



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 07:36 AM JST

PDB ID : 6L9I
Title : Crystal Structure of Lactobacillus farciminis Oxalate Decarboxylase Formate Complex
Authors : Wu, F.; Cheng, L.K.; Wang, C.Y.
Deposited on : 2019-11-10
Resolution : 2.79 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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

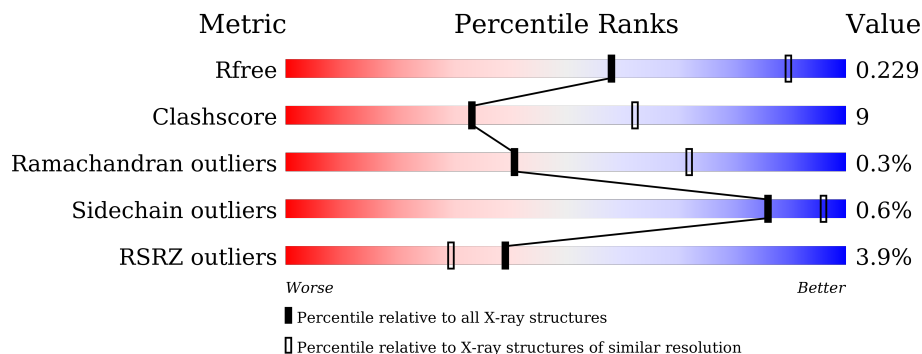
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 ≥ 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	360	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 75% 18% • 6%</p>
1	B	360	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 74% 19% • 6%</p>
1	C	360	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 73% 20% • 6%</p>
1	D	360	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 71% 22% • 6%</p>
1	E	360	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 78% 16% • 6%</p>
1	F	360	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 76% 18% 6%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMT	D	401	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16298 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 Oxalate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2670	1714	447	501	8	4	0	0
1	B	338	2670	1714	447	501	8	4	0	0
1	C	338	2670	1714	447	501	8	4	0	0
1	D	338	2670	1714	447	501	8	4	0	0
1	E	338	2670	1714	447	501	8	4	0	0
1	F	338	2670	1714	447	501	8	4	0	0

There are 48 discrepancies between the modelled and reference sequences:

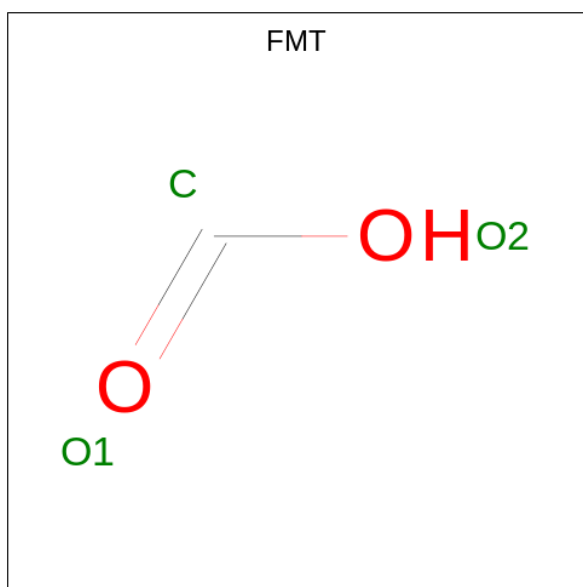
Chain	Residue	Modelled	Actual	Comment	Reference
A	374	LEU	-	expression tag	UNP A0A0H4LHD1
A	375	GLU	-	expression tag	UNP A0A0H4LHD1
A	376	HIS	-	expression tag	UNP A0A0H4LHD1
A	377	HIS	-	expression tag	UNP A0A0H4LHD1
A	378	HIS	-	expression tag	UNP A0A0H4LHD1
A	379	HIS	-	expression tag	UNP A0A0H4LHD1
A	380	HIS	-	expression tag	UNP A0A0H4LHD1
A	381	HIS	-	expression tag	UNP A0A0H4LHD1
B	374	LEU	-	expression tag	UNP A0A0H4LHD1
B	375	GLU	-	expression tag	UNP A0A0H4LHD1
B	376	HIS	-	expression tag	UNP A0A0H4LHD1
B	377	HIS	-	expression tag	UNP A0A0H4LHD1
B	378	HIS	-	expression tag	UNP A0A0H4LHD1
B	379	HIS	-	expression tag	UNP A0A0H4LHD1
B	380	HIS	-	expression tag	UNP A0A0H4LHD1
B	381	HIS	-	expression tag	UNP A0A0H4LHD1
C	374	LEU	-	expression tag	UNP A0A0H4LHD1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	375	GLU	-	expression tag	UNP A0A0H4LHD1
C	376	HIS	-	expression tag	UNP A0A0H4LHD1
C	377	HIS	-	expression tag	UNP A0A0H4LHD1
C	378	HIS	-	expression tag	UNP A0A0H4LHD1
C	379	HIS	-	expression tag	UNP A0A0H4LHD1
C	380	HIS	-	expression tag	UNP A0A0H4LHD1
C	381	HIS	-	expression tag	UNP A0A0H4LHD1
D	374	LEU	-	expression tag	UNP A0A0H4LHD1
D	375	GLU	-	expression tag	UNP A0A0H4LHD1
D	376	HIS	-	expression tag	UNP A0A0H4LHD1
D	377	HIS	-	expression tag	UNP A0A0H4LHD1
D	378	HIS	-	expression tag	UNP A0A0H4LHD1
D	379	HIS	-	expression tag	UNP A0A0H4LHD1
D	380	HIS	-	expression tag	UNP A0A0H4LHD1
D	381	HIS	-	expression tag	UNP A0A0H4LHD1
E	374	LEU	-	expression tag	UNP A0A0H4LHD1
E	375	GLU	-	expression tag	UNP A0A0H4LHD1
E	376	HIS	-	expression tag	UNP A0A0H4LHD1
E	377	HIS	-	expression tag	UNP A0A0H4LHD1
E	378	HIS	-	expression tag	UNP A0A0H4LHD1
E	379	HIS	-	expression tag	UNP A0A0H4LHD1
E	380	HIS	-	expression tag	UNP A0A0H4LHD1
E	381	HIS	-	expression tag	UNP A0A0H4LHD1
F	374	LEU	-	expression tag	UNP A0A0H4LHD1
F	375	GLU	-	expression tag	UNP A0A0H4LHD1
F	376	HIS	-	expression tag	UNP A0A0H4LHD1
F	377	HIS	-	expression tag	UNP A0A0H4LHD1
F	378	HIS	-	expression tag	UNP A0A0H4LHD1
F	379	HIS	-	expression tag	UNP A0A0H4LHD1
F	380	HIS	-	expression tag	UNP A0A0H4LHD1
F	381	HIS	-	expression tag	UNP A0A0H4LHD1

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 3 1 2	0	0
2	B	1	Total C O 3 1 2	0	0
2	C	1	Total C O 3 1 2	0	0
2	D	1	Total C O 3 1 2	0	0
2	E	1	Total C O 3 1 2	0	0
2	F	1	Total C O 3 1 2	0	0

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

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

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

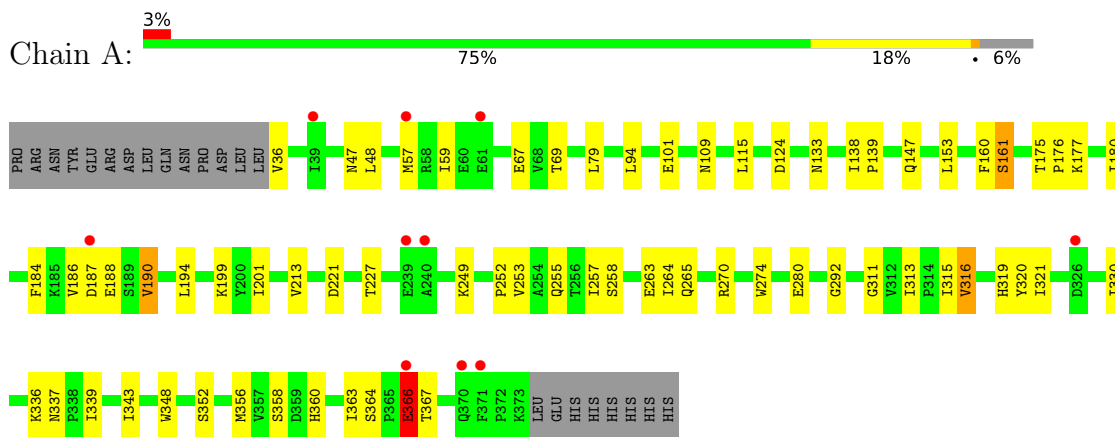
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	61	Total	O	0	0
			61	61		
4	C	39	Total	O	0	0
			39	39		
4	D	43	Total	O	0	0
			43	43		
4	E	35	Total	O	0	0
			35	35		
4	F	27	Total	O	0	0
			27	27		

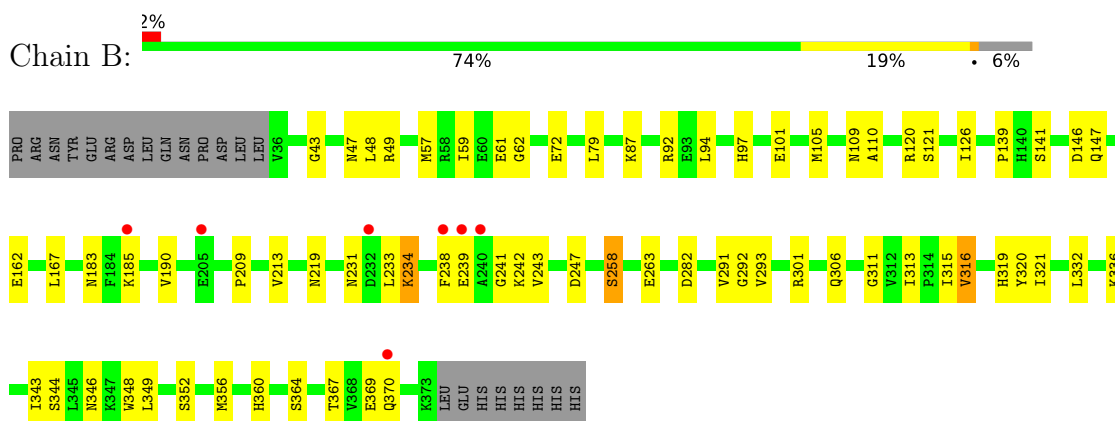
3 Residue-property plots [i](#)

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.

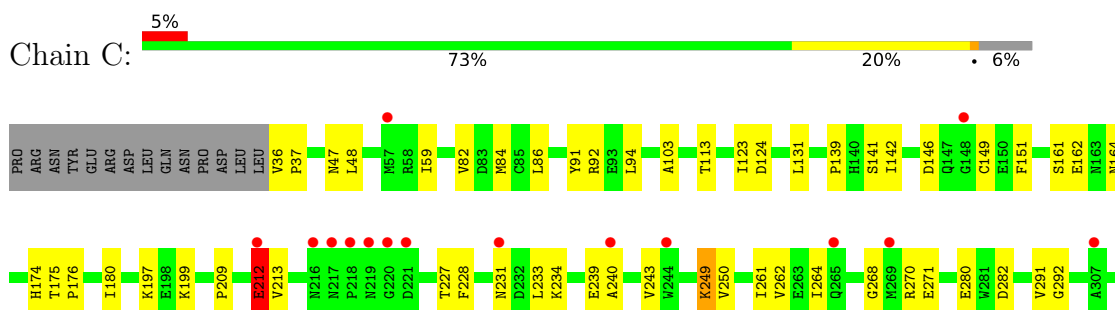
• Molecule 1: Oxalate decarboxylase



• Molecule 1: Oxalate decarboxylase

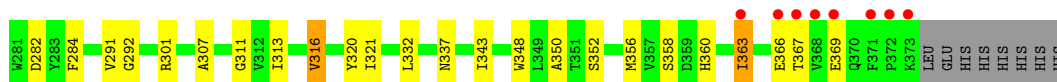
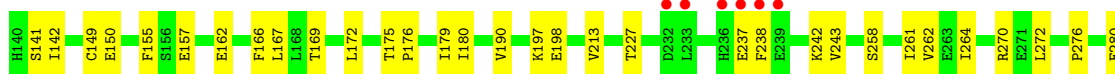


• Molecule 1: Oxalate decarboxylase

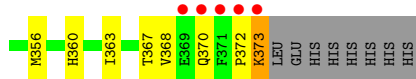
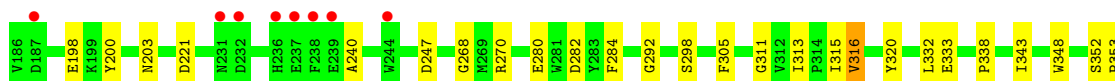
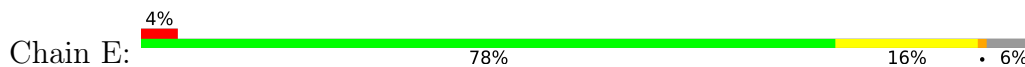




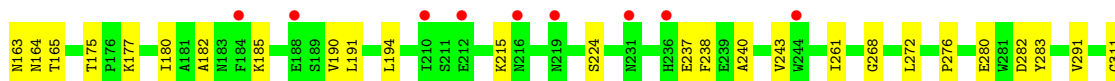
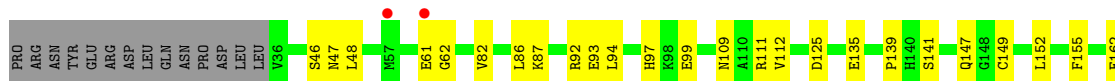
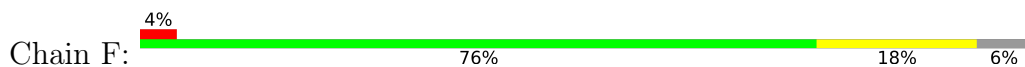
• Molecule 1: Oxalate decarboxylase



