%)	9 (3%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	299/308 (97%)	291 (97%)	8 (3%)	40	74
1	I	299/308 (97%)	293 (98%)	6 (2%)	50	81
1	J	299/308 (97%)	295 (99%)	4 (1%)	65	88
All	All	2990/3080 (97%)	2934 (98%)	56 (2%)	52	82

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	367	THR
1	J	386	LEU
1	G	295	LEU
1	J	128	SER
1	I	177	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	177	ASN
1	H	379	GLN
1	J	294	ASN
1	H	270	GLN
1	I	276	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 oligosaccharides in this entry.



## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	384/393 (97%)	-0.63	2 (0%) 87 83	17, 29, 47, 73	0
1	B	384/393 (97%)	-0.52	1 (0%) 90 87	15, 30, 52, 73	0
1	C	384/393 (97%)	-0.42	3 (0%) 82 77	16, 32, 59, 78	0
1	D	384/393 (97%)	0.10	19 (4%) 36 28	21, 42, 79, 102	0
1	E	384/393 (97%)	-0.16	2 (0%) 87 83	25, 44, 69, 83	0
1	F	384/393 (97%)	-0.34	1 (0%) 90 87	22, 40, 62, 77	0
1	G	384/393 (97%)	0.20	3 (0%) 82 77	26, 50, 73, 95	0
1	H	384/393 (97%)	0.54	24 (6%) 27 21	33, 61, 101, 120	0
1	I	384/393 (97%)	0.37	15 (3%) 44 36	32, 59, 88, 99	0
1	J	384/393 (97%)	0.28	18 (4%) 37 30	27, 54, 91, 106	0
All	All	3840/3930 (97%)	-0.06	88 (2%) 61 52	15, 43, 85, 120	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	386	LEU	5.3
1	J	119	ILE	4.2
1	H	166	VAL	4.1
1	I	386	LEU	4.0
1	D	159	ARG	3.9

### 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 [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

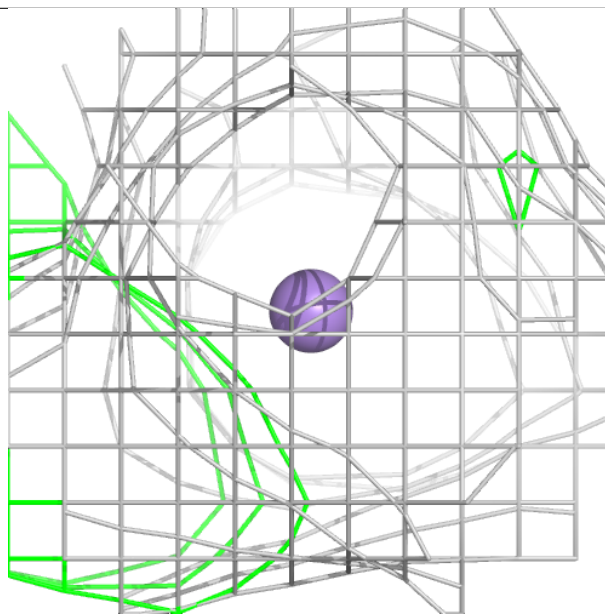
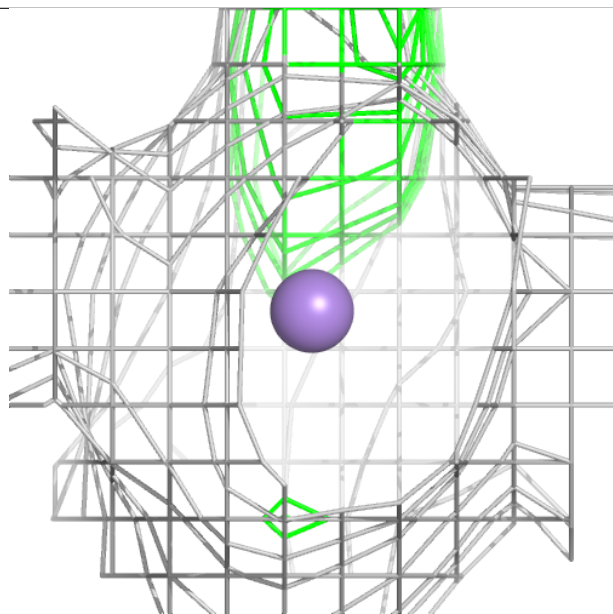
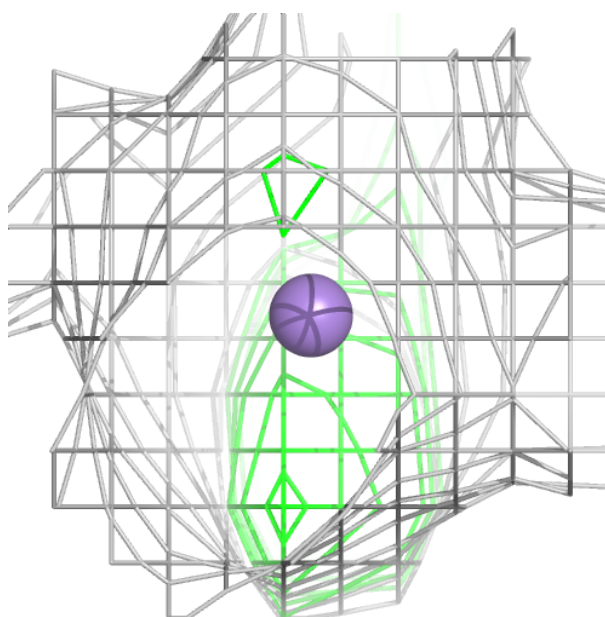
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MN	D	401	1/1	0.96	0.05	36,36,36,36	0
2	MN	E	401	1/1	0.96	0.04	43,43,43,43	0
3	NA	A	402	1/1	0.97	0.20	41,41,41,41	0
2	MN	C	401	1/1	0.98	0.03	29,29,29,29	0
2	MN	F	401	1/1	0.98	0.04	31,31,31,31	0
2	MN	G	401	1/1	0.98	0.03	44,44,44,44	0
2	MN	I	401	1/1	0.98	0.04	54,54,54,54	0
