wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 01:27 AM JST

PDB ID	:	6L0J
Title	:	Crystal structure of Dihydroorotase in complex with malate at pH7.5 from Saccharomyces cerevisiae
Authors	:	Guan, H.H.; Huang, Y.H.; Huang, C.Y.; Chen, C.J.
Deposited on	:	2019-09-26
Resolution	:	1.93 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

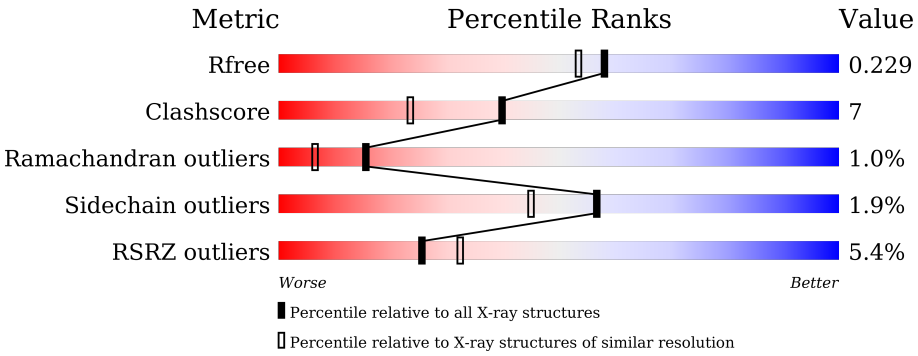
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	372	3% 82% 13%
1	B	372	3% 84% 12%
1	C	372	11% 82% 14%
1	D	372	4% 81% 15%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LMR	A	403	-	X	-	-
3	LMR	B	403	-	X	-	-
3	LMR	D	403	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12616 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 Dihydroorotase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2836	1823	470	532	11			
1	D	364	Total	C	N	O	S	0	0	0
			2844	1829	471	533	11			
1	B	364	Total	C	N	O	S	0	0	0
			2844	1829	471	533	11			
1	C	363	Total	C	N	O	S	0	0	0
			2836	1823	470	532	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	LEU	-	expression tag	UNP P20051
A	366	GLU	-	expression tag	UNP P20051
A	367	HIS	-	expression tag	UNP P20051
A	368	HIS	-	expression tag	UNP P20051
A	369	HIS	-	expression tag	UNP P20051
A	370	HIS	-	expression tag	UNP P20051
A	371	HIS	-	expression tag	UNP P20051
A	372	HIS	-	expression tag	UNP P20051
D	365	LEU	-	expression tag	UNP P20051
D	366	GLU	-	expression tag	UNP P20051
D	367	HIS	-	expression tag	UNP P20051
D	368	HIS	-	expression tag	UNP P20051
D	369	HIS	-	expression tag	UNP P20051
D	370	HIS	-	expression tag	UNP P20051
D	371	HIS	-	expression tag	UNP P20051
D	372	HIS	-	expression tag	UNP P20051
B	365	LEU	-	expression tag	UNP P20051
B	366	GLU	-	expression tag	UNP P20051
B	367	HIS	-	expression tag	UNP P20051
B	368	HIS	-	expression tag	UNP P20051
B	369	HIS	-	expression tag	UNP P20051

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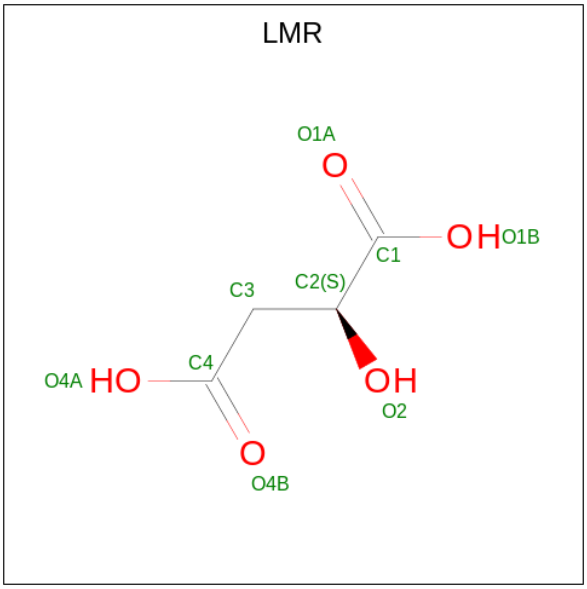
Chain	Residue	Modelled	Actual	Comment	Reference
B	370	HIS	-	expression tag	UNP P20051
B	371	HIS	-	expression tag	UNP P20051
B	372	HIS	-	expression tag	UNP P20051
C	365	LEU	-	expression tag	UNP P20051
C	366	GLU	-	expression tag	UNP P20051
C	367	HIS	-	expression tag	UNP P20051
C	368	HIS	-	expression tag	UNP P20051
C	369	HIS	-	expression tag	UNP P20051
C	370	HIS	-	expression tag	UNP P20051
C	371	HIS	-	expression tag	UNP P20051
C	372	HIS	-	expression tag	UNP P20051

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0

- Molecule 3 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: $C_4H_6O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 4 5	0	0
3	D	1	Total C O 9 4 5	0	0
3	B	1	Total C O 9 4 5	0	0
3	C	1	Total C O 9 4 5	0	0

- Molecule 4 is water.

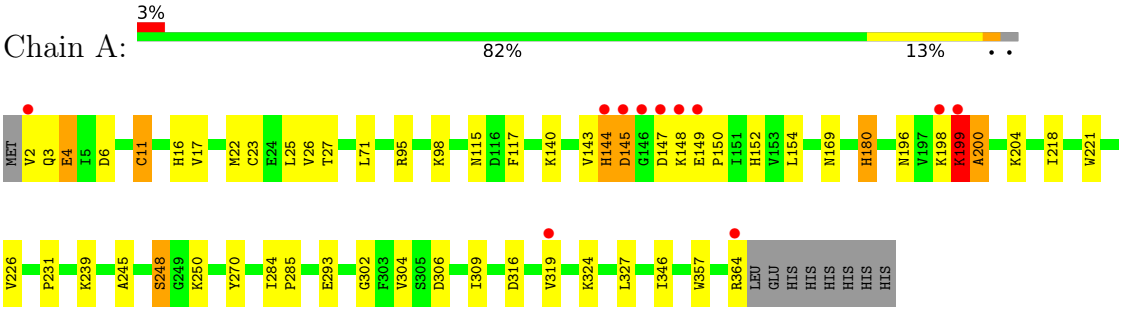
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	388	Total O 388 388	0	0
4	D	355	Total O 355 355	0	0
4	B	270	Total O 270 270	0	0
4	C	199	Total O 199 199	0	0

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.

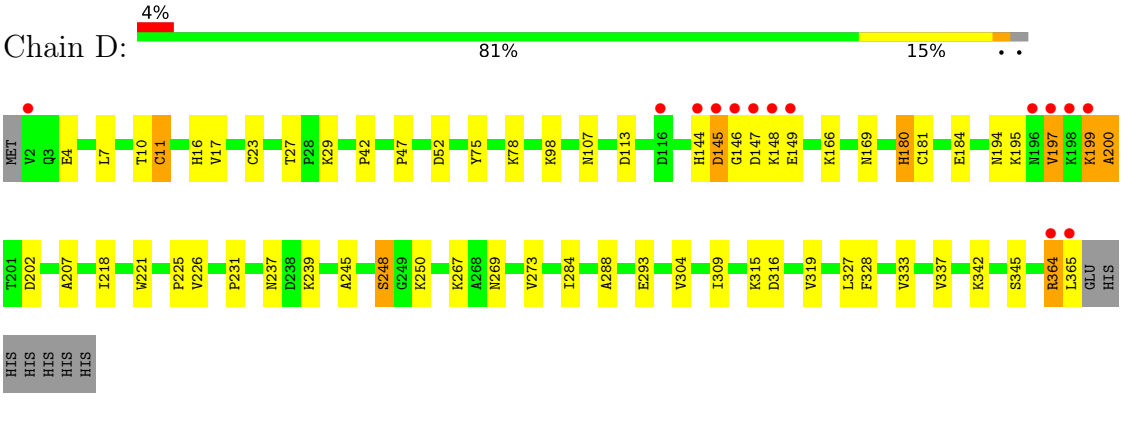
• Molecule 1: Dihydroorotase

Chain A:



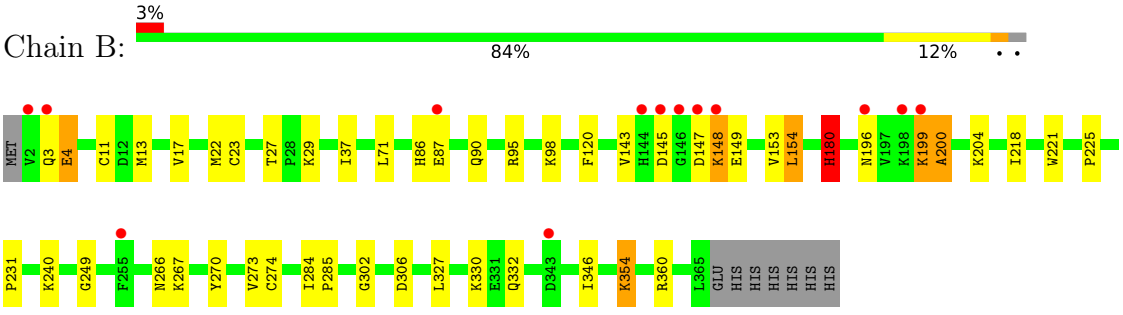
• Molecule 1: Dihydroorotase

Chain D:



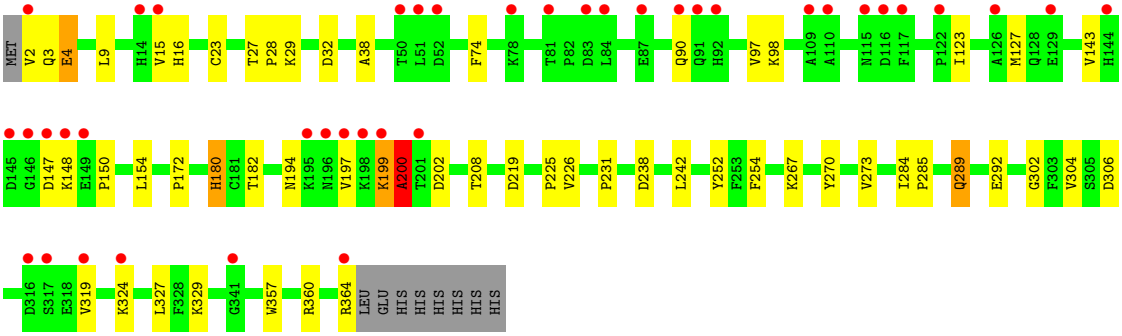
• Molecule 1: Dihydroorotase

Chain B:



• Molecule 1: Dihydroorotase

Chain C:


MET V2 Q3 E4 L9 H14 V15 H16 C23 T27 P28 K29 D32 A38 T50 L51 D52 F74 K78 T81 P82 D83 L84 E87 Q90 Q91 H92 V97 K98 A109 A110 N115 D116 F117 P122 I123 A126 M127 Q128 E129 V143 H144
D145 G146 D147 K148 E149 P150 L154 P172 H180 C181 T182 N194 K195 N196 V197 K198 K199 A200 T201 D202 T208 D219 P225 V226 P231 D238 L242 Y252 F253 F254 K267 Y270 V273 I284 P285 Q289 E292 G302 F303 V304 S305 D306
D316 S317 E318 V319 K324 L327 P328 K329 G341 W357 R360 R364 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.55Å 88.34Å 103.19Å 90.00° 95.60° 90.00°	Depositor
Resolution (Å)	28.30 – 1.93 28.31 – 1.93	Depositor EDS
% Data completeness (in resolution range)	88.0 (28.30-1.93) 88.0 (28.31-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 1.93Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.183 , 0.229 0.183 , 0.229	Depositor DCC
R_{free} test set	4795 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12616	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: KCX, LMR, ZN

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	0.47	2/2892 (0.1%)	0.59	0/3926
1	B	0.39	0/2900	0.56	0/3937
1	C	0.38	0/2892	0.55	1/3926 (0.0%)
1	D	0.47	2/2900 (0.1%)	0.58	0/3937
All	All	0.43	4/11584 (0.0%)	0.57	1/15726 (0.0%)

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	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	319	VAL	CB-CG2	6.64	1.66	1.52
1	A	319	VAL	CB-CG2	5.66	1.64	1.52
1	A	11	CYS	CB-SG	-5.63	1.72	1.81
1	D	11	CYS	CB-SG	-5.60	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	200	ALA	N-CA-C	-5.27	96.78	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	HIS	Peptide
1	D	197	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2836	0	2832	48	0
1	B	2844	0	2843	34	0
1	C	2836	0	2832	43	0
1	D	2844	0	2843	46	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	9	0	4	2	0
3	B	9	0	4	0	0
3	C	9	0	4	1	0
3	D	9	0	4	2	0
4	A	388	0	0	11	4
4	B	270	0	0	11	2
4	C	199	0	0	10	0
4	D	355	0	0	17	4
All	All	12616	0	11366	166	5

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 7.

The worst 5 of 166 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:MET:SD	4:A:794:HOH:O	2.16	1.03
1:A:199:LYS:HD2	1:A:200:ALA:HB2	1.41	1.00
1:D:202:ASP:OD2	4:D:502:HOH:O	1.88	0.92
1:A:22:MET:HE1	1:A:346:ILE:HD11	1.53	0.90
1:D:293:GLU:OE2	4:D:501:HOH:O	1.88	0.90

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:804:HOH:O	4:B:648:HOH:O[2_555]	1.81	0.39
4:A:710:HOH:O	4:D:764:HOH:O[2_556]	2.02	0.18
4:A:755:HOH:O	4:B:673:HOH:O[2_555]	2.02	0.18
4:A:528:HOH:O	4:D:678:HOH:O[2_556]	2.07	0.13
4:A:791:HOH:O	4:D:624:HOH:O[2_555]	2.10	0.10

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	360/372 (97%)	346 (96%)	10 (3%)	4 (1%)	14	5
1	B	361/372 (97%)	346 (96%)	11 (3%)	4 (1%)	14	5
1	C	360/372 (97%)	343 (95%)	14 (4%)	3 (1%)	19	9
1	D	361/372 (97%)	344 (95%)	13 (4%)	4 (1%)	14	5
All	All	1442/1488 (97%)	1379 (96%)	48 (3%)	15 (1%)	15	6

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	199	LYS
1	B	200	ALA
1	C	4	GLU
1	A	145	ASP
1	A	200	ALA

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	311/320 (97%)	305 (98%)	6 (2%)	57	45
1	B	312/320 (98%)	306 (98%)	6 (2%)	57	45
1	C	311/320 (97%)	309 (99%)	2 (1%)	86	85
1	D	312/320 (98%)	302 (97%)	10 (3%)	39	25
All	All	1246/1280 (97%)	1222 (98%)	24 (2%)	57	45

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	342	LYS
1	B	154	LEU
1	B	148	LYS
1	B	180	HIS
1	D	52	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	D	295	ASN
1	B	115	ASN
1	B	144	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	KCX	A	98	2,1	9,11,12	1.16	1 (11%)	5,12,14	1.66	1 (20%)
1	KCX	C	98	2,1	9,11,12	0.86	0	5,12,14	1.95	2 (40%)
1	KCX	B	98	2,1	9,11,12	0.89	0	5,12,14	1.50	1 (20%)
1	KCX	D	98	2,1	9,11,12	1.11	1 (11%)	5,12,14	1.76	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	98	2,1	-	0/9/10/12	-
1	KCX	C	98	2,1	-	0/9/10/12	-
1	KCX	B	98	2,1	-	1/9/10/12	-
1	KCX	D	98	2,1	-	1/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	KCX	OQ1-CX	2.64	1.26	1.21
1	D	98	KCX	CE-NZ	2.58	1.52	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	98	KCX	OQ1-CX-NZ	-3.65	119.30	124.96
1	D	98	KCX	OQ1-CX-NZ	-3.32	119.81	124.96
1	A	98	KCX	OQ1-CX-NZ	-2.63	120.87	124.96
1	B	98	KCX	OQ1-CX-NZ	-2.55	121.00	124.96
1	C	98	KCX	CE-NZ-CX	-2.21	118.33	121.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	98	KCX	CG-CD-CE-NZ
1	D	98	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	LMR	B	403	2	8,8,8	1.40	1 (12%)	10,10,10	2.58	7 (70%)
3	LMR	A	403	2	8,8,8	1.41	1 (12%)	10,10,10	2.75	6 (60%)
3	LMR	D	403	2	8,8,8	1.78	3 (37%)	10,10,10	2.32	5 (50%)
3	LMR	C	403	2	8,8,8	1.27	1 (12%)	10,10,10	2.34	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMR	B	403	2	-	4/8/8/8	-
3	LMR	A	403	2	-	4/8/8/8	-
3	LMR	D	403	2	-	4/8/8/8	-
3	LMR	C	403	2	-	4/8/8/8	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	LMR	C2-C1	2.98	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	LMR	C2-C1	2.54	1.56	1.52
3	A	403	LMR	C2-C1	2.40	1.55	1.52
3	D	403	LMR	O1A-C1	2.15	1.28	1.22
3	D	403	LMR	O4B-C4	2.10	1.29	1.22