• Molecule 1: Oxalate decarboxylase



• Molecule 1: Oxalate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.96Å 122.84Å 115.22Å 90.00° 92.47° 90.00°	Depositor
Resolution (Å)	48.00 – 2.79 48.00 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.00-2.79) 96.9 (48.00-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.197 , 0.229 0.197 , 0.229	Depositor DCC
R_{free} test set	3104 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtrriage
Anisotropy	0.690	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.058 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16298	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: FMT, 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	0.42	2/2751 (0.1%)	0.64	4/3750 (0.1%)
1	B	0.39	1/2751 (0.0%)	0.68	7/3750 (0.2%)
1	C	0.39	2/2751 (0.1%)	0.64	6/3750 (0.2%)
1	D	0.38	0/2751	0.64	3/3750 (0.1%)
1	E	0.36	0/2751	0.63	5/3750 (0.1%)
1	F	0.38	0/2751	0.62	1/3750 (0.0%)
All	All	0.39	5/16506 (0.0%)	0.64	26/22500 (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	B	0	1
1	C	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	GLU	CD-OE1	7.82	1.34	1.25
1	B	234	LYS	CG-CD	5.94	1.72	1.52
1	C	212	GLU	CD-OE2	5.88	1.32	1.25
1	A	190	VAL	CB-CG1	-5.73	1.40	1.52
1	C	249	LYS	CD-CE	5.68	1.65	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	373	LYS	CD-CE-NZ	-10.48	87.59	111.70
1	B	234	LYS	CA-CB-CG	9.71	134.75	113.40
1	B	234	LYS	CD-CE-NZ	-9.64	89.53	111.70
1	B	234	LYS	CB-CG-CD	9.29	135.75	111.60
1	D	98	LYS	CD-CE-NZ	-8.54	92.05	111.70
1	E	49	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	366	GLU	CG-CD-OE2	-8.30	101.70	118.30
1	B	233	LEU	C-N-CA	-8.21	101.17	121.70
1	E	49	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	D	363	ILE	CG1-CB-CG2	-7.53	94.84	111.40
1	C	234	LYS	CD-CE-NZ	-7.51	94.44	111.70
1	C	231	ASN	CB-CA-C	-7.25	95.90	110.40
1	A	366	GLU	CG-CD-OE1	6.66	131.61	118.30
1	F	61	GLU	CA-CB-CG	6.58	127.88	113.40
1	B	239	GLU	CA-CB-CG	6.29	127.23	113.40
1	B	234	LYS	CG-CD-CE	6.22	130.56	111.90
1	A	187	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	E	185	LYS	CB-CG-CD	6.08	127.42	111.60
1	C	233	LEU	C-N-CA	-5.94	106.86	121.70
1	D	363	ILE	CA-CB-CG1	5.51	121.47	111.00
1	B	61	GLU	CA-CB-CG	5.49	125.47	113.40
1	C	234	LYS	CB-CG-CD	-5.44	97.45	111.60
1	A	161	SER	N-CA-CB	5.41	118.61	110.50
1	C	249	LYS	CA-CB-CG	-5.33	101.68	113.40
1	C	249	LYS	CG-CD-CE	-5.29	96.03	111.90
1	E	373	LYS	CA-CB-CG	-5.16	102.05	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	GLU	Sidechain
1	B	231	ASN	Sidechain
1	C	212	GLU	Sidechain

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	2670	0	2552	52	0
1	B	2670	0	2552	52	0
1	C	2670	0	2552	56	0
1	D	2670	0	2552	63	0
1	E	2670	0	2552	45	0
1	F	2670	0	2552	48	0
2	A	3	0	1	0	0
2	B	3	0	1	1	0
2	C	3	0	1	0	0
2	D	3	0	1	2	0
2	E	3	0	1	1	0
2	F	3	0	1	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	43	0	0	6	0
4	B	61	0	0	7	0
4	C	39	0	0	4	0
4	D	43	0	0	5	0
4	E	35	0	0	3	0
4	F	27	0	0	3	0
All	All	16298	0	15318	269	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.

All (269) 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:47:ASN:O	4:F:501:HOH:O	1.91	0.87
1:E:55:ALA:O	4:E:501:HOH:O	1.95	0.84
1:D:213:VAL:O	4:D:501:HOH:O	1.96	0.83
1:B:367:THR:O	1:B:370:GLN:HB2	1.82	0.80
1:B:349:LEU:O	4:B:501:HOH:O	2.05	0.74
1:E:198:GLU:OE2	4:E:502:HOH:O	2.04	0.74
1:E:221:ASP:OD1	4:E:503:HOH:O	2.06	0.72
1:D:237:GLU:HG3	1:D:238:PHE:N	2.03	0.71
1:A:221:ASP:OD1	4:A:501:HOH:O	2.09	0.71
1:B:242:LYS:NZ	4:B:505:HOH:O	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ILE:HG12	1:C:316:VAL:HG13	1.74	0.70
1:F:135:GLU:O	4:F:502:HOH:O	2.11	0.69
1:B:146:ASP:OD1	4:B:502:HOH:O	2.12	0.68
1:A:364:SER:HB2	1:A:366:GLU:HG2	1.74	0.68
1:B:238:PHE:HE1	1:B:243:VAL:HG23	1.57	0.68
1:B:49:ARG:NH1	4:B:504:HOH:O	2.27	0.68
1:A:352:SER:OG	4:A:502:HOH:O	2.11	0.68
1:B:94:LEU:HD21	1:C:356:MET:HE3	1.75	0.68
1:A:265:GLN:NE2	4:A:505:HOH:O	2.24	0.67
1:F:238:PHE:HE1	1:F:243:VAL:HG23	1.60	0.67
1:A:358:SER:OG	1:A:363:ILE:O	2.08	0.67
1:A:36:VAL:N	4:A:506:HOH:O	2.27	0.67
1:C:47:ASN:O	4:C:501:HOH:O	2.13	0.67
1:D:343:ILE:HD13	1:F:139:PRO:HD3	1.76	0.66
1:A:188:GLU:O	4:A:504:HOH:O	2.13	0.66
1:E:92:ARG:NH2	2:E:401:FMT:O2	2.30	0.64
1:C:261:ILE:HG12	1:C:332:LEU:HD22	1.79	0.63
1:D:358:SER:OG	1:D:363:ILE:O	2.13	0.63
1:C:36:VAL:N	4:C:508:HOH:O	2.31	0.63
1:C:249:LYS:HE3	1:C:339:ILE:HD12	1.80	0.63
1:D:237:GLU:OE1	1:D:242:LYS:HG2	1.99	0.62
1:C:291:VAL:HG22	1:C:321:ILE:HG12	1.81	0.62
1:D:261:ILE:HG12	1:D:332:LEU:HD22	1.81	0.62
1:D:49:ARG:NH1	4:D:509:HOH:O	2.33	0.62
1:B:306:GLN:NE2	4:B:510:HOH:O	2.31	0.61
1:C:199:LYS:NZ	1:E:360:HIS:O	2.30	0.61
1:A:67:GLU:OE1	1:A:161:SER:HB2	2.00	0.61
1:B:315:ILE:HG12	1:B:316:VAL:HG13	1.83	0.61
1:B:185:LYS:HD2	1:C:372:PRO:HG3	1.84	0.60
1:D:175:THR:HB	1:D:180:ILE:HD11	1.83	0.60
1:C:240:ALA:HB1	1:C:268:GLY:HA3	1.83	0.60
1:D:61:GLU:HG3	1:D:61:GLU:O	2.02	0.60
1:B:348:TRP:CE2	1:E:139:PRO:HB2	2.36	0.60
1:C:243:VAL:HG23	1:C:262:VAL:HG22	1.85	0.59
1:B:183:ASN:O	1:B:185:LYS:NZ	2.33	0.59
1:A:249:LYS:HE3	1:A:339:ILE:HD12	1.85	0.59
1:C:146:ASP:OD1	4:C:502:HOH:O	2.17	0.59
1:A:315:ILE:HG12	1:A:316:VAL:HG13	1.84	0.58
1:B:110:ALA:HB3	1:B:126:ILE:HD11	1.85	0.58
1:C:270:ARG:NH2	1:C:333:GLU:OE1	2.35	0.58
1:D:118:GLU:OE1	1:D:120:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:GLY:HA2	1:F:87:LYS:HD2	1.85	0.58
1:B:356:MET:HE3	1:E:94:LEU:HD21	1.85	0.57
1:C:209:PRO:HD2	1:C:212:GLU:OE1	2.04	0.57
1:B:247:ASP:HA	1:B:258:SER:HB2	1.87	0.57
1:F:92:ARG:HH22	1:F:165:THR:HG21	1.68	0.57
1:F:175:THR:HB	1:F:180:ILE:HD11	1.85	0.56
1:F:238:PHE:CE1	1:F:243:VAL:HG23	2.40	0.56
1:D:86:LEU:HB2	1:D:149:CYS:SG	2.46	0.56
1:D:115:LEU:O	1:D:139:PRO:HD2	2.06	0.56
1:C:59:ILE:HD11	1:D:37:PRO:HD2	1.86	0.56
1:A:47:ASN:HB2	1:B:72:GLU:HG3	1.88	0.55
1:D:101:GLU:HG3	1:D:155:PHE:CE2	2.41	0.55
1:E:61:GLU:HG2	1:E:203:ASN:ND2	2.22	0.55
1:C:91:TYR:CE1	1:E:356:MET:HG3	2.42	0.55
1:E:372:PRO:O	1:E:373:LYS:HG2	2.07	0.55
1:C:175:THR:HB	1:C:180:ILE:HD11	1.87	0.55
1:A:356:MET:HE3	1:D:94:LEU:HD21	1.89	0.54
1:A:315:ILE:HG21	1:D:98:LYS:HD2	1.90	0.54
1:B:190:VAL:HG11	1:C:367:THR:HG21	1.90	0.54
1:D:172:LEU:HD22	1:D:180:ILE:HD13	1.90	0.54
1:E:280:GLU:HB3	1:E:313:ILE:HB	1.88	0.54
1:D:258:SER:OG	1:D:337:ASN:O	2.21	0.54
1:E:372:PRO:C	1:E:373:LYS:HG2	2.27	0.54
1:F:240:ALA:HB1	1:F:268:GLY:HA3	1.90	0.54
1:B:352:SER:HB3	1:B:356:MET:HE2	1.90	0.54
1:A:57:MET:HG2	1:A:59:ILE:HG13	1.91	0.53
1:B:47:ASN:OD1	4:B:504:HOH:O	2.18	0.53
1:B:190:VAL:CG1	1:C:367:THR:HG21	2.38	0.53
1:A:366:GLU:HG3	1:A:367:THR:H	1.73	0.53
1:B:282:ASP:HA	1:B:332:LEU:O	2.09	0.53
1:F:280:GLU:HB3	1:F:313:ILE:HB	1.90	0.53
1:E:292:GLY:HA3	1:E:320:TYR:CE1	2.44	0.53
1:E:352:SER:HB3	1:E:356:MET:HE2	1.89	0.53
1:A:124:ASP:OD2	1:A:227:THR:HG21	2.08	0.53
1:A:139:PRO:HD3	1:F:343:ILE:HD13	1.89	0.53
1:C:124:ASP:OD2	1:C:227:THR:HG21	2.08	0.53
1:D:157:GLU:OE2	4:D:504:HOH:O	2.19	0.53
1:A:264:ILE:HD11	1:A:270:ARG:HB2	1.91	0.53
1:A:366:GLU:HG3	1:A:367:THR:N	2.24	0.53
1:A:258:SER:OG	1:A:337:ASN:O	2.15	0.53
1:C:161:SER:HB3	1:C:164:ASN:HD22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLU:HG3	1:F:47:ASN:HB2	1.91	0.53
1:E:97:HIS:CE1	1:E:101:GLU:HG3	2.44	0.52
1:A:348:TRP:CE2	1:D:139:PRO:HB2	2.44	0.52
1:C:280:GLU:HB3	1:C:313:ILE:HB	1.91	0.52
1:F:291:VAL:HG22	1:F:321:ILE:HG12	1.92	0.52
1:F:353:PRO:HD2	1:F:356:MET:HE2	1.91	0.52
1:B:43:GLY:O	1:B:301:ARG:NH2	2.40	0.51
1:C:271:GLU:OE1	4:C:503:HOH:O	2.19	0.51
1:D:367:THR:HG21	1:F:190:VAL:CG1	2.39	0.51
1:F:177:LYS:HE3	1:F:191:LEU:HB2	1.92	0.51
1:F:272:LEU:HD23	1:F:320:TYR:HB3	1.92	0.51
1:E:97:HIS:HE1	1:E:101:GLU:HG3	1.74	0.51
1:F:224:SER:OG	4:F:503:HOH:O	2.12	0.51
1:B:79:LEU:HD21	1:B:336:LYS:HB2	1.93	0.51
1:A:263:GLU:HG3	1:A:330:ILE:HG12	1.93	0.51
1:A:343:ILE:HD12	1:D:139:PRO:HD3	1.91	0.51
1:D:264:ILE:HD11	1:D:270:ARG:HB2	1.92	0.51
1:D:291:VAL:HG22	1:D:321:ILE:HG23	1.93	0.51
1:B:97:HIS:CE1	1:B:101:GLU:HG3	2.45	0.51
1:C:103:ALA:O	1:C:131:LEU:HA	2.11	0.51
1:C:176:PRO:O	1:C:180:ILE:HG13	2.11	0.50
1:F:86:LEU:HB2	1:F:149:CYS:SG	2.52	0.50
1:F:97:HIS:NE2	1:F:155:PHE:HE2	2.09	0.50
1:C:94:LEU:HD23	1:C:141:SER:HB3	1.93	0.49
1:D:280:GLU:HB3	1:D:313:ILE:HB	1.94	0.49
1:E:282:ASP:HA	1:E:332:LEU:O	2.12	0.49
1:E:284:PHE:CE1	1:E:305:PHE:CD2	3.00	0.49
1:C:213:VAL:HG22	1:E:353:PRO:HB3	1.94	0.49
1:C:352:SER:HB3	1:C:356:MET:CE	2.43	0.49
1:D:162:GLU:OE1	2:D:401:FMT:O2	2.29	0.49
1:B:105:MET:SD	1:B:126:ILE:HD13	2.51	0.49
1:B:139:PRO:HD3	1:C:343:ILE:HD13	1.95	0.49
1:E:94:LEU:HD23	1:E:141:SER:HB3	1.94	0.49
1:F:261:ILE:HG12	1:F:332:LEU:HD23	1.95	0.49
1:A:175:THR:HB	1:A:180:ILE:HD11	1.93	0.49
1:B:343:ILE:HD12	1:E:139:PRO:HD3	1.94	0.49
1:C:86:LEU:HB2	1:C:149:CYS:SG	2.52	0.49
1:A:280:GLU:HB3	1:A:313:ILE:HB	1.96	0.48
1:C:139:PRO:HD3	1:E:343:ILE:HD13	1.95	0.48
1:F:163:ASN:C	1:F:164:ASN:HD22	2.15	0.48
1:B:139:PRO:HB2	1:C:348:TRP:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:CYS:HB2	1:D:150:GLU:HG3	1.95	0.48
1:B:92:ARG:HH12	1:B:167:LEU:HD21	1.77	0.48
1:E:270:ARG:NH2	1:E:333:GLU:OE1	2.45	0.48
1:B:48:LEU:O	1:B:311:GLY:HA2	2.14	0.48
1:A:213:VAL:HG13	1:F:353:PRO:HB3	1.96	0.48
1:D:352:SER:HB3	1:D:356:MET:HE2	1.96	0.48
1:B:352:SER:O	4:B:501:HOH:O	2.20	0.47
1:D:356:MET:HE3	1:F:94:LEU:HD11	1.96	0.47
1:F:82:VAL:HG11	1:F:162:GLU:HG3	1.95	0.47
1:C:197:LYS:HB3	1:C:197:LYS:HE2	1.52	0.47
1:A:360:HIS:CD2	1:D:93:GLU:HG3	2.49	0.47
1:D:92:ARG:HH12	1:D:167:LEU:HD21	1.79	0.47
1:E:240:ALA:HB1	1:E:268:GLY:HA3	1.97	0.47
1:C:94:LEU:CD2	1:C:141:SER:HB3	2.45	0.47
1:C:264:ILE:HD12	1:C:331:PHE:HE1	1.80	0.47
1:D:124:ASP:OD2	1:D:227:THR:HG21	2.15	0.47
1:D:197:LYS:HG3	4:D:528:HOH:O	2.14	0.47
1:D:276:PRO:HA	1:D:316:VAL:HG12	1.96	0.46
1:D:348:TRP:CE2	1:F:139:PRO:HB2	2.50	0.46
1:D:126:ILE:HD11	1:D:132:TRP:HE3	1.80	0.46
1:D:126:ILE:HD11	1:D:132:TRP:CE3	2.50	0.46
1:D:243:VAL:HG13	1:D:262:VAL:HG22	1.96	0.46
1:A:252:PRO:O	1:A:255:GLN:NE2	2.41	0.46
1:C:352:SER:HB3	1:C:356:MET:HE2	1.96	0.46
1:E:315:ILE:HG12	1:E:316:VAL:HG13	1.97	0.46
1:B:109:ASN:OD1	1:B:147:GLN:HB2	2.16	0.46
1:B:291:VAL:HG22	1:B:321:ILE:HG23	1.98	0.46
1:B:292:GLY:HA3	1:B:320:TYR:CE1	2.51	0.46
1:C:174:HIS:CE1	1:E:298:SER:HB3	2.50	0.46
1:A:292:GLY:HA3	1:A:320:TYR:CE1	2.51	0.46
1:E:109:ASN:OD1	1:E:147:GLN:HB2	2.16	0.46
1:C:361:LEU:HB2	1:C:363:ILE:HG12	1.98	0.45
1:F:48:LEU:O	1:F:311:GLY:HA2	2.17	0.45
1:F:282:ASP:HA	1:F:332:LEU:O	2.17	0.45
1:A:184:PHE:O	1:A:186:VAL:HG13	2.16	0.45
1:D:43:GLY:O	1:D:301:ARG:NH2	2.49	0.45
1:A:48:LEU:O	1:A:311:GLY:HA2	2.16	0.45
1:A:274:TRP:CH2	1:D:139:PRO:HB3	2.51	0.45
1:B:346:ASN:OD1	1:E:183:ASN:ND2	2.49	0.45
1:F:191:LEU:HD22	1:F:194:LEU:HD11	1.99	0.45
1:A:270:ARG:HB3	1:A:321:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:VAL:HA	1:E:37:PRO:HD3	1.85	0.45
1:F:182:ALA:O	1:F:185:LYS:HD3	2.17	0.45
1:B:57:MET:HG2	1:B:59:ILE:HG12	1.98	0.45
1:F:152:LEU:HD22	1:F:283:TYR:CD2	2.51	0.45
1:E:363:ILE:HG13	1:E:368:VAL:HG23	1.99	0.45
1:F:366:GLU:O	1:F:370:GLN:HG3	2.17	0.45
1:D:366:GLU:HA	1:D:369:GLU:OE1	2.17	0.45
1:C:92:ARG:HB3	1:C:142:ILE:HB	1.98	0.44
1:D:103:ALA:O	1:D:131:LEU:HA	2.16	0.44
1:D:82:VAL:HG21	1:D:162:GLU:HG2	1.98	0.44
1:A:79:LEU:HD21	1:A:336:LYS:HB2	1.98	0.44
1:C:228:PHE:CE2	1:C:250:VAL:HG12	2.53	0.44
1:D:284:PHE:O	1:D:307:ALA:O	2.34	0.44
1:F:177:LYS:HB3	1:F:177:LYS:HE2	1.56	0.44
1:C:292:GLY:O	1:C:319:HIS:HA	2.17	0.44
1:F:62:GLY:CA	1:F:87:LYS:HD2	2.47	0.44
1:A:177:LYS:HE3	1:A:194:LEU:HD12	2.00	0.44
1:B:162:GLU:OE1	2:B:401:FMT:O2	2.34	0.44
1:B:48:LEU:CD1	1:B:293:VAL:HG11	2.48	0.44
1:B:291:VAL:HG13	1:B:321:ILE:HG12	1.99	0.44
1:C:94:LEU:HD21	1:E:356:MET:HE3	1.99	0.44
1:A:115:LEU:O	1:A:139:PRO:HD2	2.18	0.43
1:A:176:PRO:O	1:A:180:ILE:HG13	2.17	0.43
1:B:62:GLY:HA2	1:B:87:LYS:HD2	2.00	0.43
1:C:366:GLU:CD	1:C:366:GLU:H	2.22	0.43
1:D:272:LEU:HD23	1:D:320:TYR:HB3	2.01	0.43
1:A:364:SER:CB	1:A:366:GLU:HG2	2.48	0.43
1:A:313:ILE:HG21	1:A:319:HIS:CE1	2.53	0.43
1:B:126:ILE:HD12	1:B:126:ILE:O	2.19	0.43
1:B:209:PRO:O	1:B:213:VAL:HG22	2.19	0.43
1:C:249:LYS:CE	1:C:339:ILE:HD12	2.46	0.43
1:D:94:LEU:HD23	1:D:141:SER:HB3	1.99	0.43
1:F:112:VAL:HA	1:F:141:SER:O	2.18	0.43
1:A:190:VAL:HG11	1:F:367:THR:HG21	2.00	0.43
1:A:364:SER:OG	1:A:366:GLU:OE2	2.22	0.43
1:E:247:ASP:HB2	1:E:338:PRO:O	2.19	0.43
1:B:315:ILE:HD13	1:E:98:LYS:HG3	2.01	0.43
1:E:48:LEU:O	1:E:311:GLY:HA2	2.18	0.43
1:D:176:PRO:HB2	1:D:179:ILE:HG12	2.01	0.42
1:D:360:HIS:CD2	1:F:93:GLU:HG3	2.54	0.42
1:D:69:THR:HG22	1:D:80:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LYS:HD2	1:C:372:PRO:CG	2.49	0.42
1:C:36:VAL:HA	1:C:37:PRO:HD3	1.84	0.42
1:B:348:TRP:CZ2	1:E:94:LEU:HD22	2.54	0.42
1:B:360:HIS:CD2	1:E:93:GLU:HG3	2.53	0.42
1:D:348:TRP:CZ2	1:F:94:LEU:HB3	2.54	0.42
1:B:364:SER:OG	1:B:367:THR:HG23	2.20	0.42
1:C:82:VAL:HG11	1:C:162:GLU:HG3	2.01	0.42
1:F:109:ASN:OD1	1:F:147:GLN:HB2	2.19	0.42
1:A:69:THR:HG21	1:A:160:PHE:O	2.20	0.42
1:A:343:ILE:HG21	1:D:139:PRO:HG3	2.01	0.42
1:B:313:ILE:HG21	1:B:319:HIS:CE1	2.54	0.42
1:D:282:ASP:HA	1:D:332:LEU:O	2.18	0.42
1:E:367:THR:O	1:E:370:GLN:HB2	2.20	0.42
1:E:84:MET:HB3	1:E:151:PHE:CE1	2.54	0.42
1:E:94:LEU:CD2	1:E:141:SER:HB3	2.49	0.42
1:C:139:PRO:HB2	1:E:348:TRP:CE2	2.55	0.42
1:A:115:LEU:O	1:A:138:ILE:HG23	2.19	0.41
1:B:120:ARG:HG2	1:B:219:ASN:O	2.20	0.41
1:B:121:SER:HB3	1:C:351:THR:HB	2.02	0.41
1:F:366:GLU:HA	1:F:369:GLU:OE1	2.20	0.41
1:C:48:LEU:O	1:C:311:GLY:HA2	2.20	0.41
1:C:113:THR:HG22	1:C:123:ILE:HG13	2.03	0.41
1:D:292:GLY:HA3	1:D:320:TYR:CE2	2.54	0.41
1:D:367:THR:HG21	1:F:190:VAL:HG11	2.01	0.41
1:B:139:PRO:HD3	1:C:343:ILE:CD1	2.50	0.41
1:D:48:LEU:O	1:D:311:GLY:HA2	2.21	0.41
1:D:95:HIS:NE2	2:D:401:FMT:H	2.34	0.41
1:D:94:LEU:CD2	1:D:141:SER:HB3	2.50	0.41
1:F:111:ARG:HE	1:F:125:ASP:CG	2.24	0.41
1:C:161:SER:HB3	1:C:164:ASN:ND2	2.34	0.41
1:F:97:HIS:ND1	1:F:99:GLU:O	2.54	0.41
1:A:94:LEU:HB3	1:F:348:TRP:CZ2	2.56	0.41
1:A:101:GLU:OE1	1:A:153:LEU:HD22	2.20	0.41
1:A:199:LYS:O	1:A:201:ILE:N	2.54	0.41
1:D:58:ARG:NH2	1:D:198:GLU:OE1	2.50	0.41
1:D:93:GLU:OE2	1:D:169:THR:OG1	2.20	0.41
1:E:65:THR:HG21	1:E:200:TYR:OH	2.21	0.41
1:A:109:ASN:ND2	1:A:147:GLN:HG3	2.35	0.40
1:A:257:ILE:N	4:A:503:HOH:O	2.13	0.40
1:D:166:PHE:HA	4:D:512:HOH:O	2.20	0.40
1:D:350:ALA:O	1:F:215:LYS:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:ARG:NH2	1:F:125:ASP:OD1	2.50	0.40
1:F:276:PRO:HA	1:F:316:VAL:HG12	2.03	0.40
1:A:94:LEU:HD21	1:F:356:MET:HE3	2.03	0.40
1:A:367:THR:HG21	1:D:190:VAL:CG1	2.51	0.40
1:B:241:GLY:HA3	1:B:263:GLU:O	2.21	0.40
1:E:58:ARG:NH2	1:E:198:GLU:OE1	2.50	0.40
1:E:93:GLU:OE1	1:E:200:TYR:N	2.39	0.40
1:E:97:HIS:CE1	1:E:155:PHE:HE2	2.40	0.40
1:A:133:ASN:HD22	1:A:253:VAL:HG23	1.86	0.40
1:C:292:GLY:HA3	1:C:320:TYR:CE2	2.57	0.40
1:D:92:ARG:HB3	1:D:142:ILE:HB	2.03	0.40
1:C:84:MET:HB3	1:C:151:PHE:CE1	2.57	0.40
1:C:282:ASP:HA	1:C:332:LEU:O	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	336/360 (93%)	328 (98%)	7 (2%)	1 (0%)	41	72
1	B	336/360 (93%)	327 (97%)	8 (2%)	1 (0%)	41	72
1	C	336/360 (93%)	325 (97%)	10 (3%)	1 (0%)	41	72
1	D	336/360 (93%)	328 (98%)	7 (2%)	1 (0%)	41	72
1	E	336/360 (93%)	325 (97%)	10 (3%)	1 (0%)	41	72
1	F	336/360 (93%)	329 (98%)	6 (2%)	1 (0%)	41	72
All	All	2016/2160 (93%)	1962 (97%)	48 (2%)	6 (0%)	41	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	316	VAL
1	D	316	VAL
1	F	316	VAL
1	A	316	VAL
1	E	316	VAL
1	B	316	VAL