2	MN	J	401	1/1	0.98	0.02	43,43,43,43	0
2	MN	B	401	1/1	0.98	0.04	26,26,26,26	0
2	MN	H	401	1/1	0.99	0.05	62,62,62,62	0
2	MN	A	401	1/1	0.99	0.02	19,19,19,19	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 D 401:**

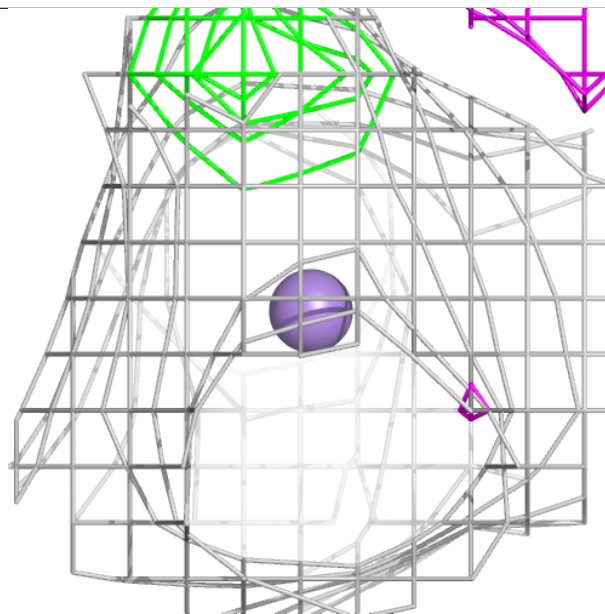
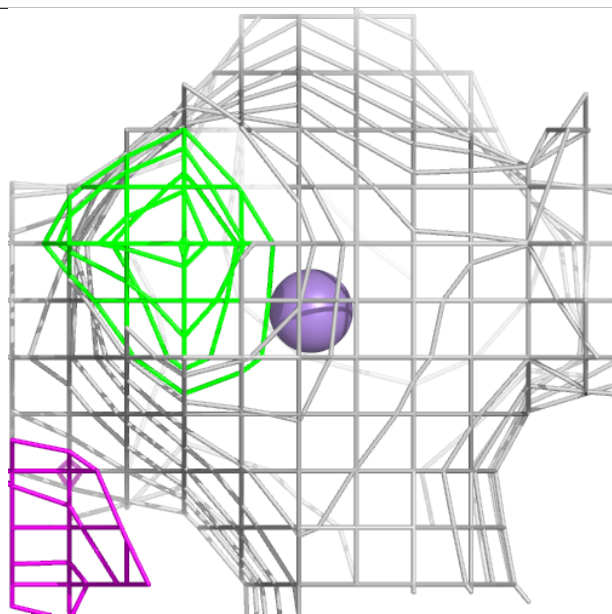
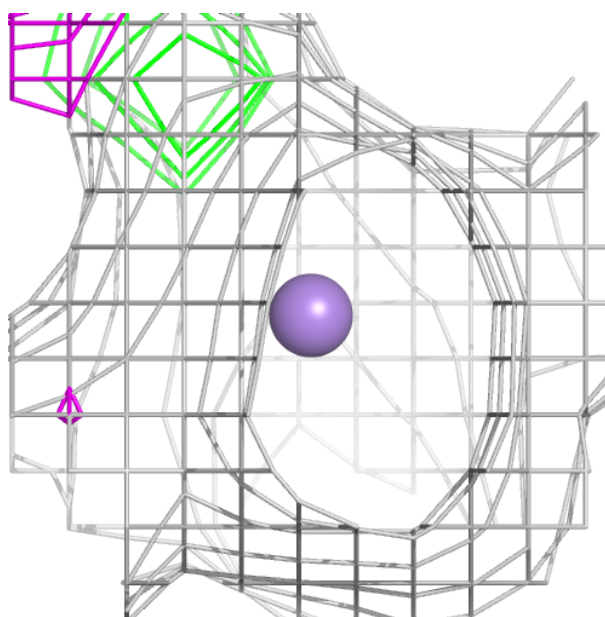
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN E 401:**

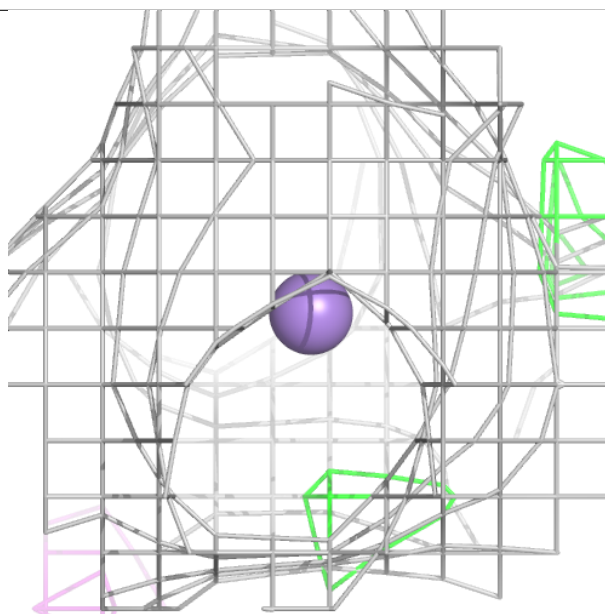