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	403	LMR	O1B-C1-C2	5.07	123.85	112.72
3	A	403	LMR	C2-C3-C4	-5.04	99.65	112.13
3	D	403	LMR	C2-C3-C4	-4.02	102.19	112.13
3	B	403	LMR	O1B-C1-O1A	-3.89	115.27	124.09
3	C	403	LMR	O1B-C1-O1A	-3.57	115.98	124.09

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	LMR	O1A-C1-C2-O2
3	B	403	LMR	O1B-C1-C2-O2
3	C	403	LMR	O1A-C1-C2-O2
3	C	403	LMR	O1A-C1-C2-C3
3	C	403	LMR	O1B-C1-C2-O2

There are no ring outliers.

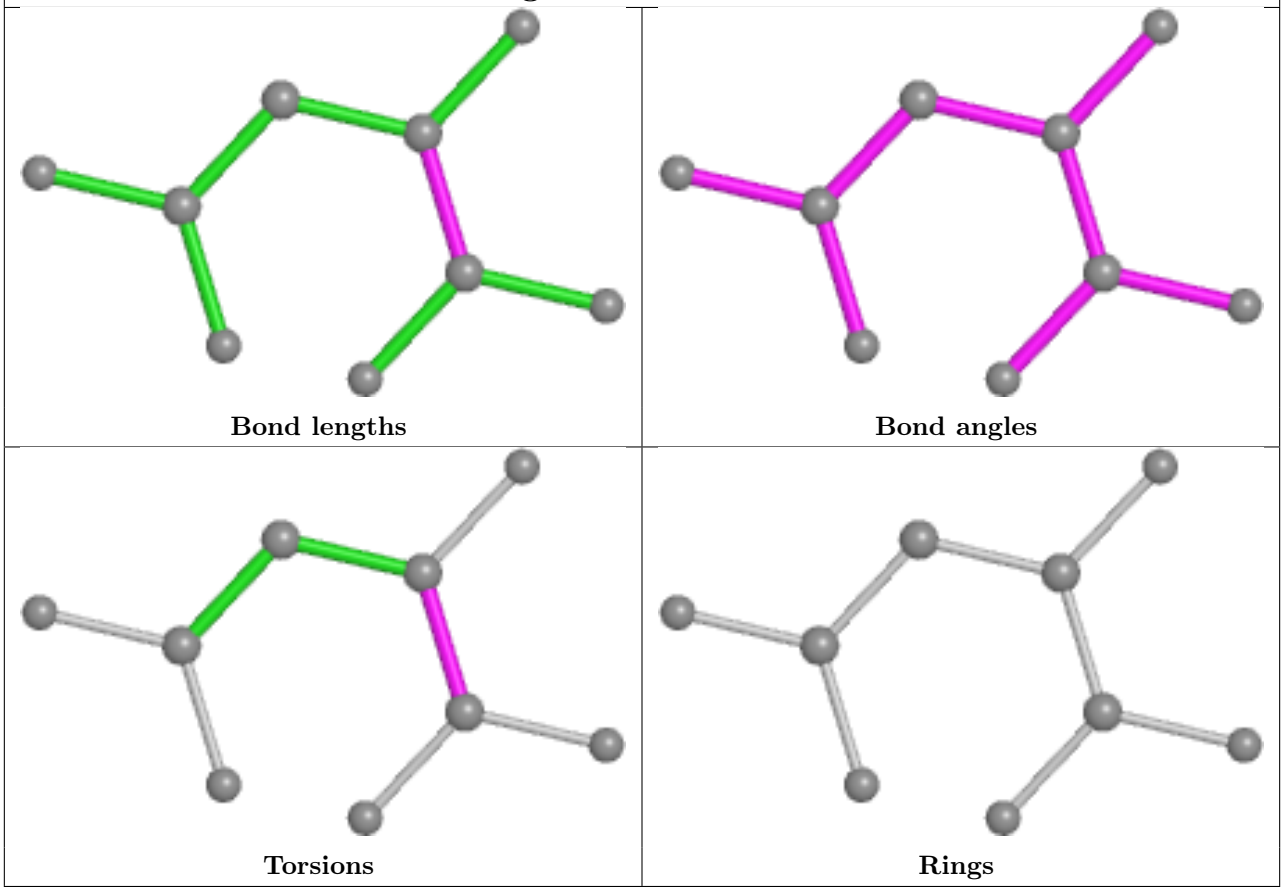
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	LMR	2	0
3	D	403	LMR	2	0
3	C	403	LMR	1	0

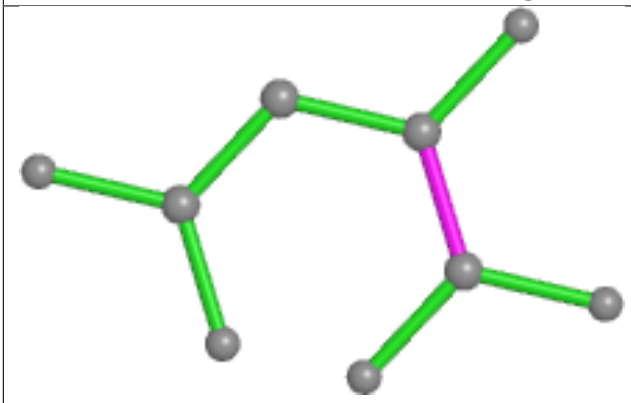
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