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	288/310 (93%)	288 (100%)	0	100	100
1	B	288/310 (93%)	283 (98%)	5 (2%)	60	87
1	C	288/310 (93%)	287 (100%)	1 (0%)	92	98
1	D	288/310 (93%)	288 (100%)	0	100	100
1	E	288/310 (93%)	286 (99%)	2 (1%)	84	95
1	F	288/310 (93%)	286 (99%)	2 (1%)	84	95
All	All	1728/1860 (93%)	1718 (99%)	10 (1%)	86	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	141	SER
1	B	234	LYS
1	B	258	SER
1	B	344	SER
1	B	369	GLU
1	C	239	GLU
1	E	66	ARG
1	E	97	HIS
1	F	46	SER
1	F	237	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	288	HIS
1	B	231	ASN
1	B	306	GLN
1	B	370	GLN
1	C	164	ASN
1	F	164	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FMT	E	401	3	2,2,2	0.73	0	1,1,1	0.36	0
2	FMT	A	401	3	2,2,2	0.70	0	1,1,1	0.29	0
2	FMT	F	401	3	2,2,2	0.72	0	1,1,1	0.18	0
2	FMT	C	401	3	2,2,2	0.71	0	1,1,1	0.25	0
2	FMT	B	401	3	2,2,2	0.71	0	1,1,1	0.22	0
2	FMT	D	401	3	2,2,2	0.74	0	1,1,1	0.38	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

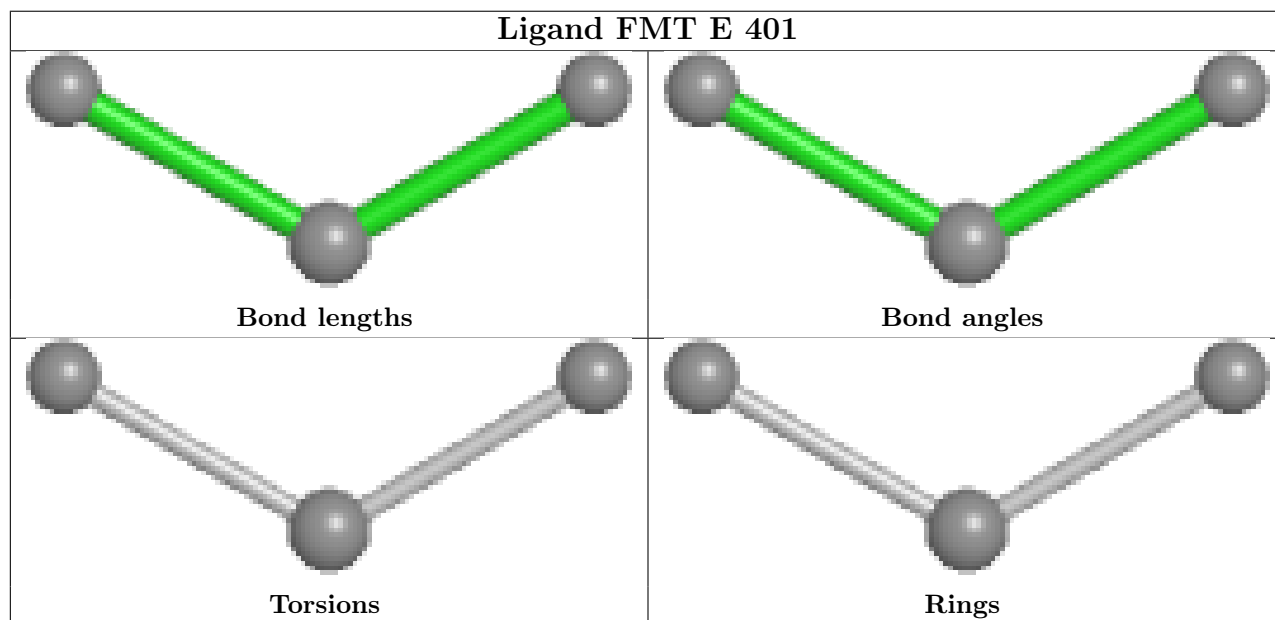
There are no torsion outliers.