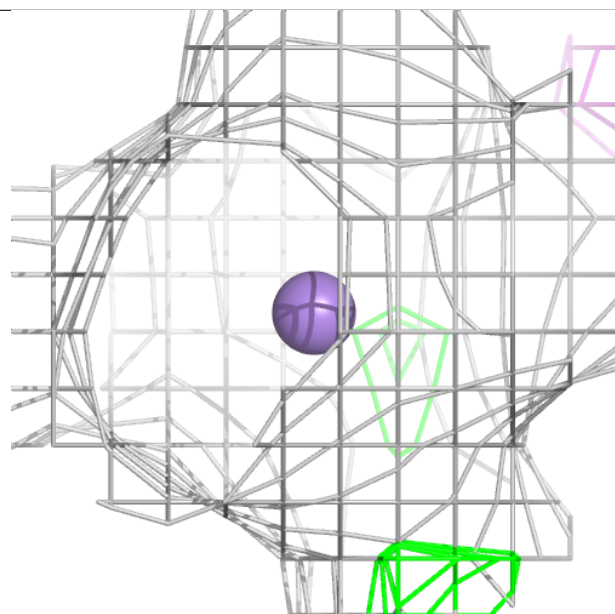
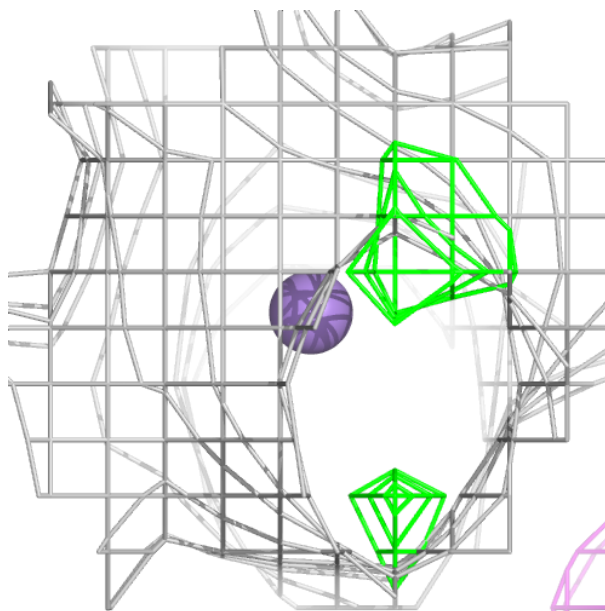
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN C 401:**

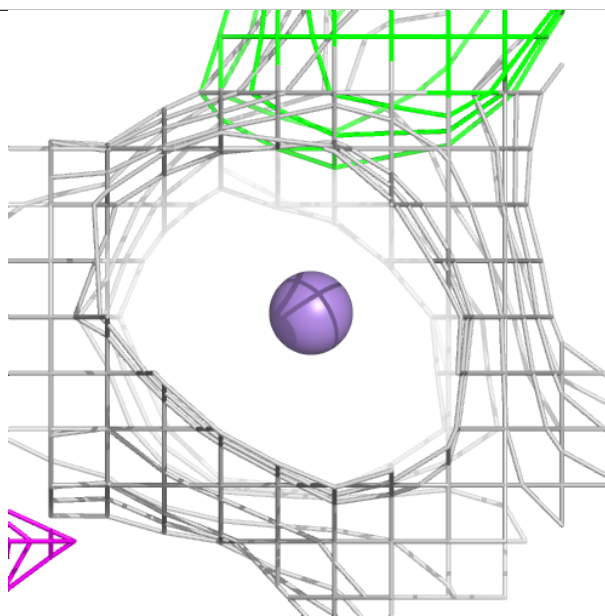
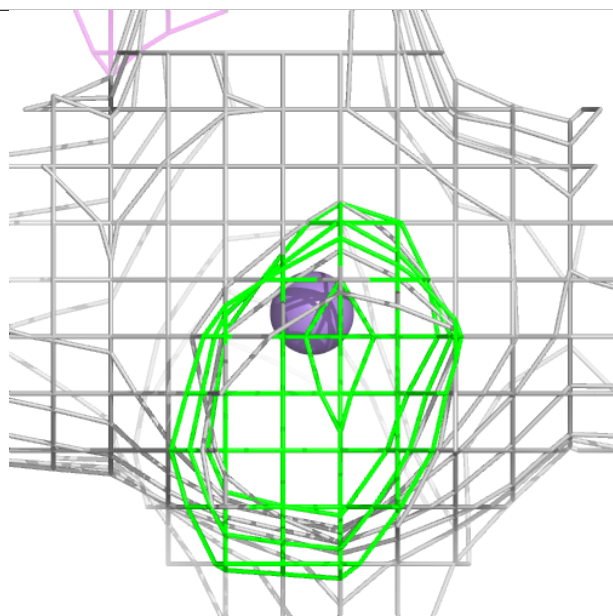
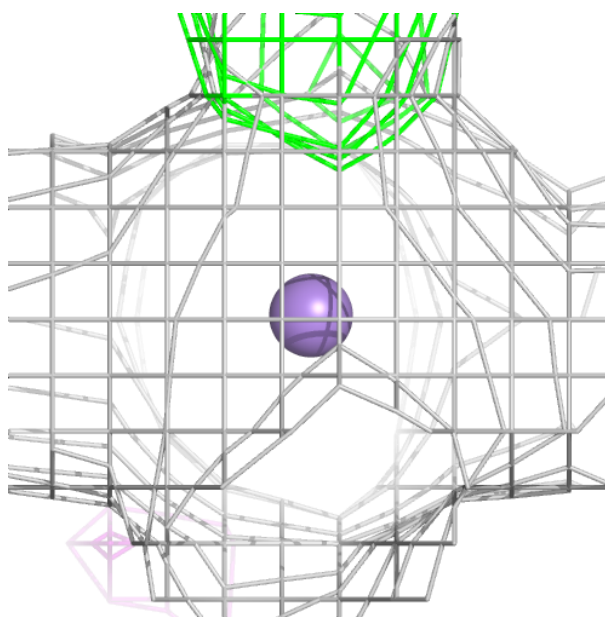
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN F 401:**

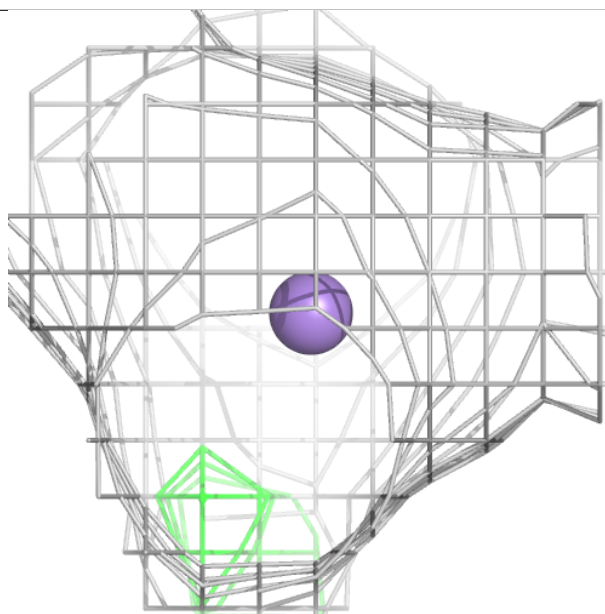
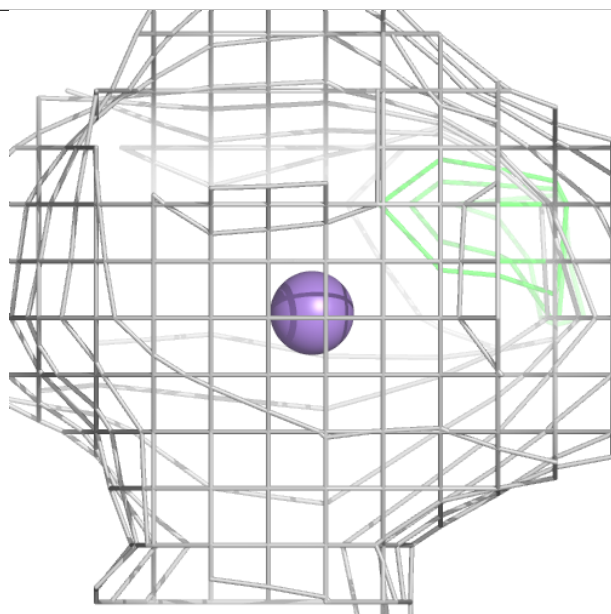
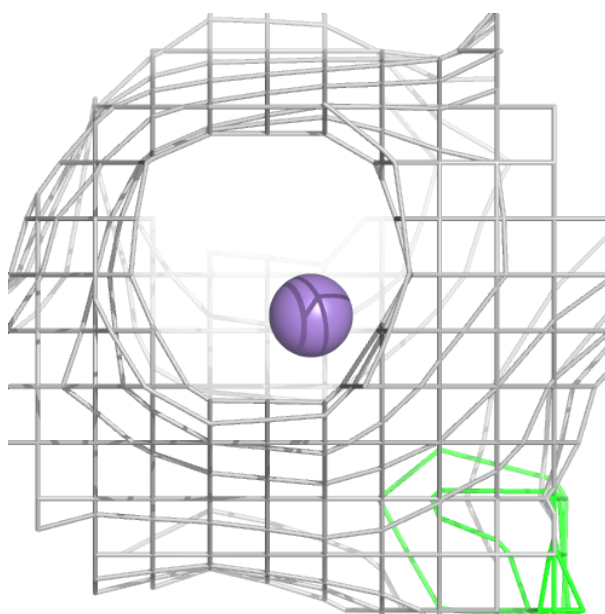