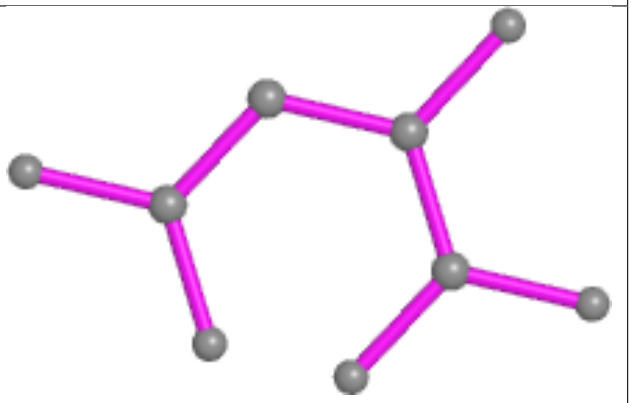
Ligand LMR B 403



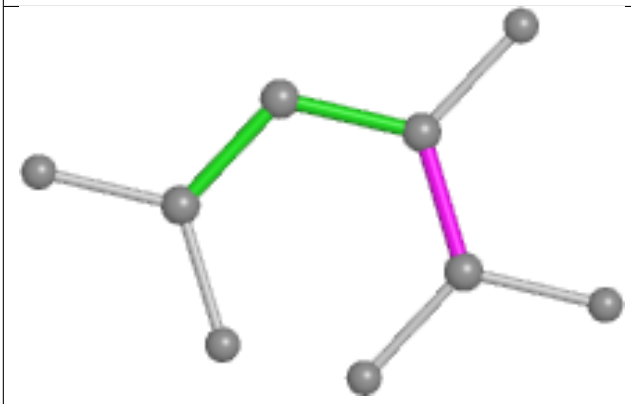
Ligand LMR A 403



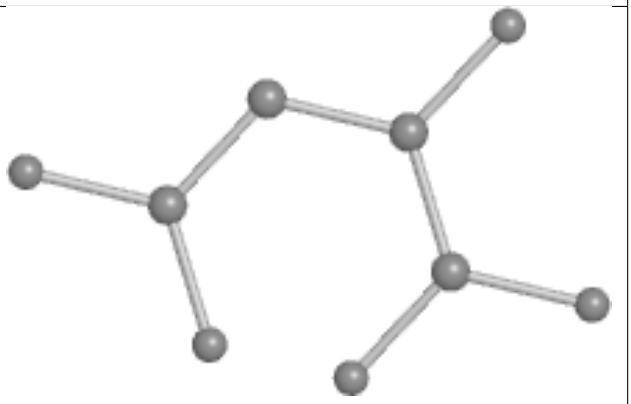
Bond lengths



Bond angles

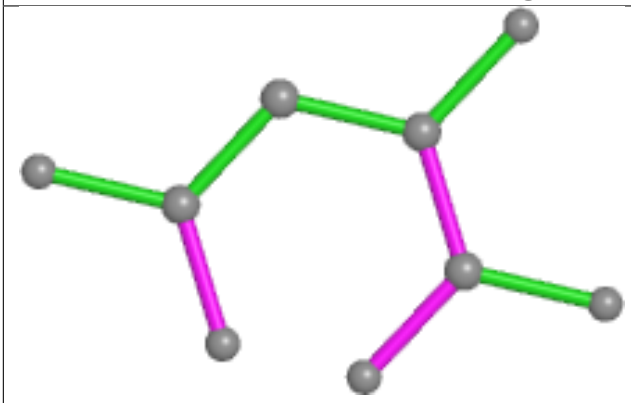


Torsions

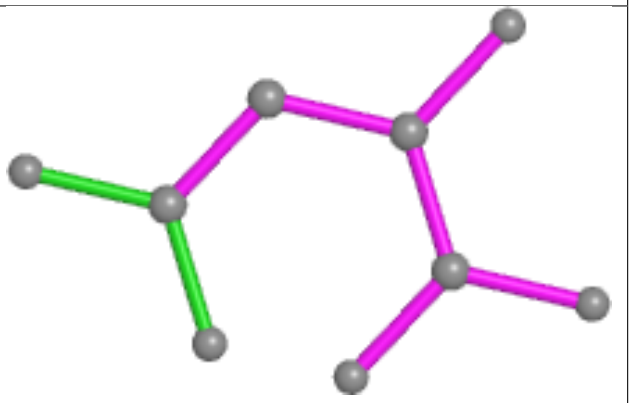


Rings

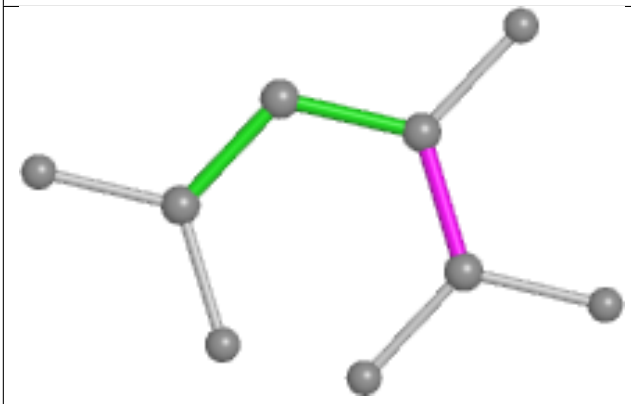
Ligand LMR D 403



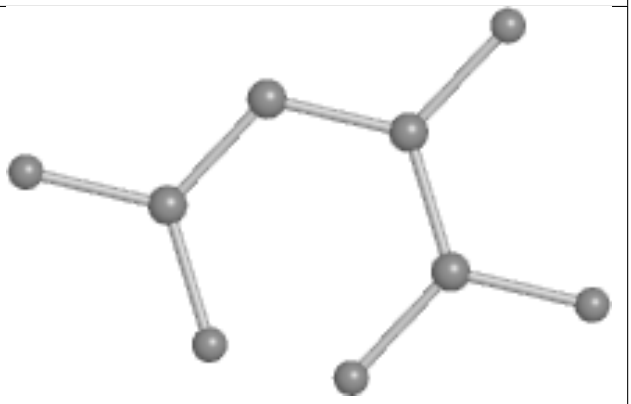
Bond lengths



Bond angles

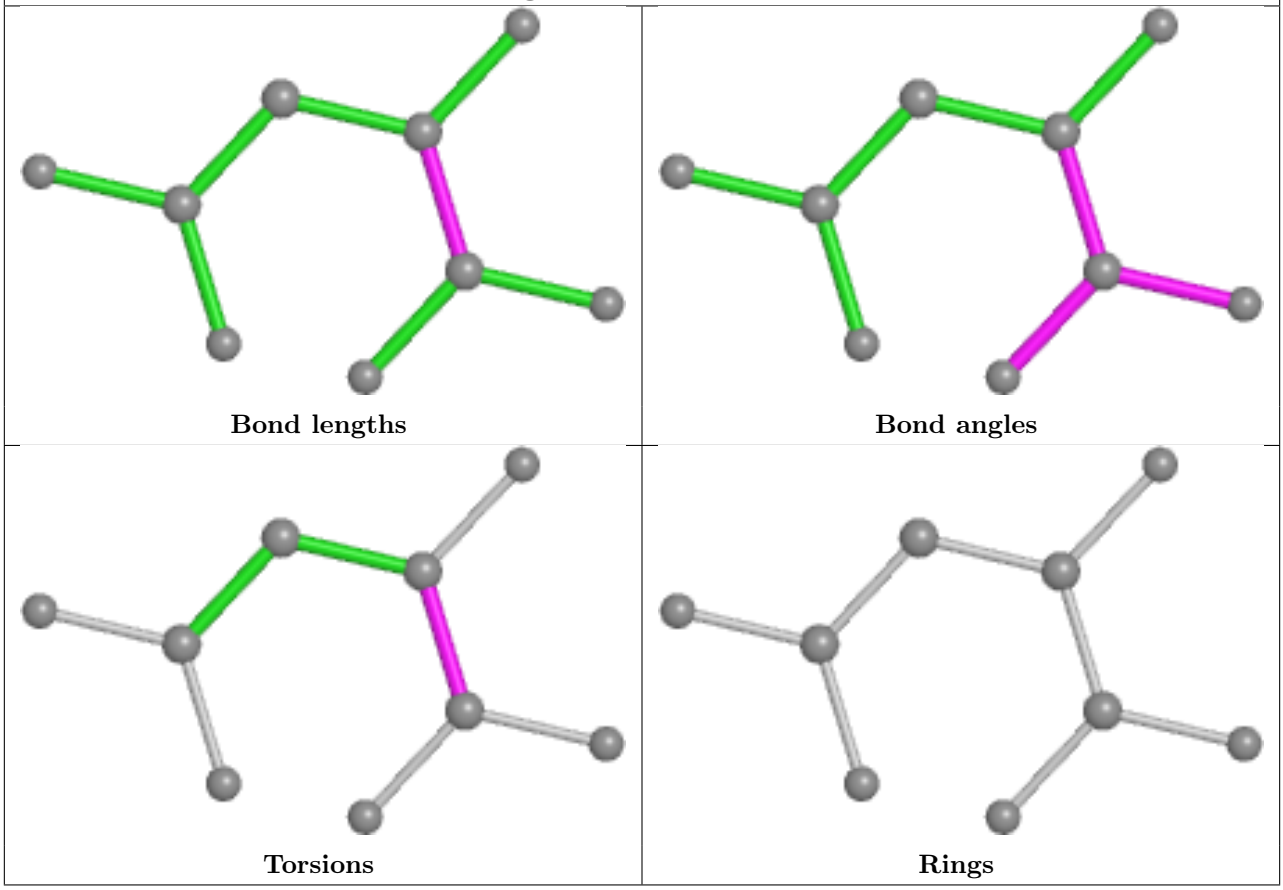


Torsions



Rings

Ligand LMR C 403



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	362/372 (97%)	-0.12	11 (3%)	50	57	7, 16, 34, 82	0
1	B	363/372 (97%)	0.18	13 (3%)	42	50	10, 24, 43, 69	0
1	C	362/372 (97%)	0.74	40 (11%)	5	8	12, 32, 56, 78	0
1	D	363/372 (97%)	-0.04	14 (3%)	39	47	7, 16, 36, 86	0
All	All	1450/1488 (97%)	0.19	78 (5%)	25	32	7, 21, 49, 86	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	VAL	10.0
1	D	146	GLY	9.7
1	A	2	VAL	7.4
1	C	144	HIS	7.3
1	D	2	VAL	7.0