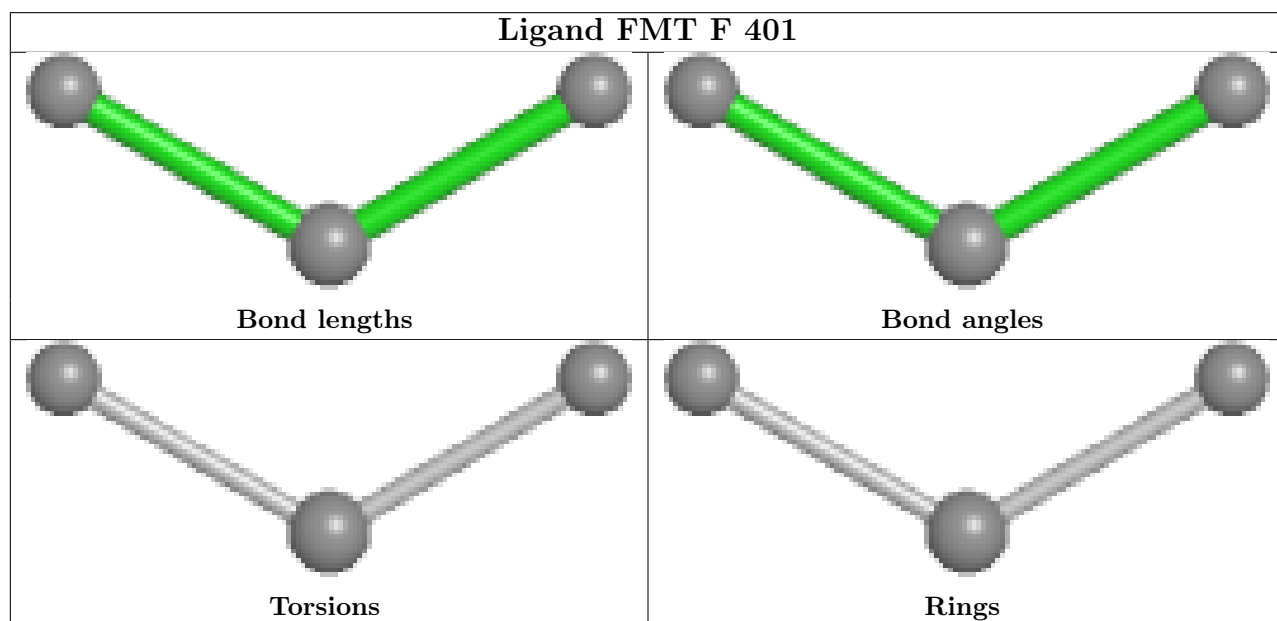
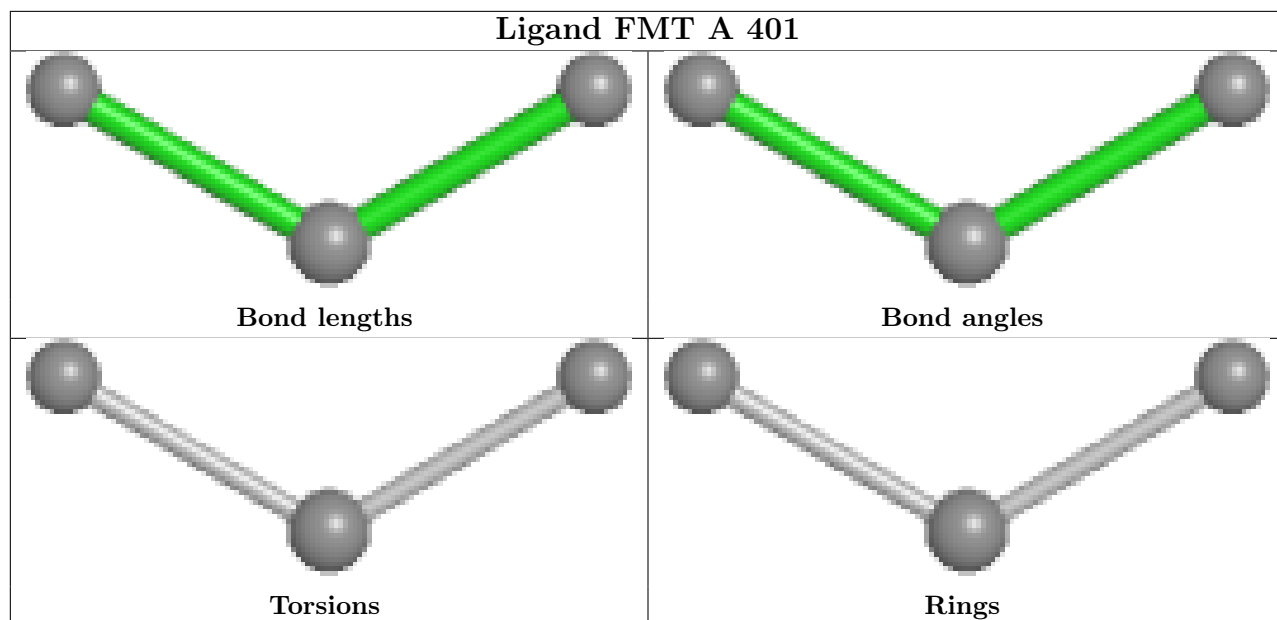
There are no ring outliers.

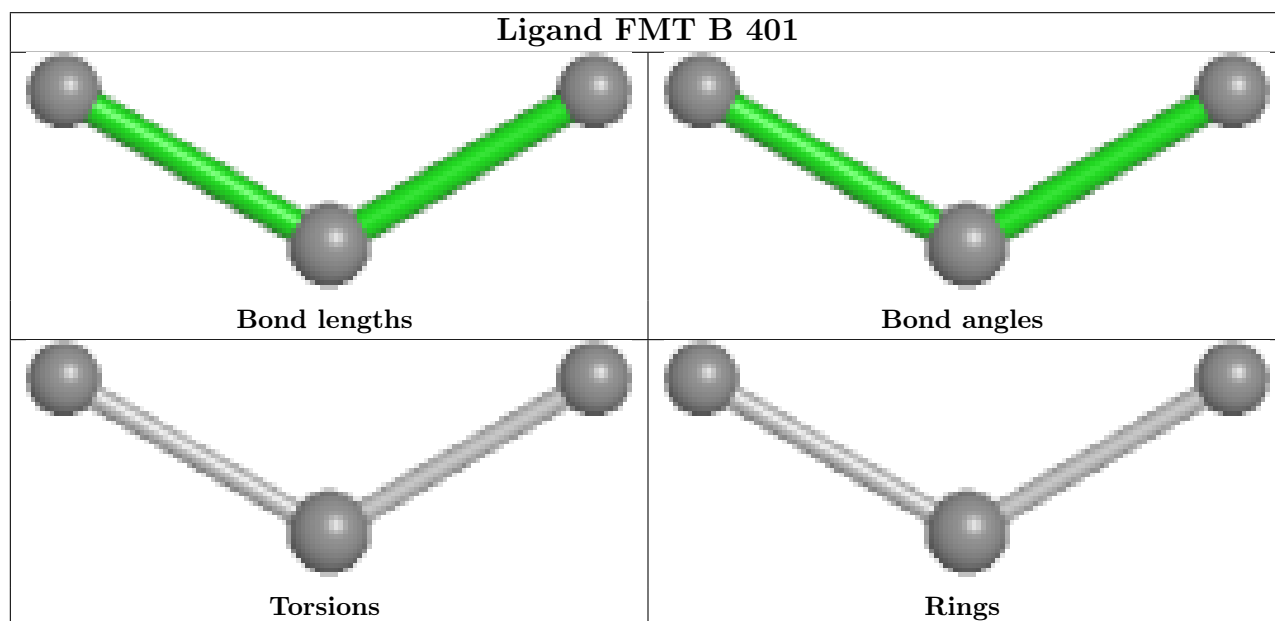
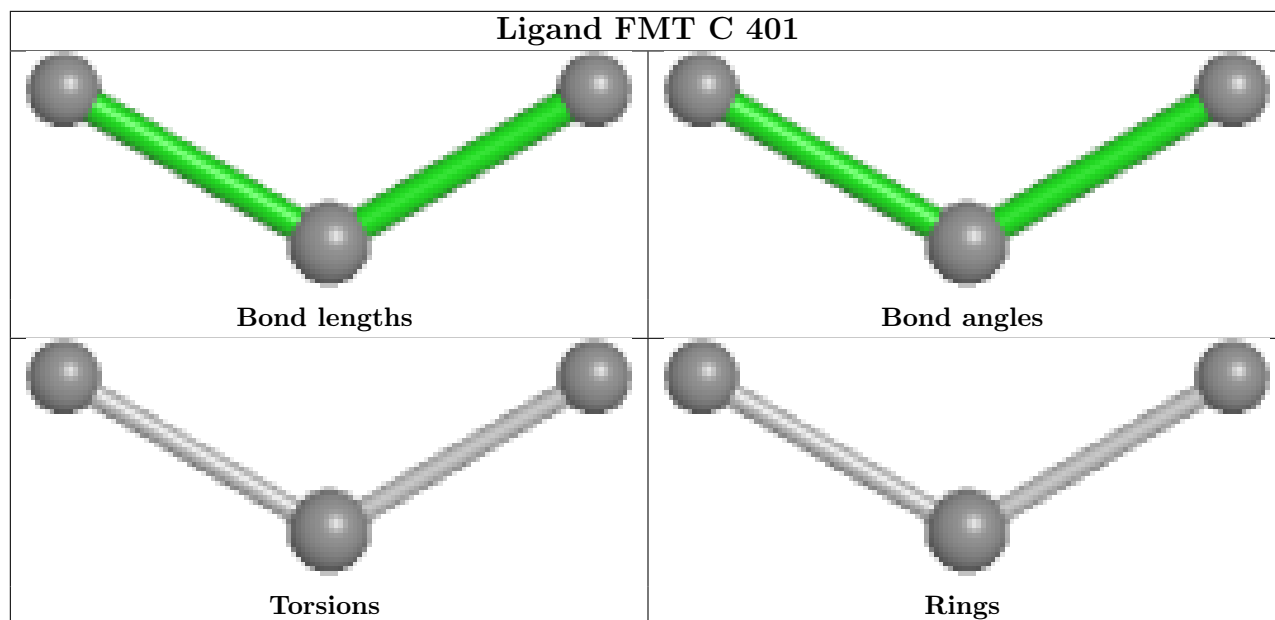
3 monomers are involved in 4 short contacts:

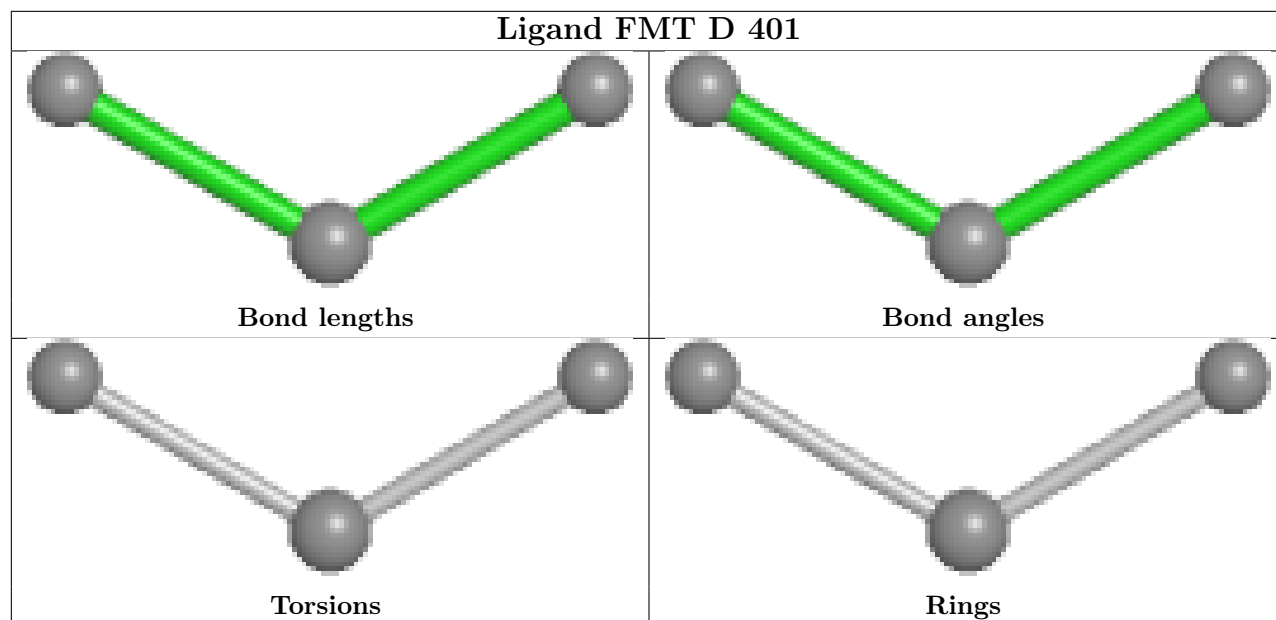
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	FMT	1	0
2	B	401	FMT	1	0
2	D	401	FMT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	338/360 (93%)	0.14	10 (2%) 50 40	16, 27, 49, 69	1 (0%)
1	B	338/360 (93%)	0.11	7 (2%) 63 54	14, 26, 45, 63	1 (0%)
1	C	338/360 (93%)	0.34	17 (5%) 28 19	17, 34, 53, 70	1 (0%)
1	D	338/360 (93%)	0.29	15 (4%) 34 24	17, 30, 57, 90	1 (0%)
1	E	338/360 (93%)	0.22	15 (4%) 34 24	19, 32, 58, 75	1 (0%)
1	F	338/360 (93%)	0.37	15 (4%) 34 24	18, 37, 60, 77	1 (0%)
All	All	2028/2160 (93%)	0.24	79 (3%) 39 29	14, 31, 55, 90	6 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	371	PHE	4.5
1	A	239	GLU	4.4
1	D	36	VAL	4.1
1	F	61	GLU	4.0
1	C	212	GLU	3.8
1	C	220	GLY	3.7
1	B	240	ALA	3.6
1	D	237	GLU	3.6
1	C	218	PRO	3.6
1	D	366	GLU	3.5
1	C	231	ASN	3.5
1	E	231	ASN	3.5
1	C	57	MET	3.4
1	A	57	MET	3.3
1	E	232	ASP	3.3
1	E	57	MET	3.2
1	C	216	ASN	3.2
1	E	371	PHE	3.1
1	C	219	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	237	GLU	3.1
1	A	187	ASP	3.1
1	F	236	HIS	3.0
1	F	366	GLU	2.9
1	F	57	MET	2.9
1	D	368	VAL	2.9
1	F	371	PHE	2.9
1	E	369	GLU	2.9
1	C	244	TRP	2.8
1	D	232	ASP	2.8
1	A	370	GLN	2.8
1	F	212	GLU	2.8
1	D	372	PRO	2.8
1	C	240	ALA	2.7
1	D	367	THR	2.7
1	D	369	GLU	2.7
1	F	327	GLU	2.7
1	D	363	ILE	2.6
1	E	39	ILE	2.6
1	F	244	TRP	2.6
1	C	307	ALA	2.6
1	E	238	PHE	2.6
1	C	217	ASN	2.5
1	F	219	ASN	2.5
1	C	328	PRO	2.5
1	B	370	GLN	2.5
1	D	236	HIS	2.5
1	F	210	ILE	2.5
1	A	371	PHE	2.5
1	C	265	GLN	2.4
1	D	239	GLU	2.4
1	F	231	ASN	2.4
1	A	61	GLU	2.4
1	B	238	PHE	2.3
1	D	238	PHE	2.3
1	B	232	ASP	2.3
1	F	184	PHE	2.3
1	E	239	GLU	2.3
1	A	326	ASP	2.3
1	E	244	TRP	2.2
1	E	372	PRO	2.2
1	F	188	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	240	ALA	2.2
1	B	185	LYS	2.2
1	F	326	ASP	2.2
1	E	373	LYS	2.2
1	E	236	HIS	2.1
1	B	239	GLU	2.1
1	A	39	ILE	2.1
1	D	373	LYS	2.1
1	E	187	ASP	2.1
1	C	221	ASP	2.1
1	C	148	GLY	2.1
1	D	233	LEU	2.1
1	A	366	GLU	2.1
1	E	370	GLN	2.0
1	C	269	MET	2.0
1	F	216	ASN	2.0
1	C	326	ASP	2.0
1	B	205	GLU	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(Å ²)	Q<0.9
2	FMT	D	401	3/3	0.89	0.27	40,40,46,46	0
2	FMT	F	401	3/3	0.90	0.24	42,42,48,49	0
3	MN	F	402	1/1	0.90	0.11	46,46,46,46	0
2	FMT	B	401	3/3	0.92	0.20	18,18,33,35	0
3	MN	C	402	1/1	0.92	0.14	41,41,41,41	0