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)





**Electron density around MN G 401:**

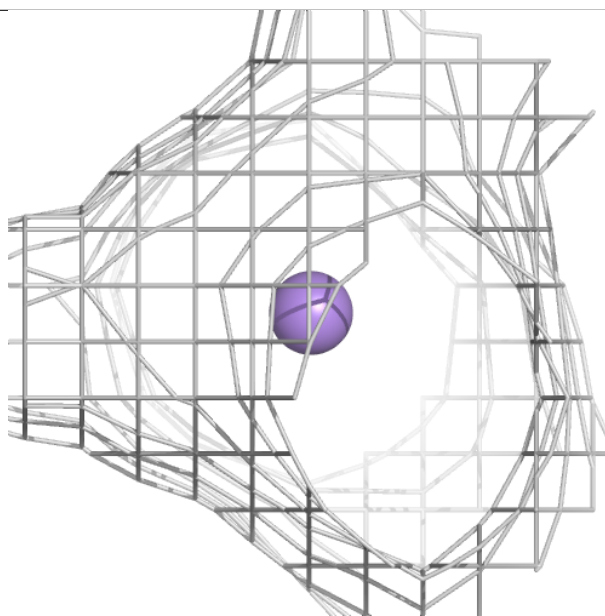
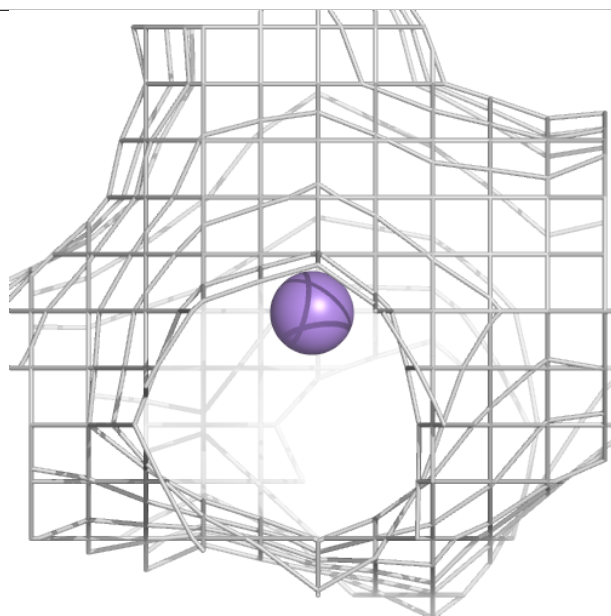
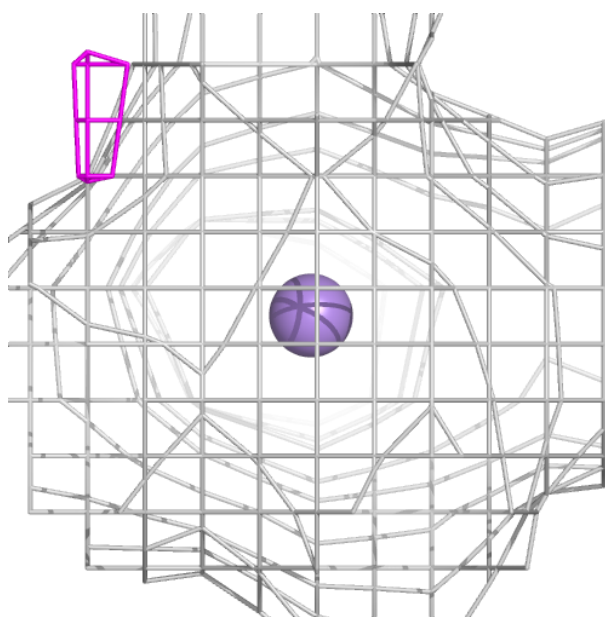
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN I 401:**

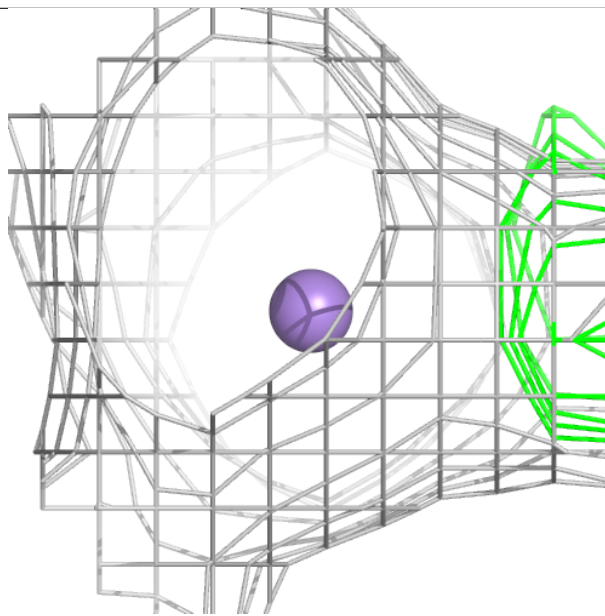
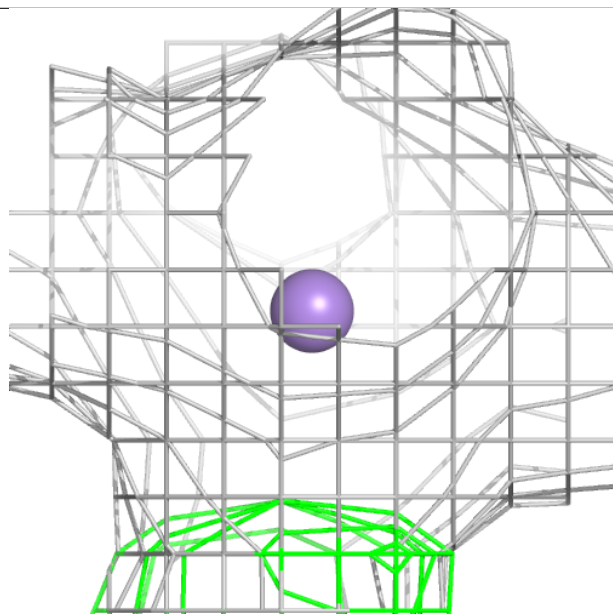
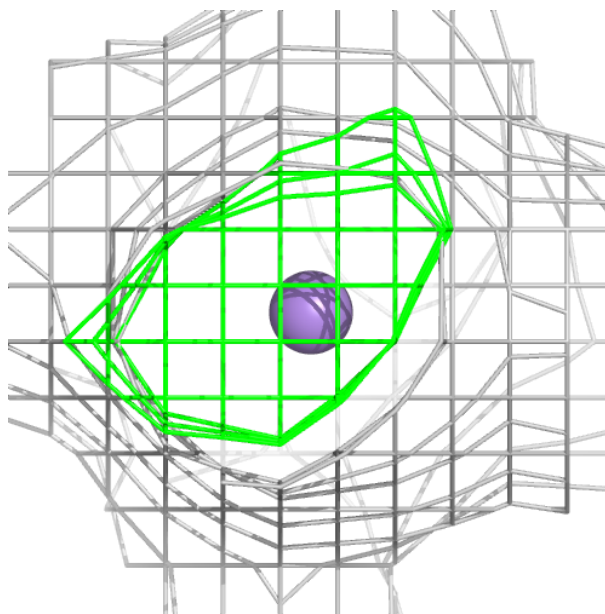
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN J 401:**