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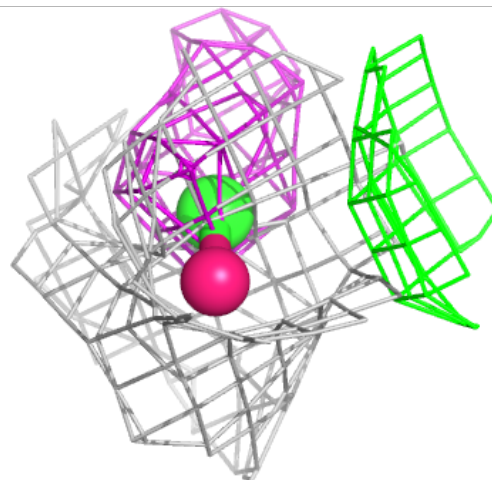
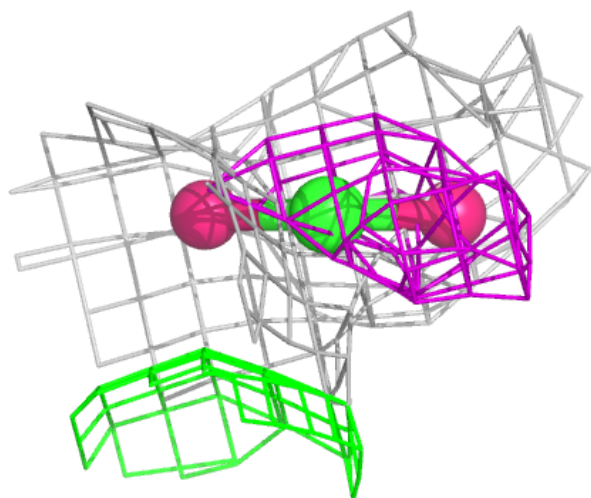
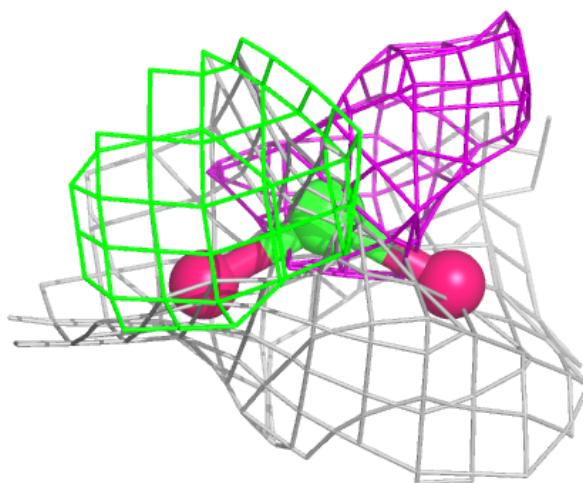
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FMT	A	401	3/3	0.92	0.24	31,31,41,41	0
2	FMT	C	401	3/3	0.93	0.16	46,46,50,50	0
3	MN	D	402	1/1	0.95	0.12	28,28,28,28	0
3	MN	B	402	1/1	0.95	0.10	23,23,23,23	0
3	MN	A	403	1/1	0.97	0.05	32,32,32,32	0
3	MN	C	403	1/1	0.97	0.06	39,39,39,39	0
2	FMT	E	401	3/3	0.97	0.26	65,65,68,74	0
3	MN	E	402	1/1	0.97	0.12	28,28,28,28	0
3	MN	B	403	1/1	0.97	0.06	36,36,36,36	0
3	MN	F	403	1/1	0.97	0.06	43,43,43,43	0
3	MN	E	403	1/1	0.98	0.07	49,49,49,49	0
3	MN	D	403	1/1	0.98	0.06	44,44,44,44	0
3	MN	A	402	1/1	0.98	0.09	30,30,30,30	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.

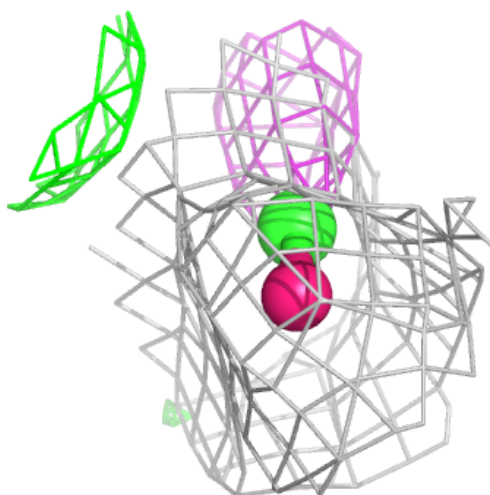
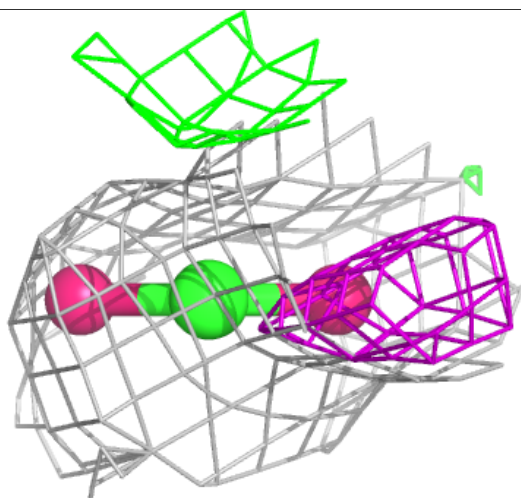
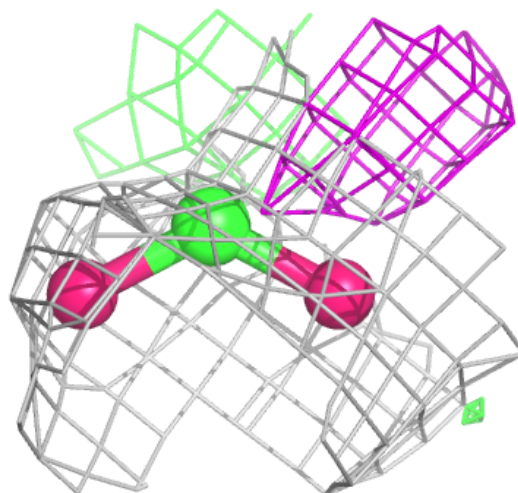
Electron density around FMT D 401:

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



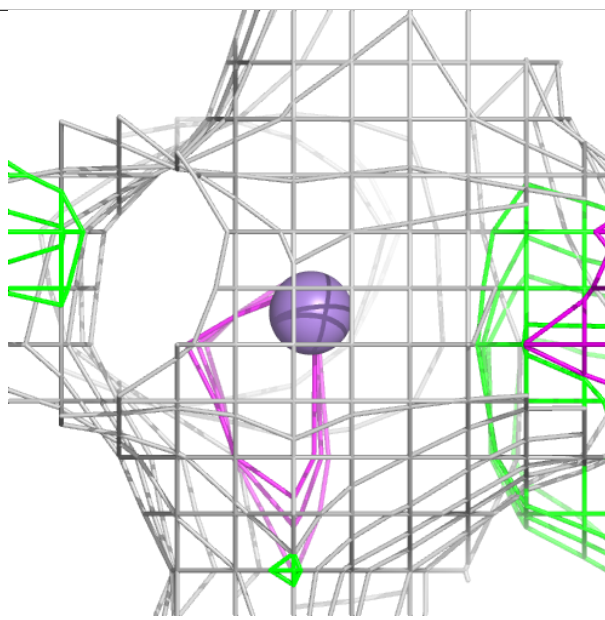
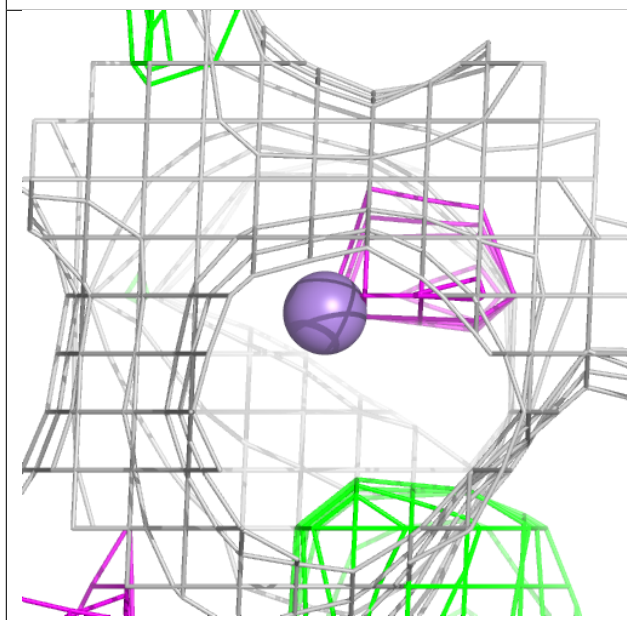
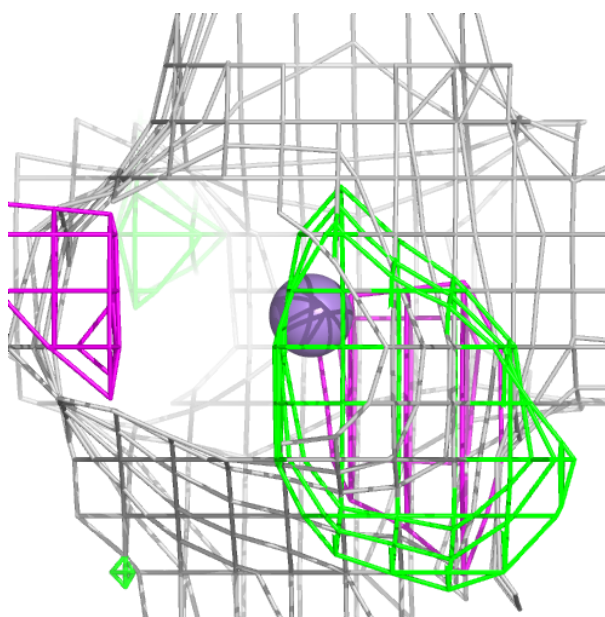
Electron density around FMT F 401:

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and green (positive)



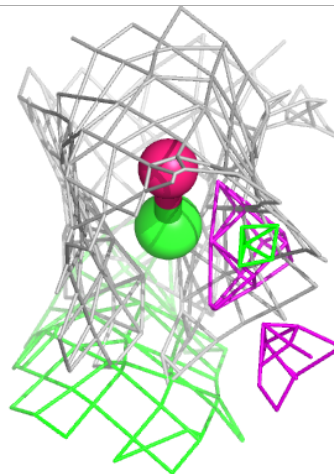
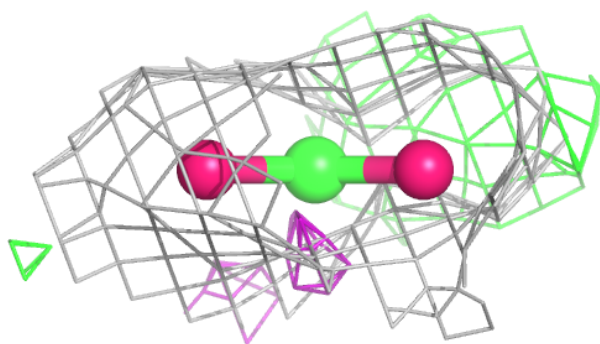
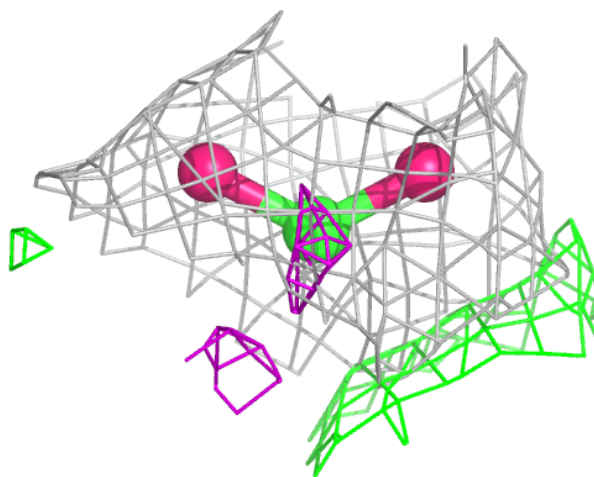
Electron density around MN F 402:

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



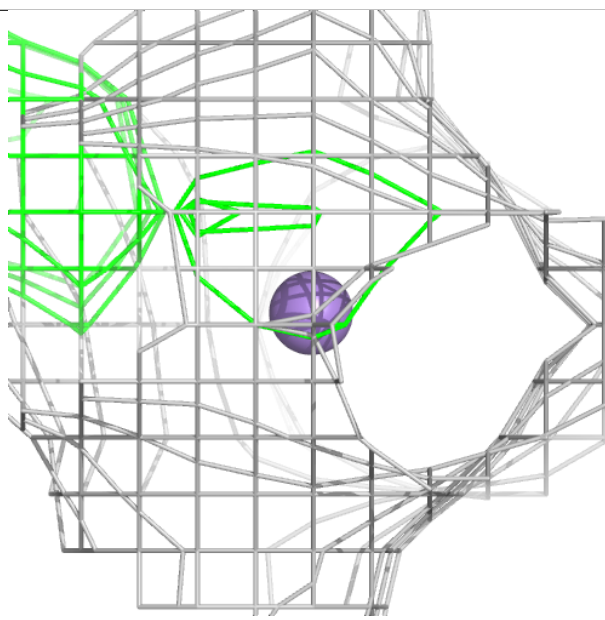
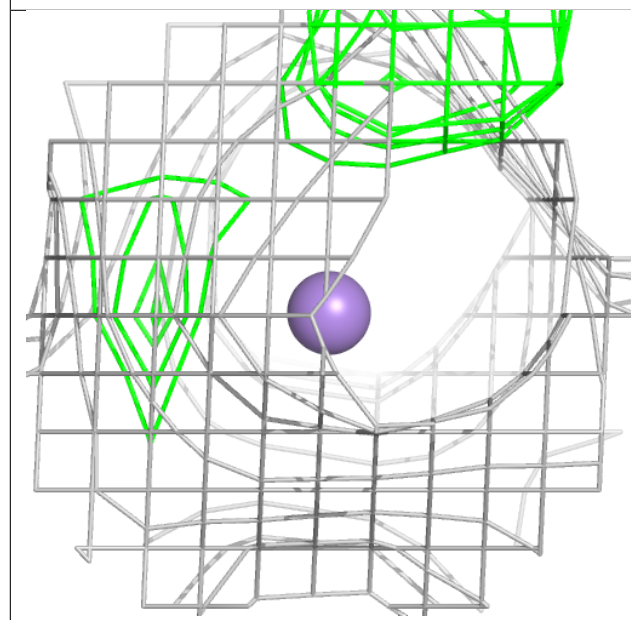
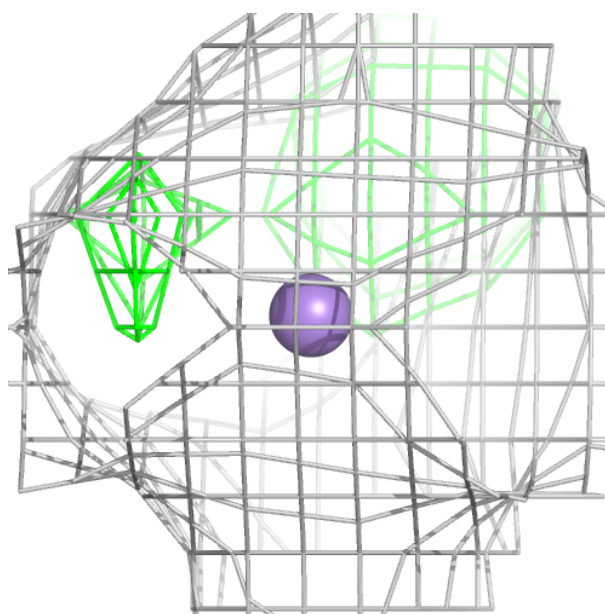
Electron density around FMT B 401:

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and green (positive)



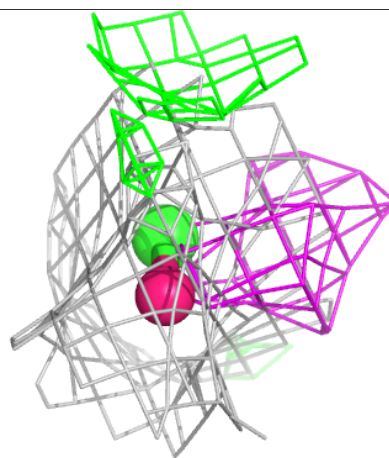
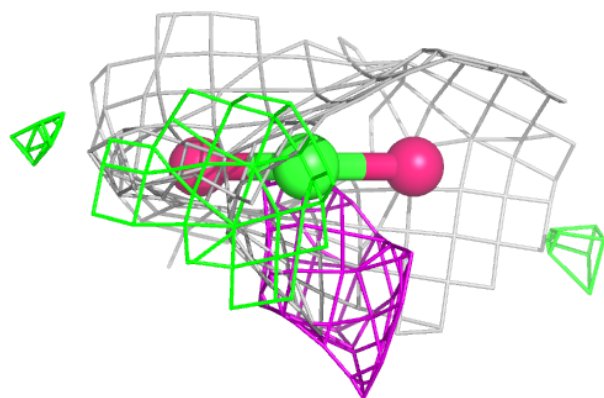
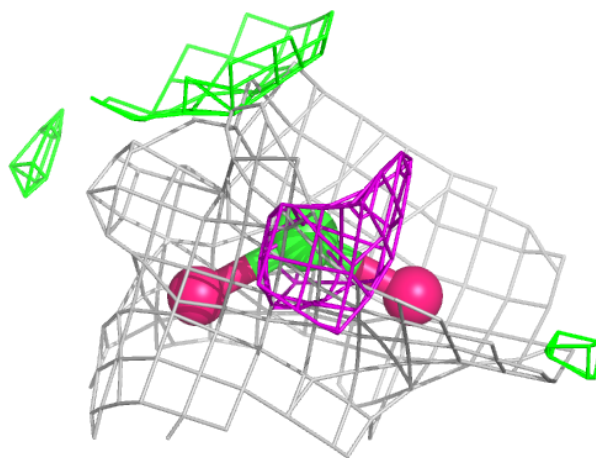
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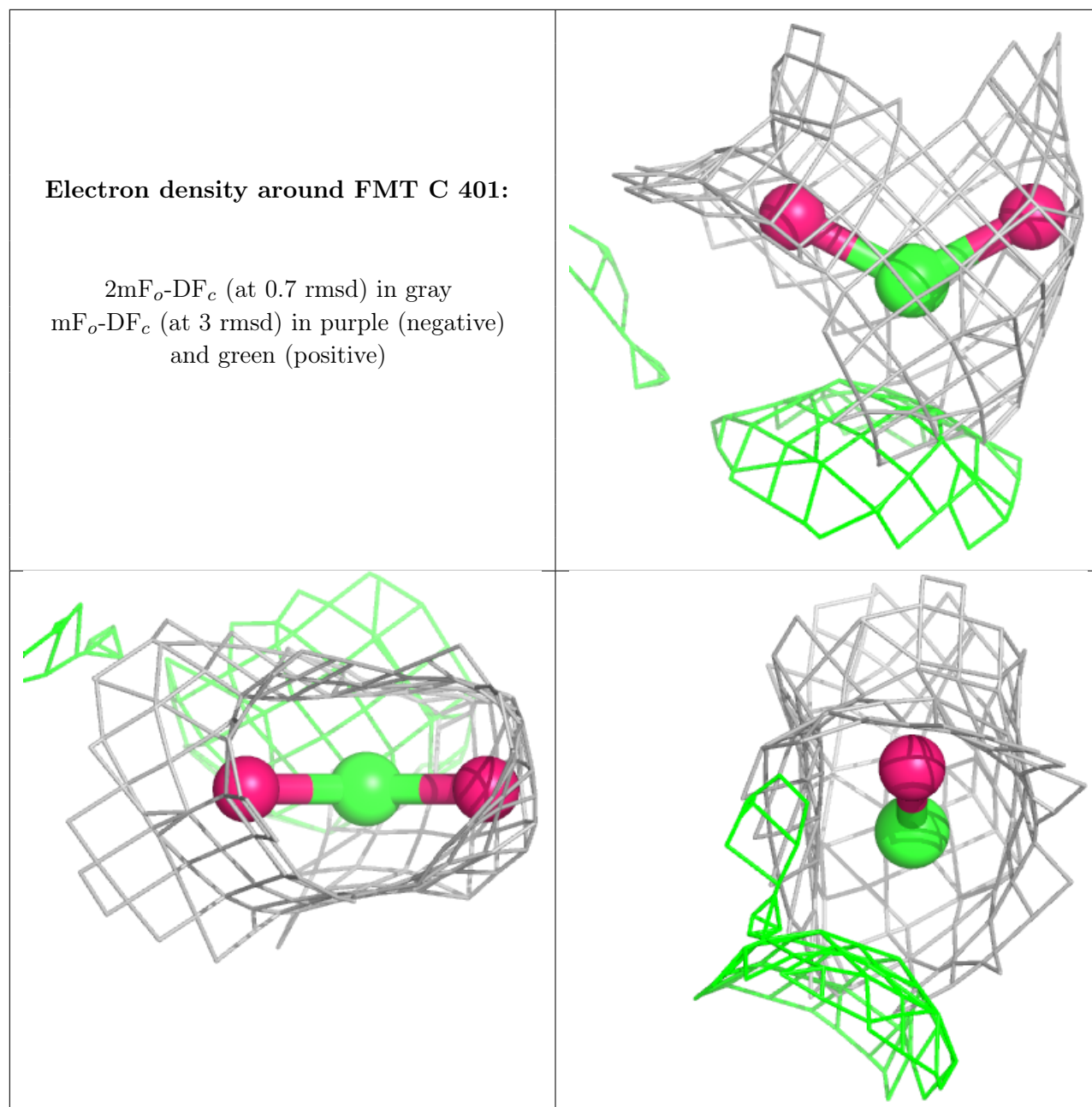
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMT A 401:

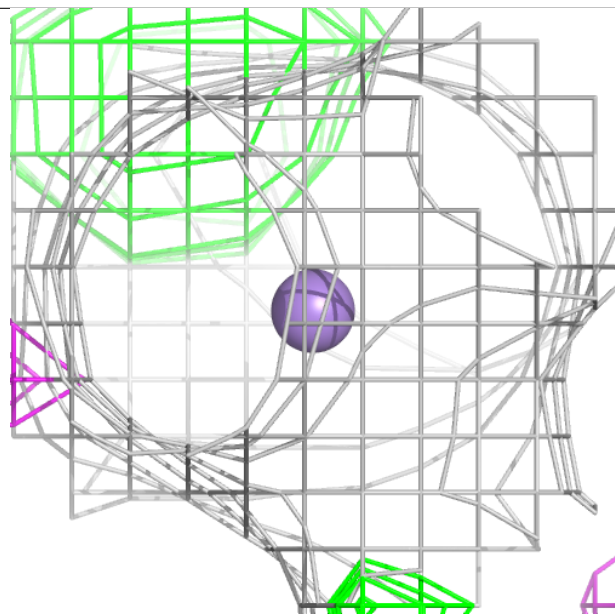
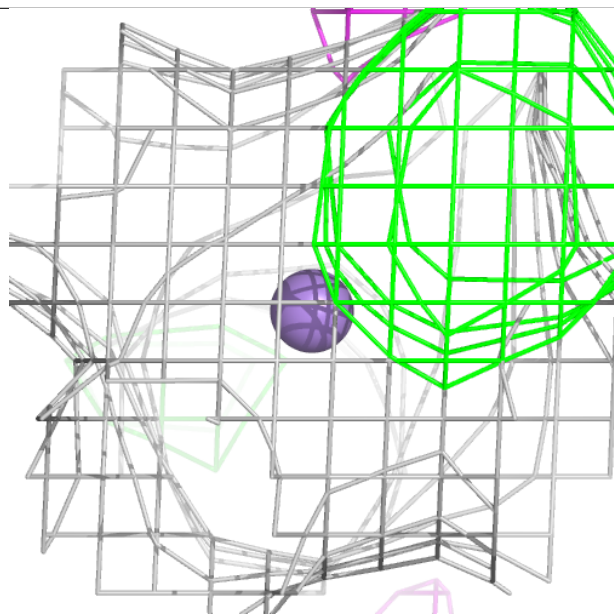
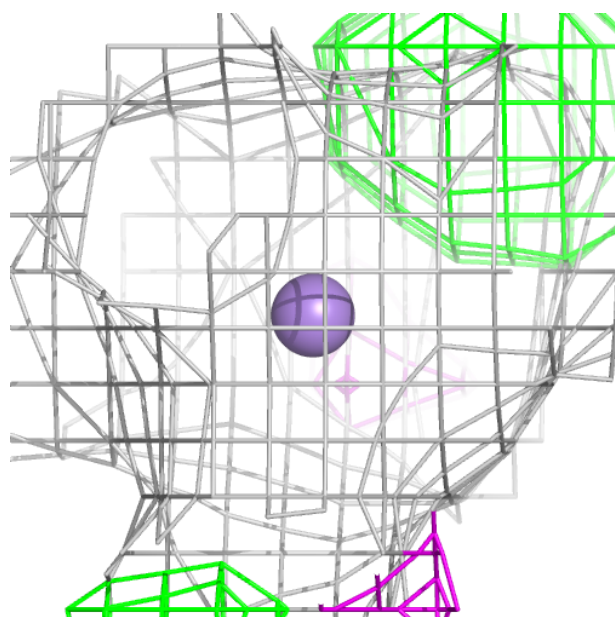
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





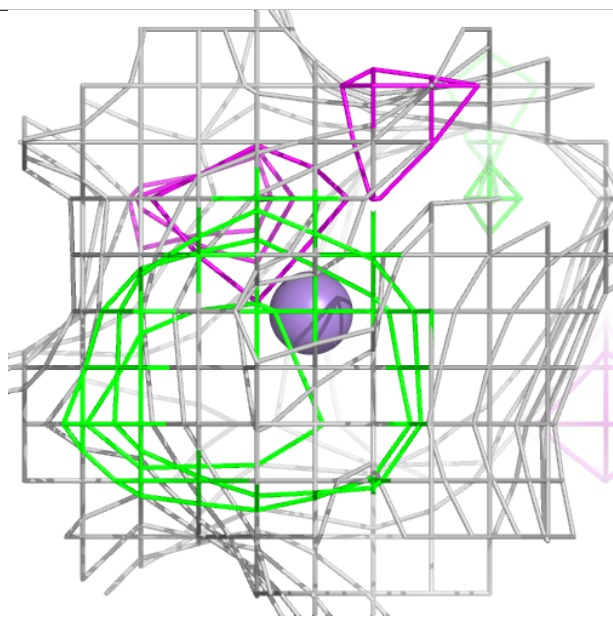
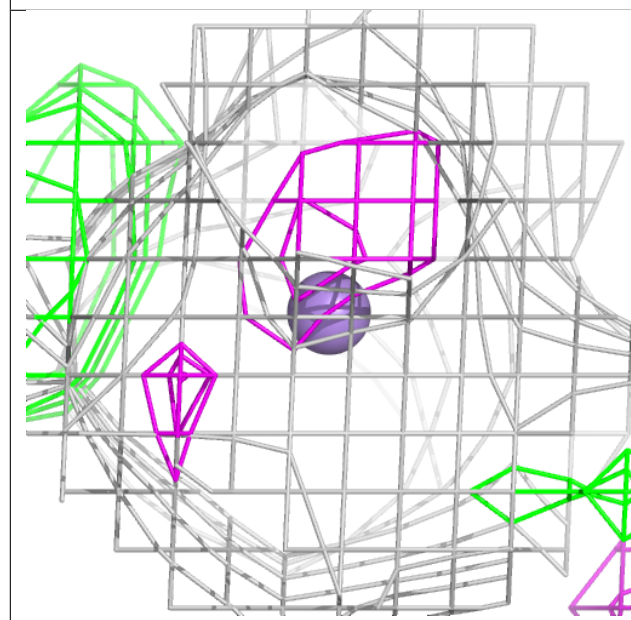
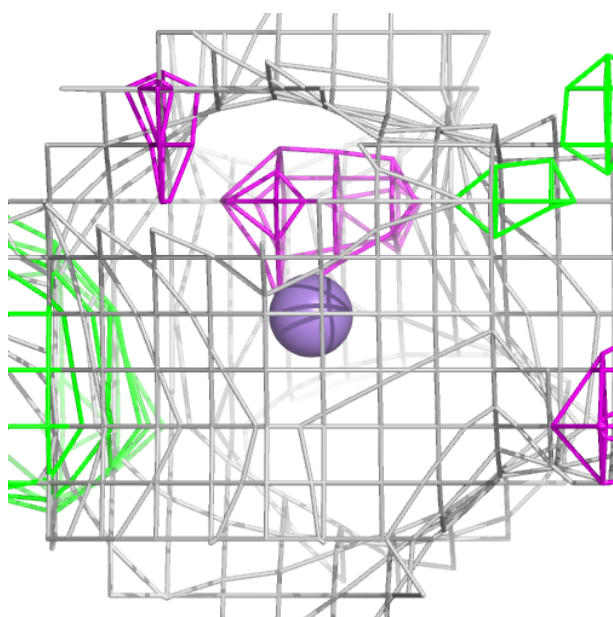
Electron density around MN D 402:

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and green (positive)