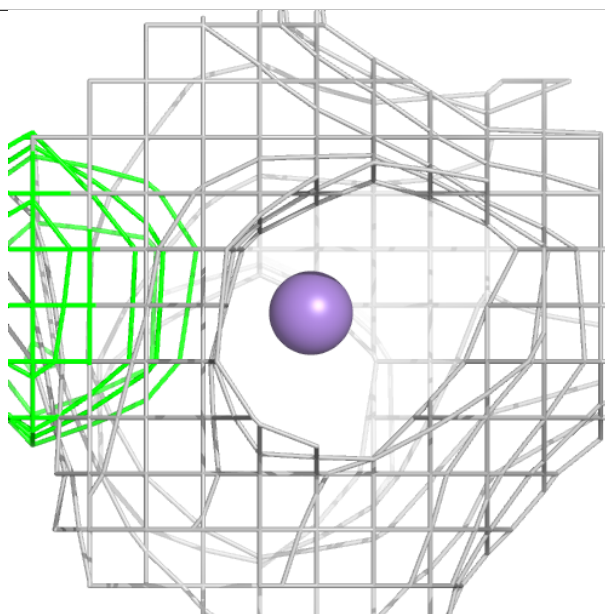
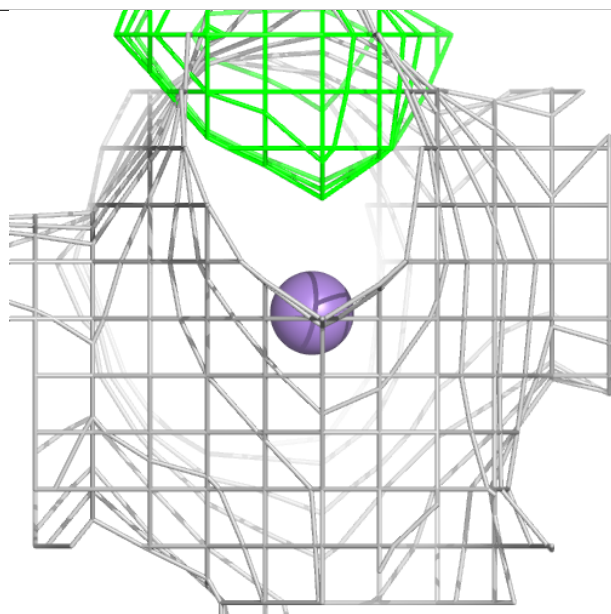
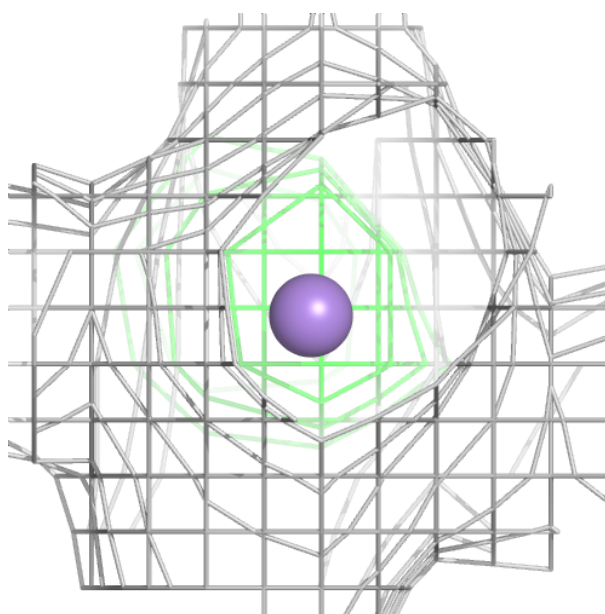
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN B 401:**

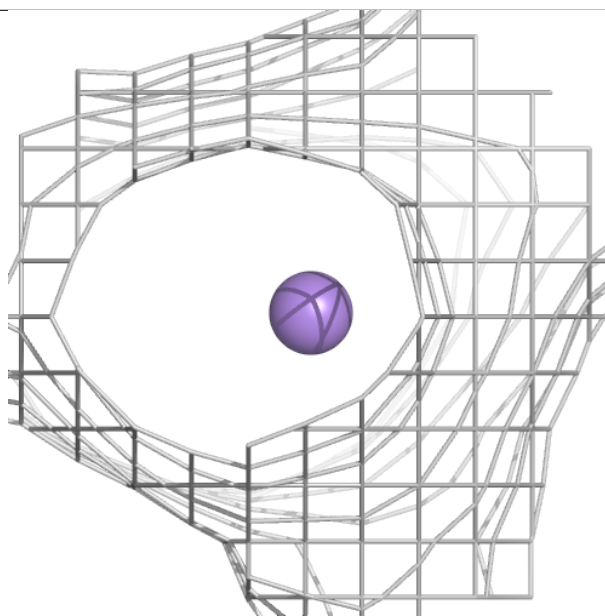
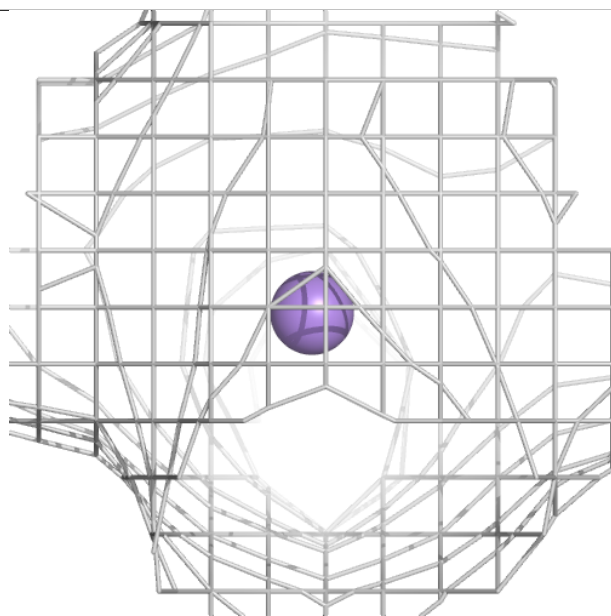
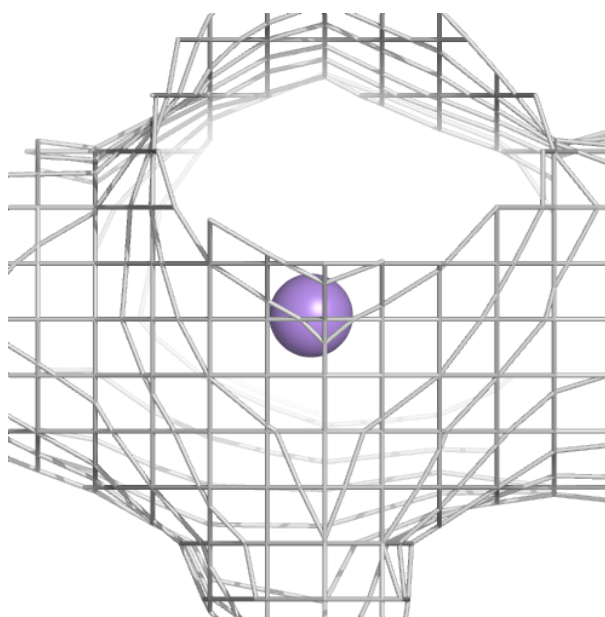
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN H 401:**

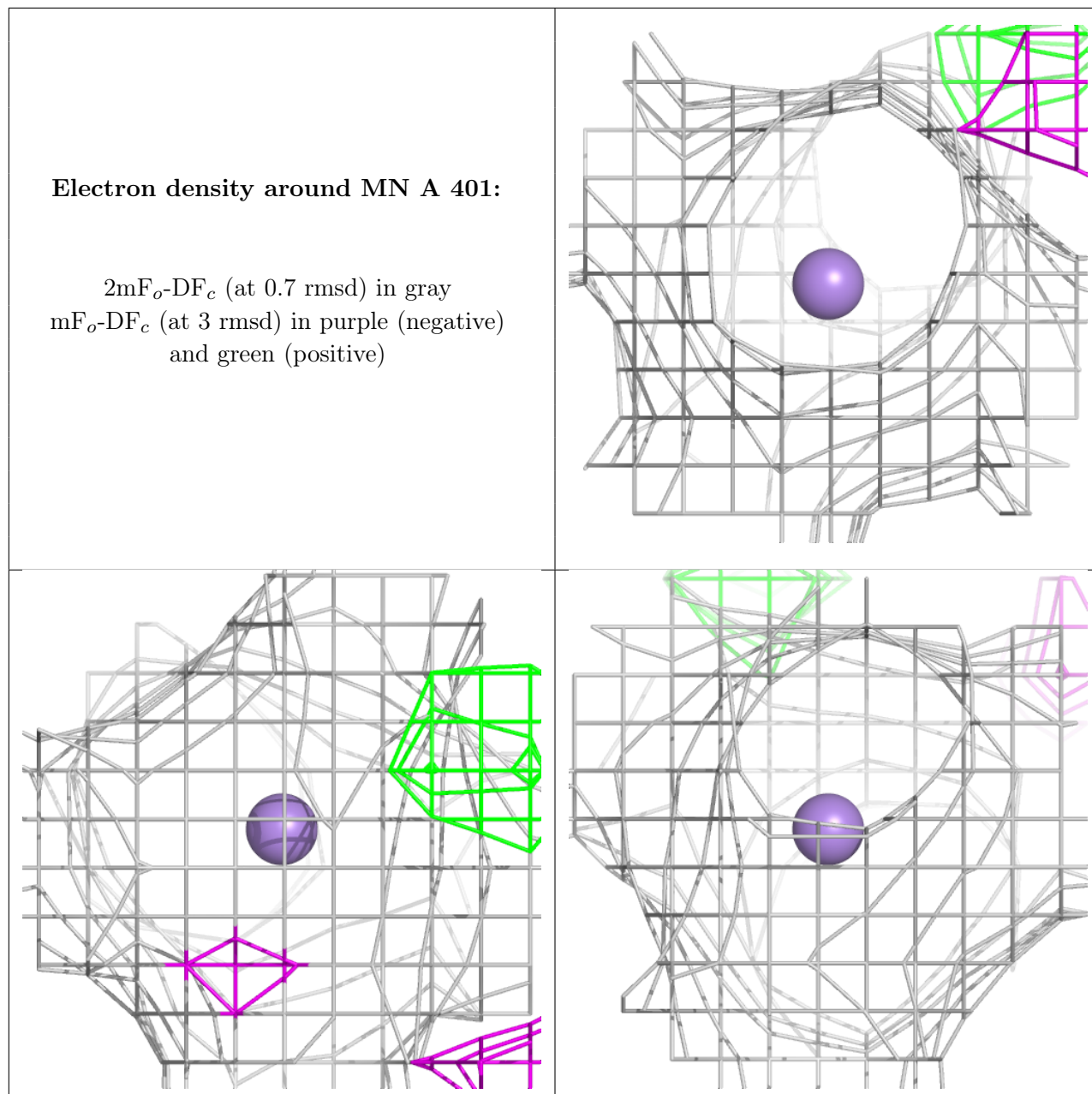
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.