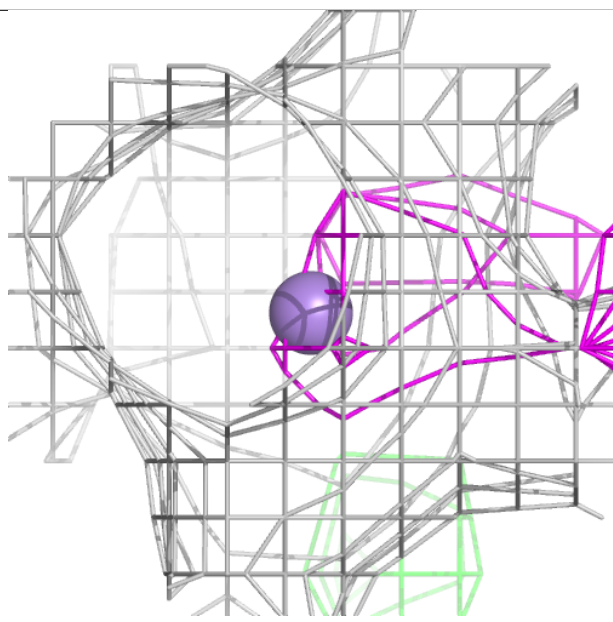
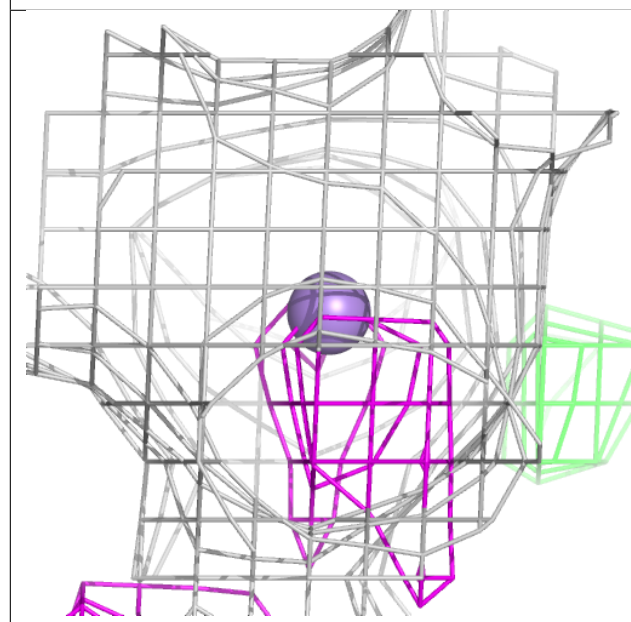
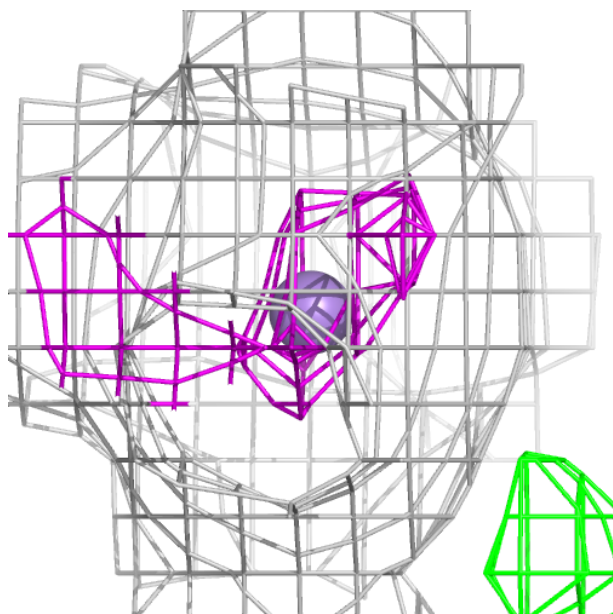
Electron density around MN B 402:

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



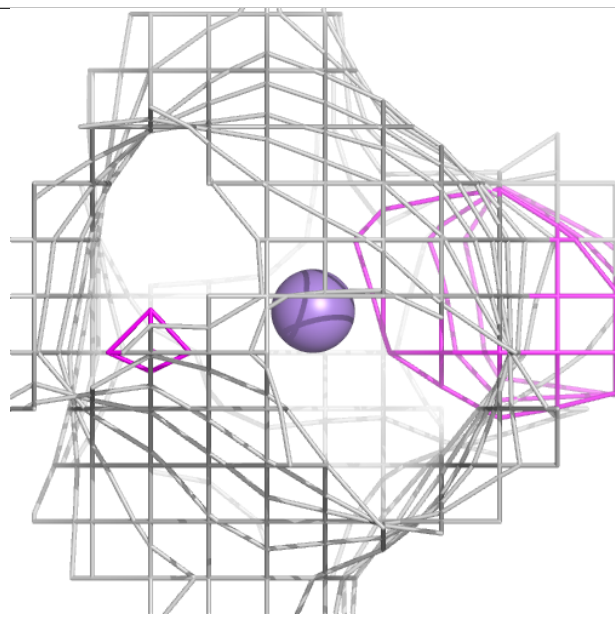
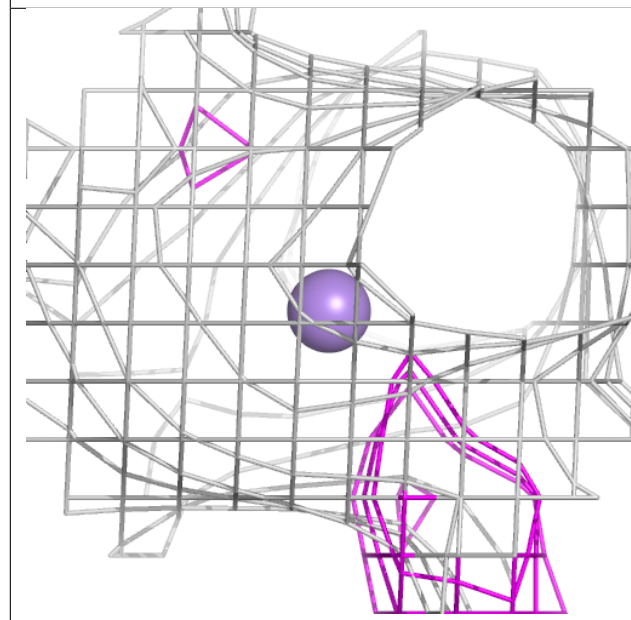
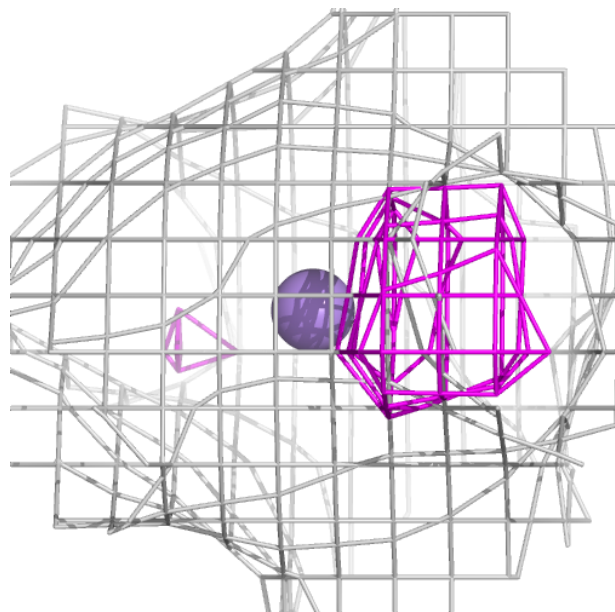
Electron density around MN A 403:

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



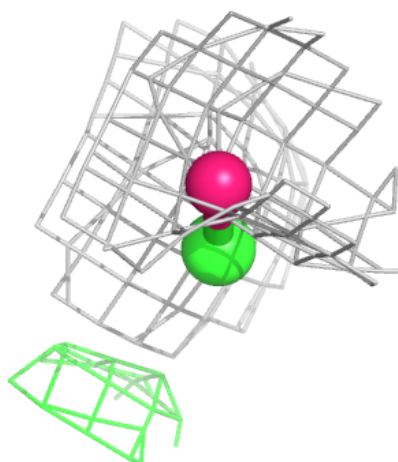
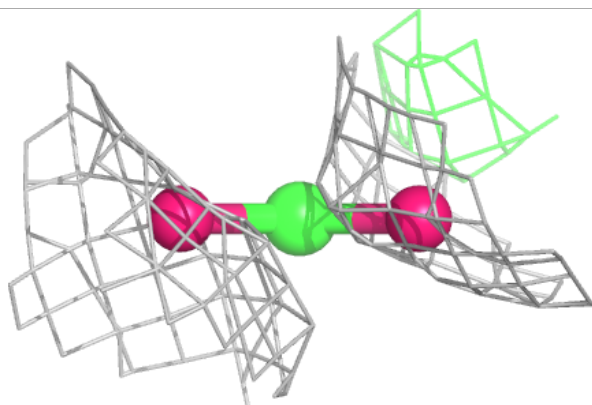
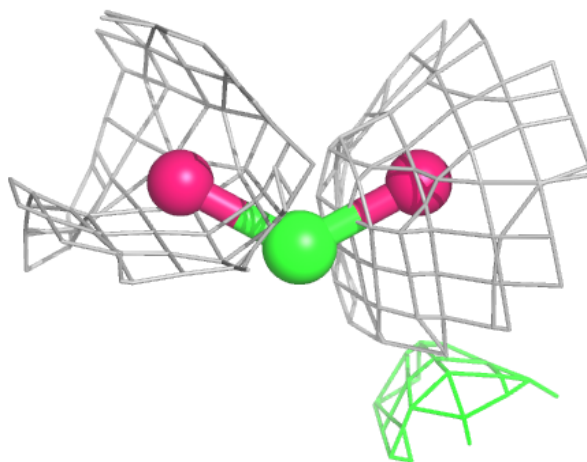
Electron density around MN C 403:

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



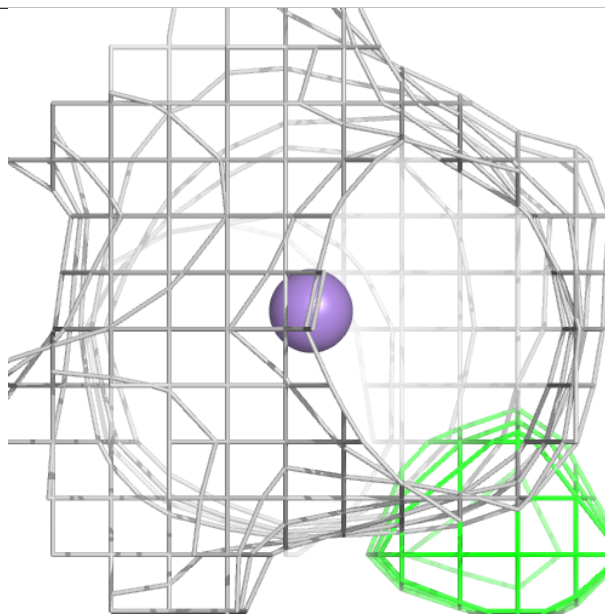
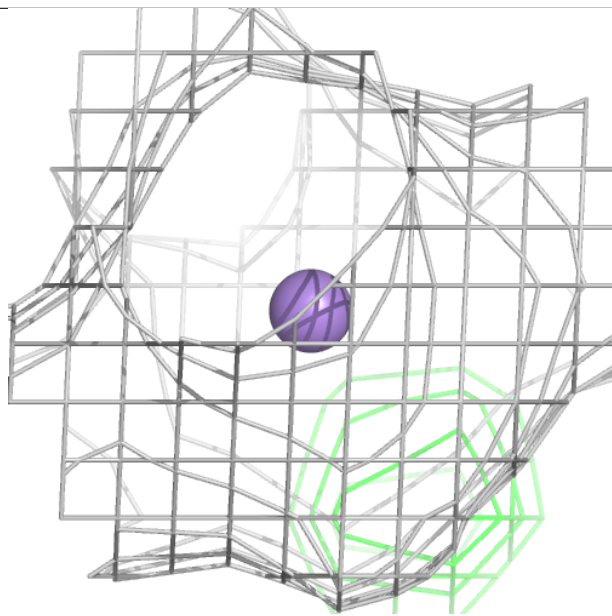
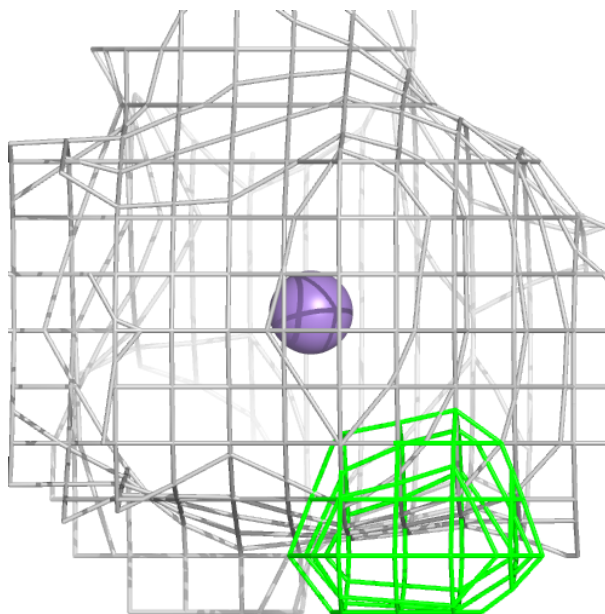
Electron density around FMT E 401:

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



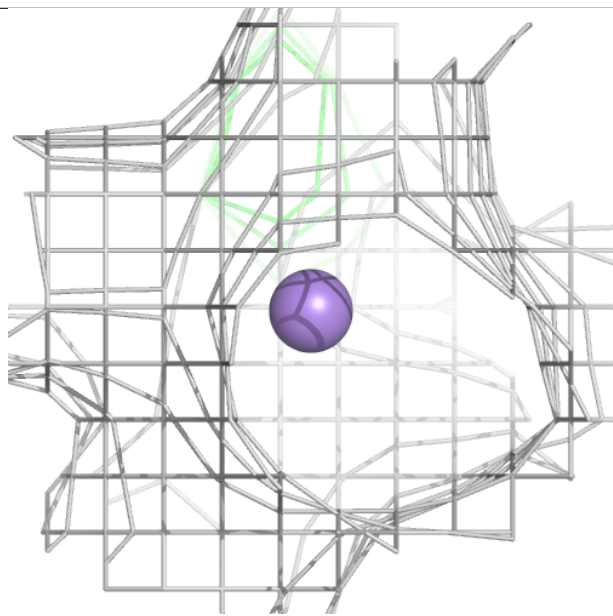
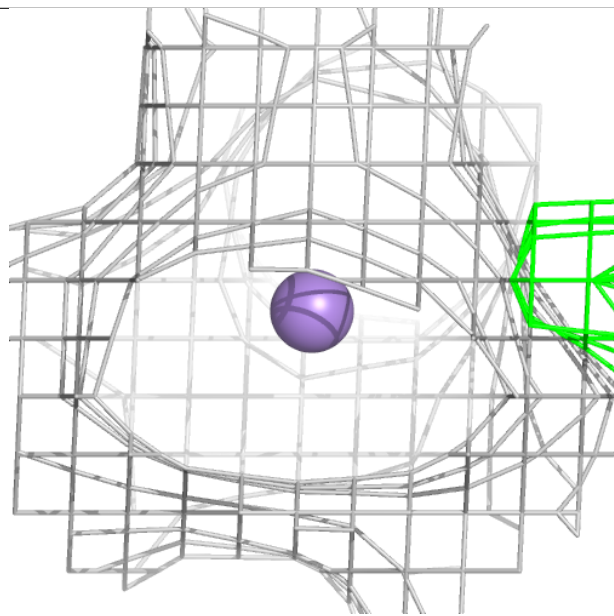
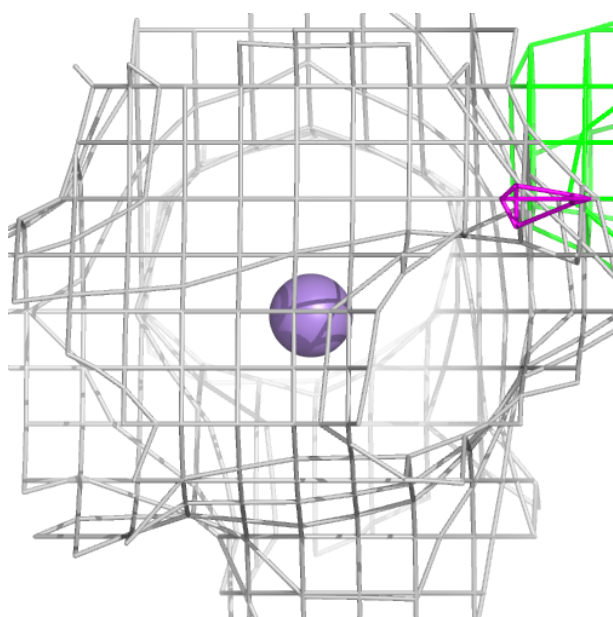
Electron density around MN E 402:

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



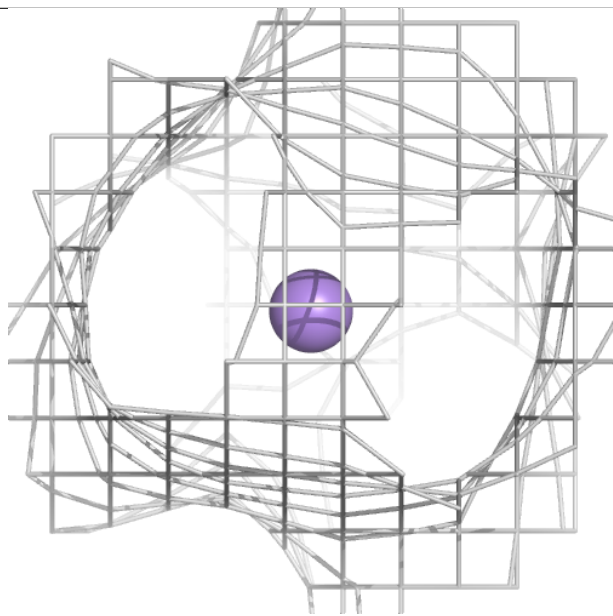
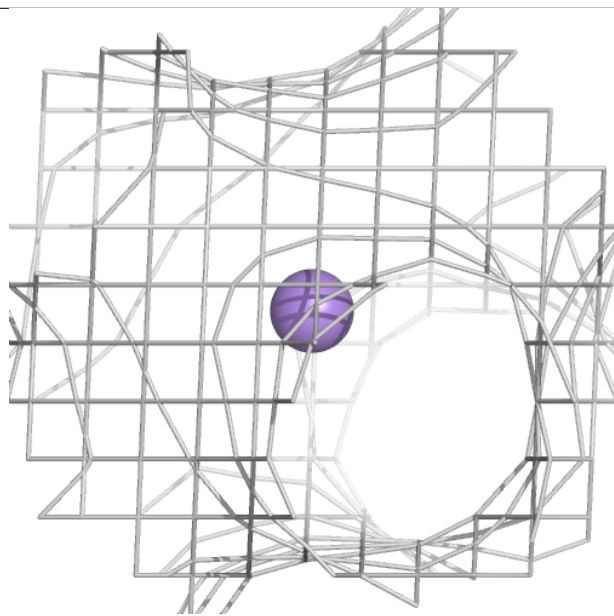
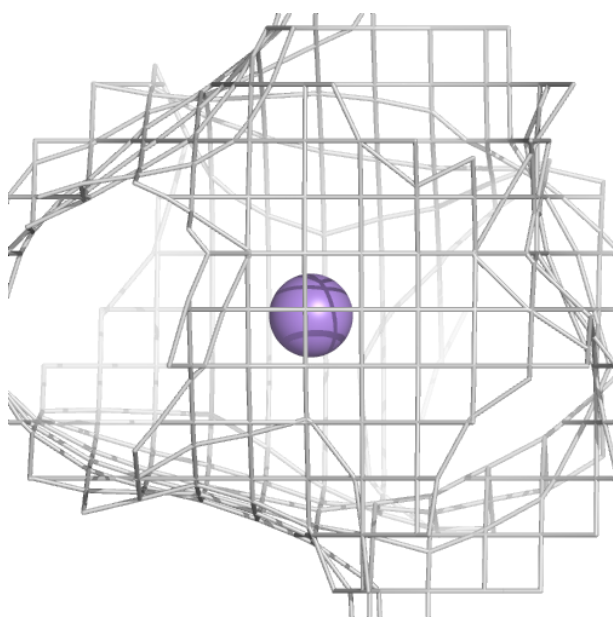
Electron density around MN B 403:

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



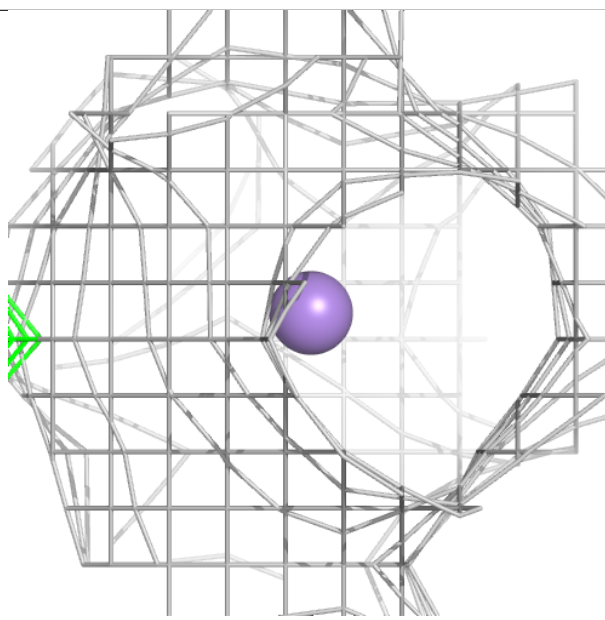
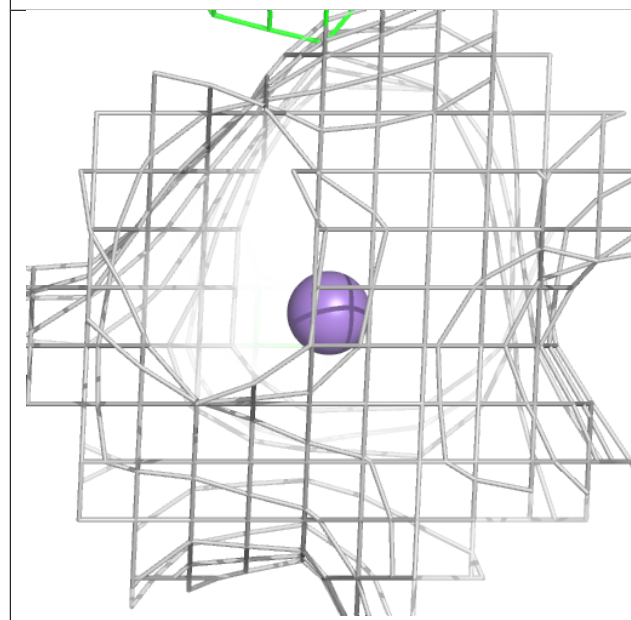
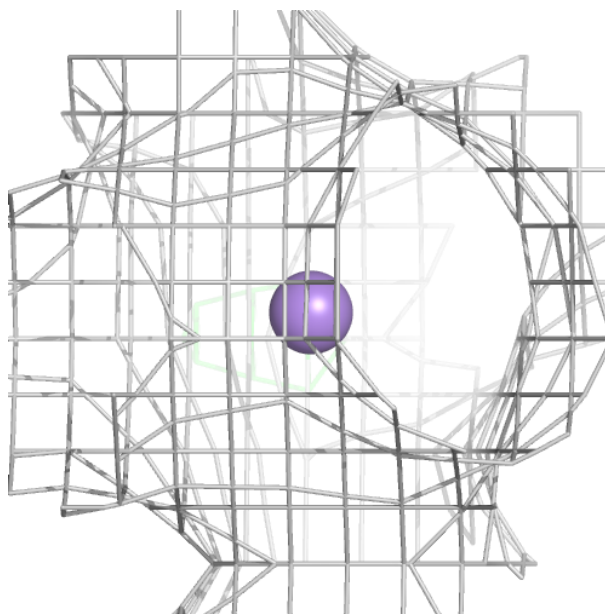
Electron density around MN F 403:

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



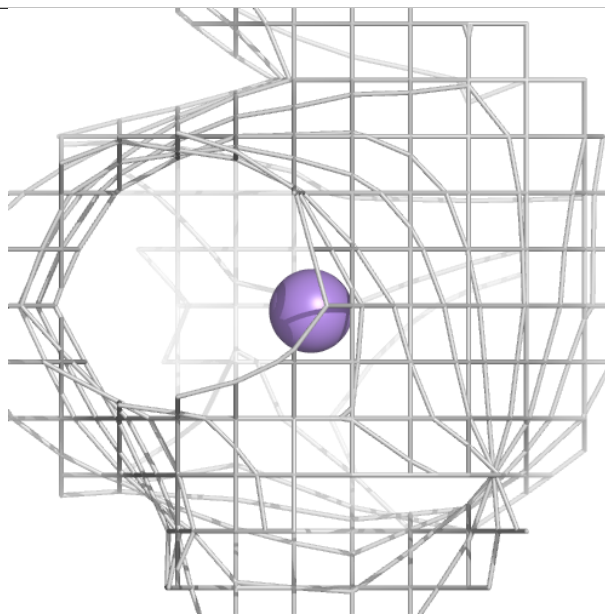
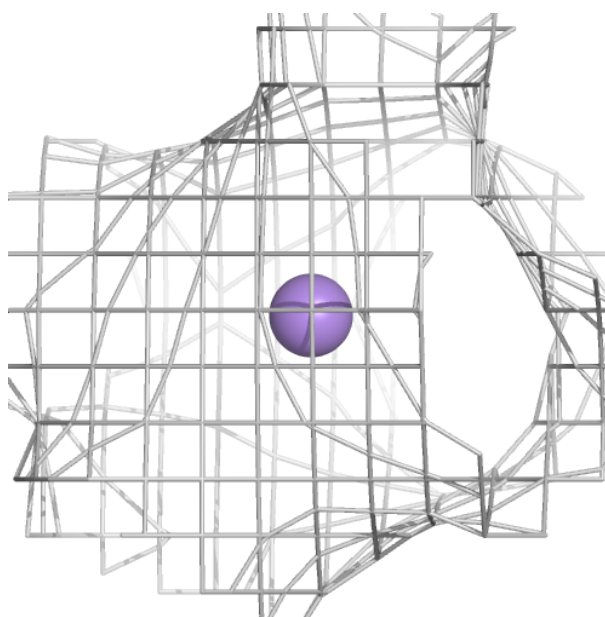
Electron density around MN E 403:

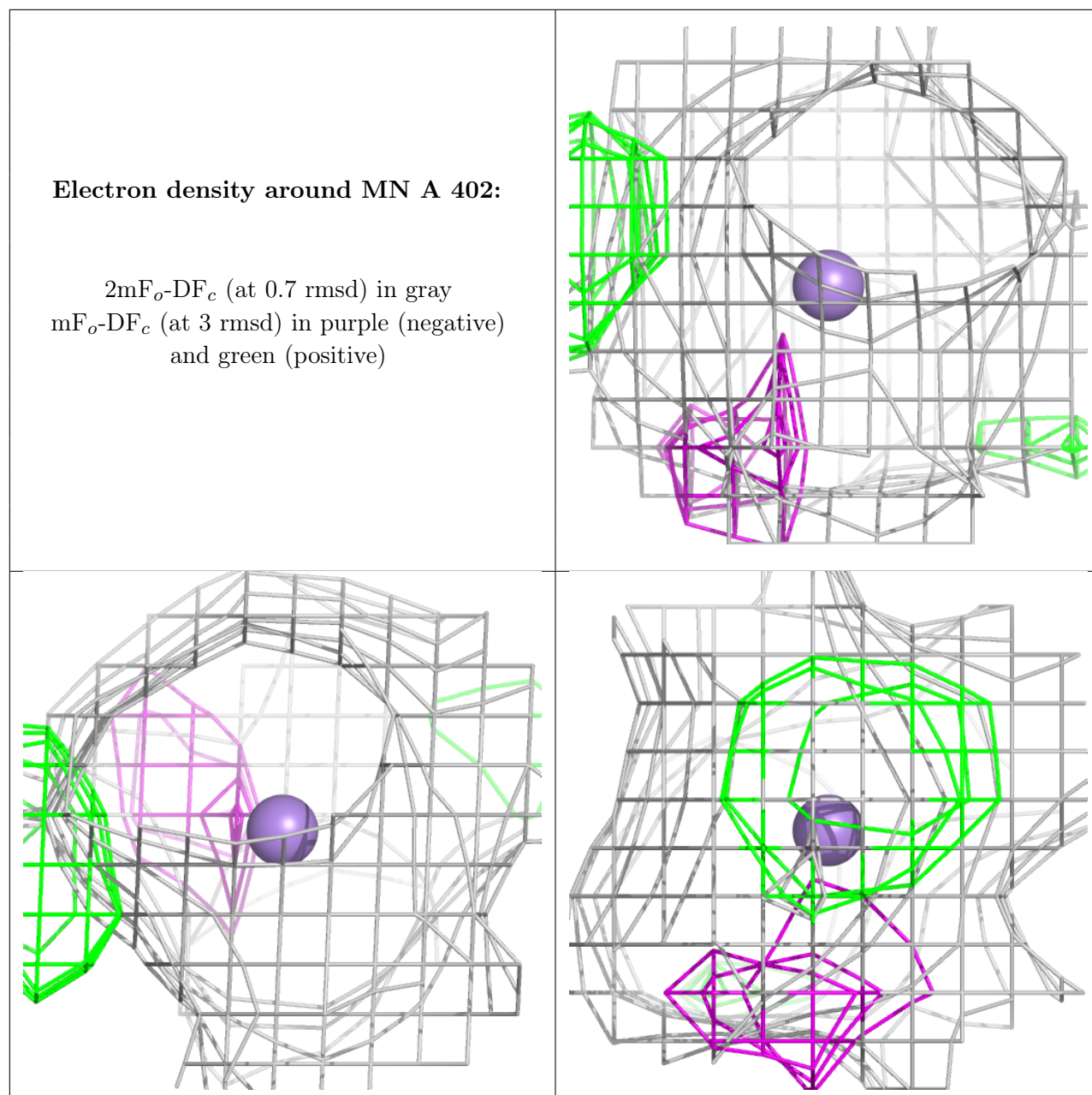
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN D 403:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.