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

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^{th} 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
1	KCX	B	98	12/13	0.94	0.17	13,16,17,20	0
1	KCX	C	98	12/13	0.95	0.12	25,28,35,35	0
1	KCX	A	98	12/13	0.98	0.10	6,9,10,10	0
1	KCX	D	98	12/13	0.98	0.13	7,9,11,12	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

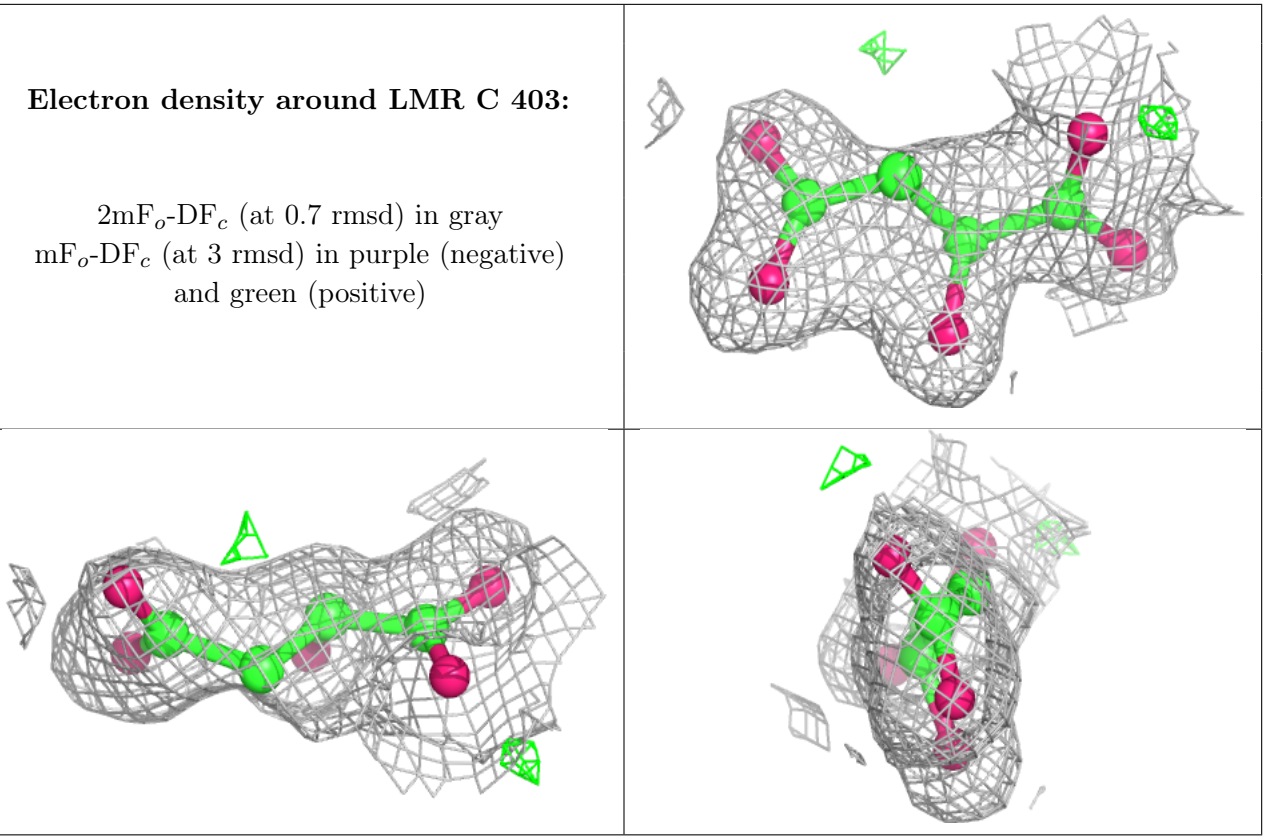
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	LMR	C	403	9/9	0.90	0.14	25,27,30,32	0
3	LMR	A	403	9/9	0.93	0.13	9,12,16,19	0
3	LMR	B	403	9/9	0.94	0.15	14,16,20,24	0
3	LMR	D	403	9/9	0.94	0.13	10,12,16,18	0
2	ZN	B	401	1/1	0.99	0.04	20,20,20,20	0
2	ZN	B	402	1/1	0.99	0.07	19,19,19,19	0
2	ZN	C	401	1/1	0.99	0.05	28,28,28,28	0
2	ZN	C	402	1/1	0.99	0.07	28,28,28,28	0
2	ZN	A	401	1/1	1.00	0.03	15,15,15,15	0
2	ZN	A	402	1/1	1.00	0.07	17,17,17,17	0
2	ZN	D	401	1/1	1.00	0.03	13,13,13,13	0
2	ZN	D	402	1/1	1.00	0.05	17,17,17,17	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.

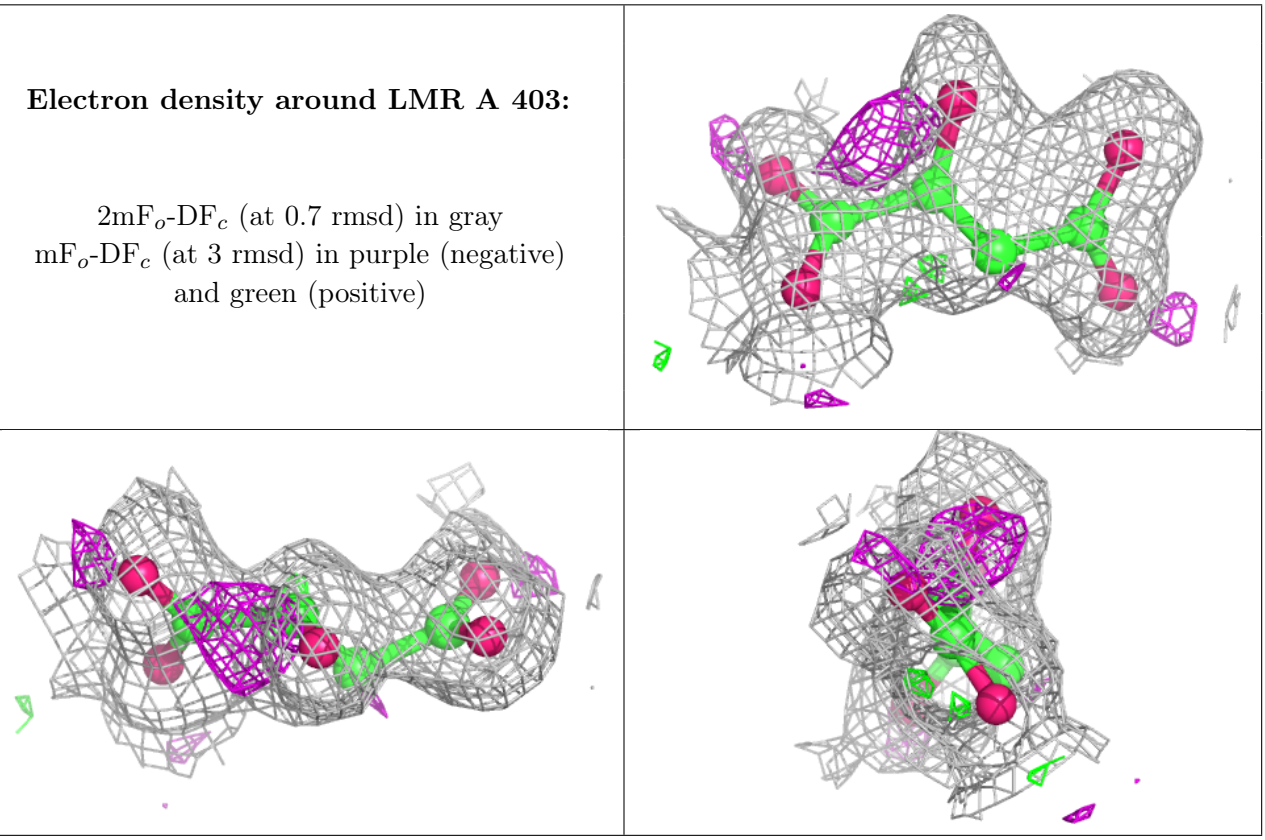
Electron density around LMR C 403:

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



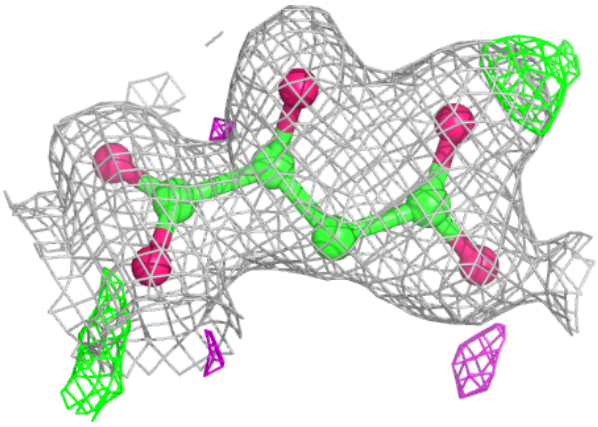
Electron density around LMR A 403:

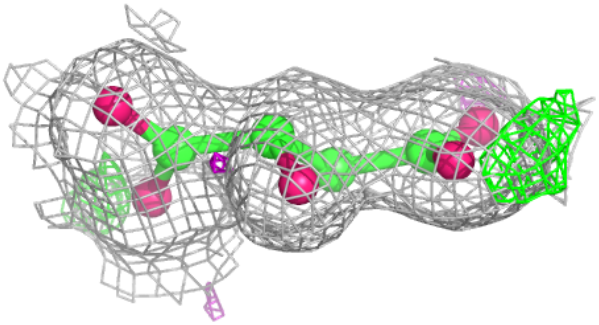
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

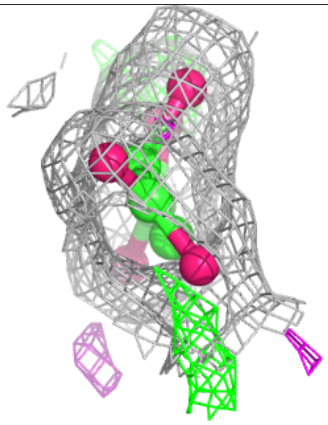


Electron density around LMR B 403:

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

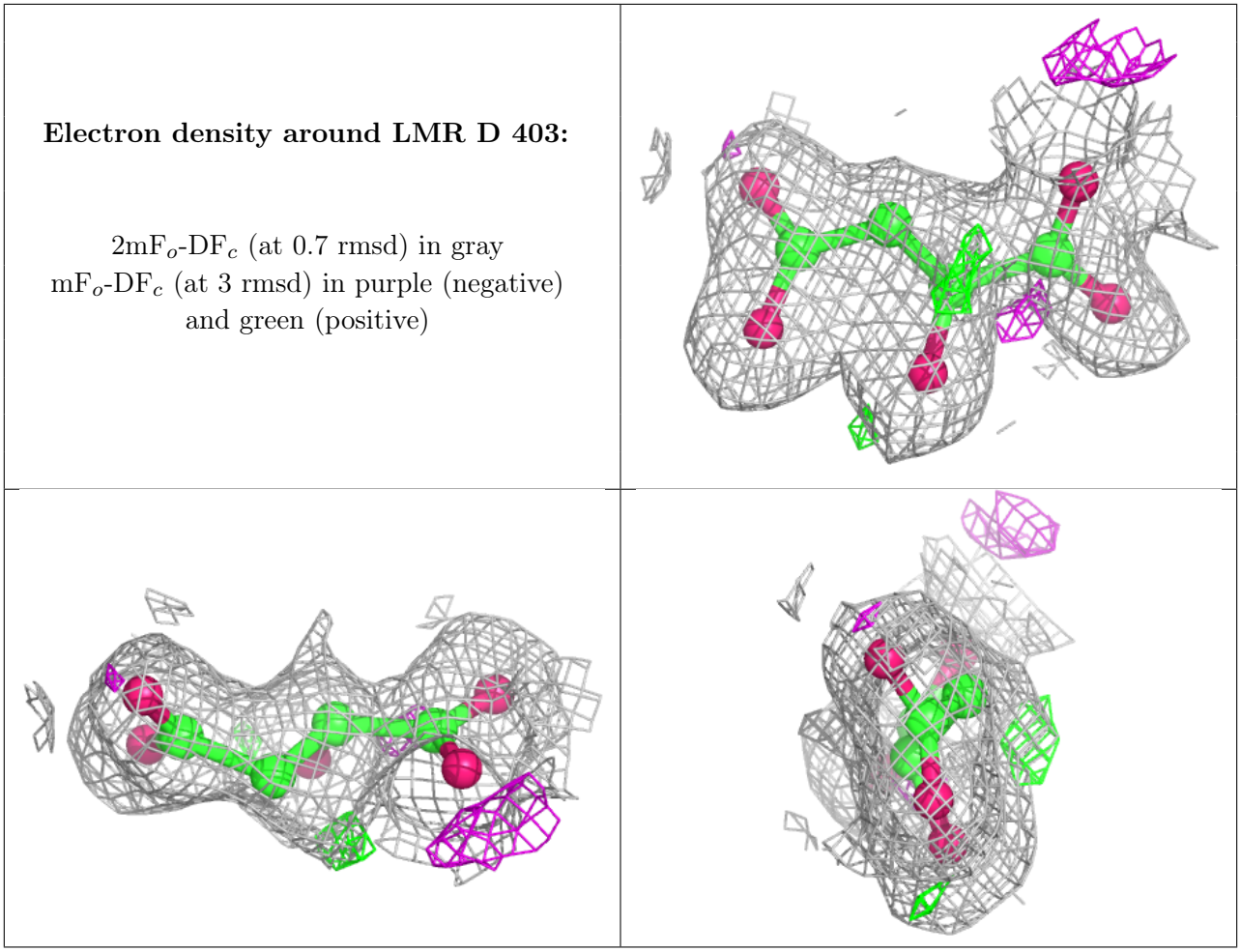






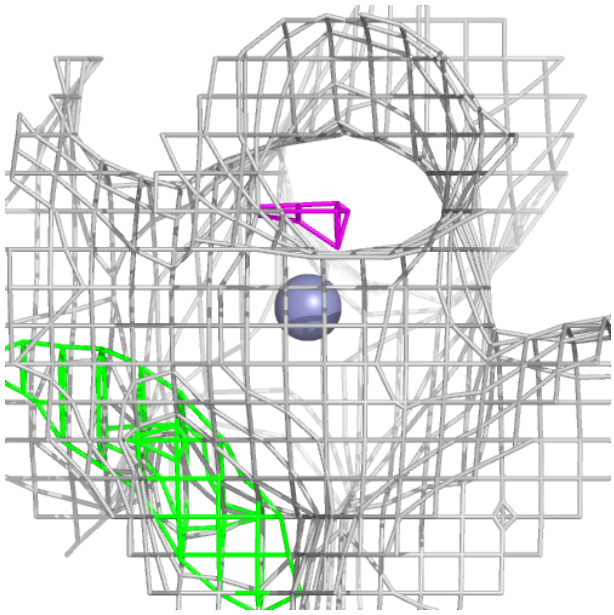
Electron density around LMR D 403:

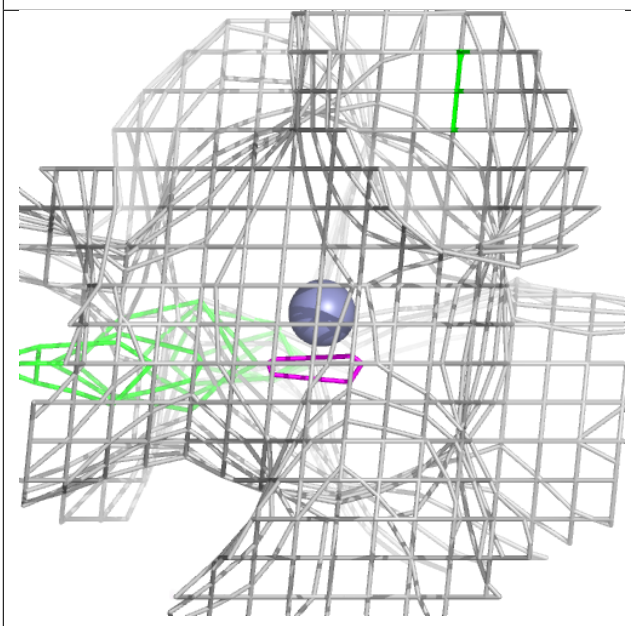
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

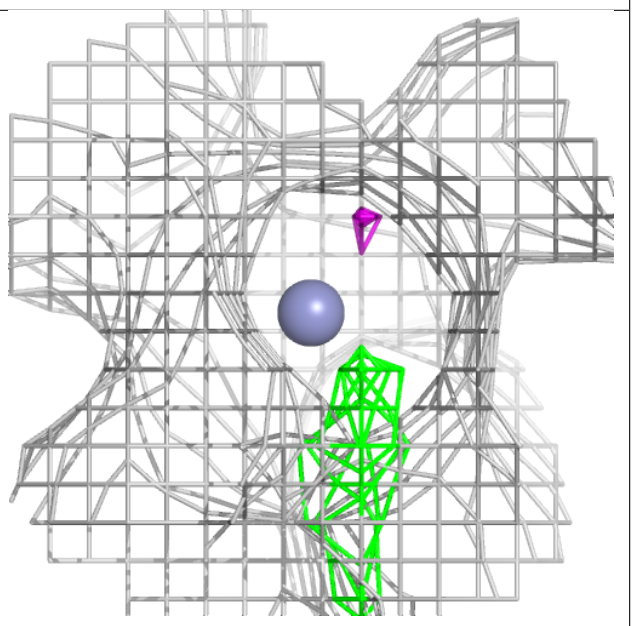


Electron density around ZN B 401:

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

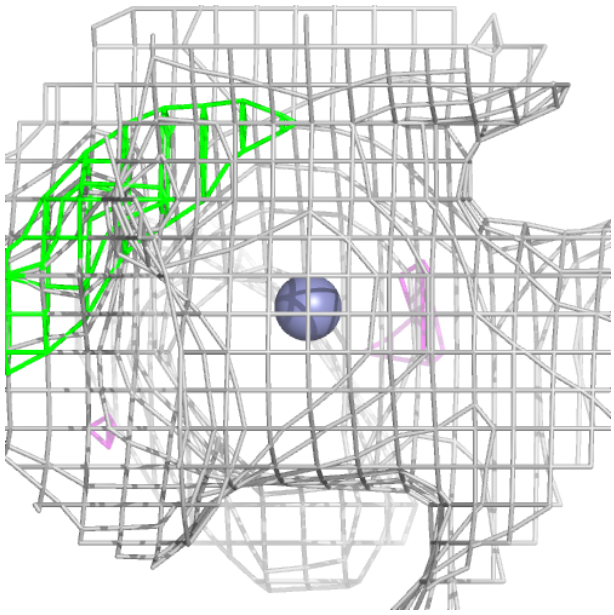


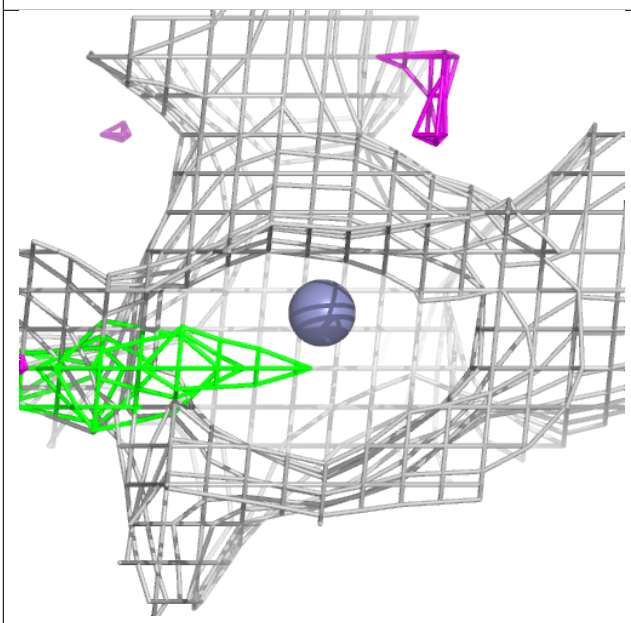


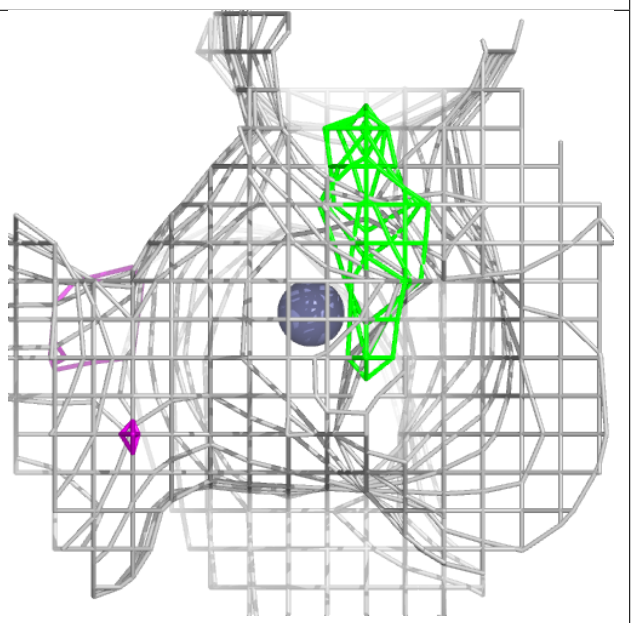


Electron density around ZN B 402:

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

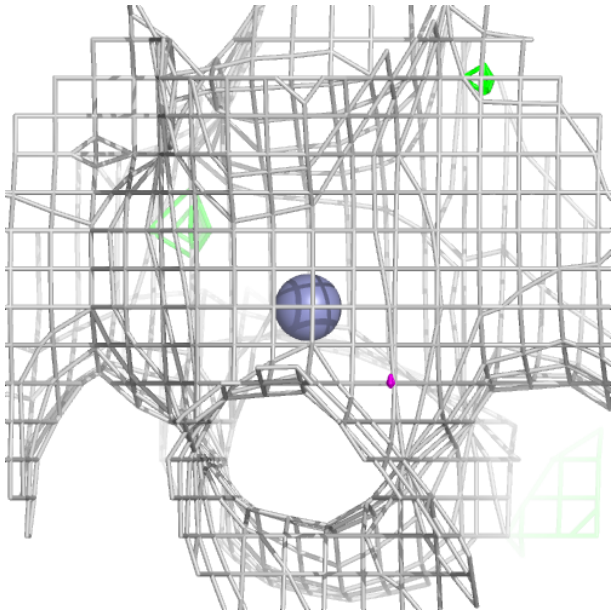


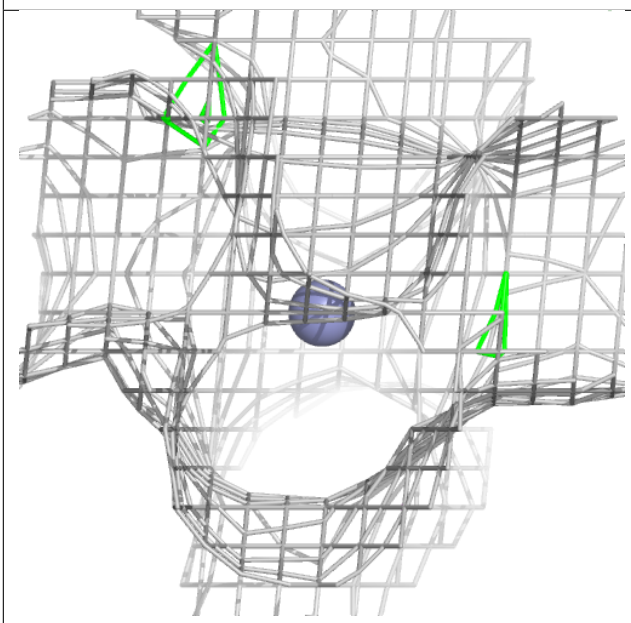


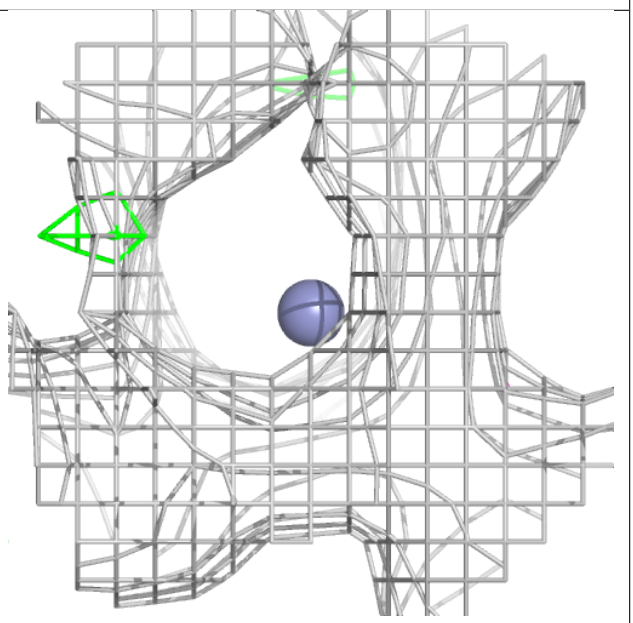


Electron density around ZN C 401:

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

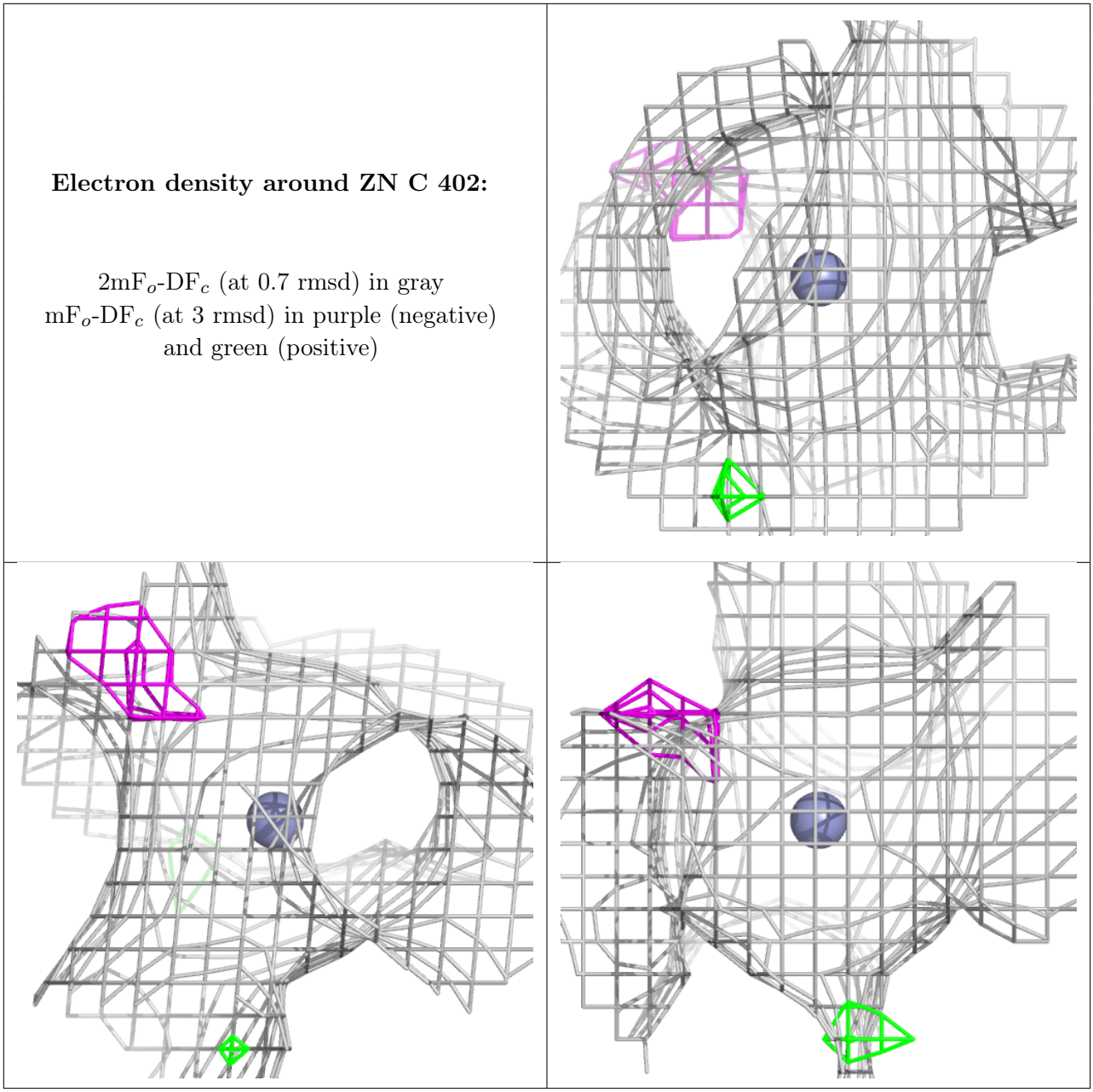






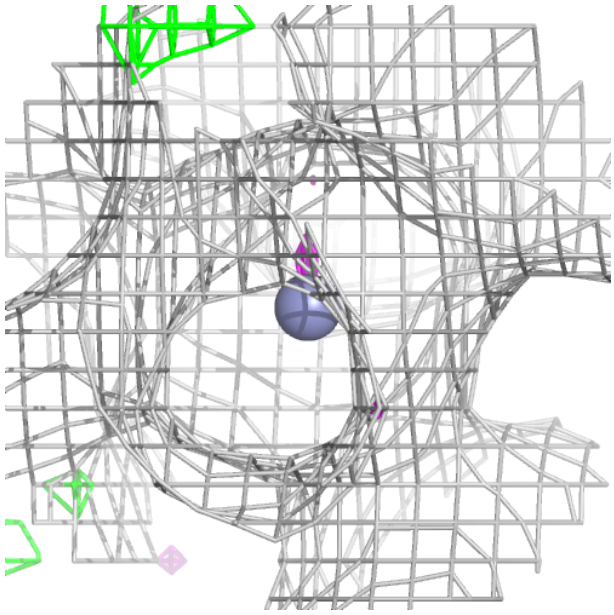
Electron density around ZN C 402:

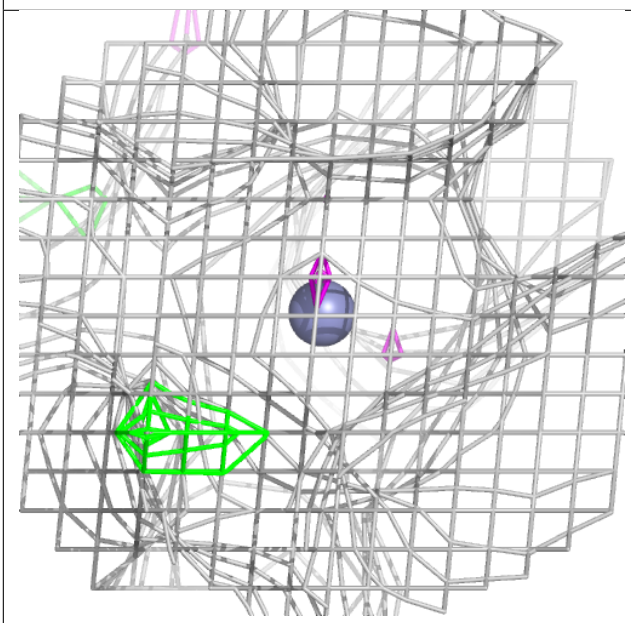
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

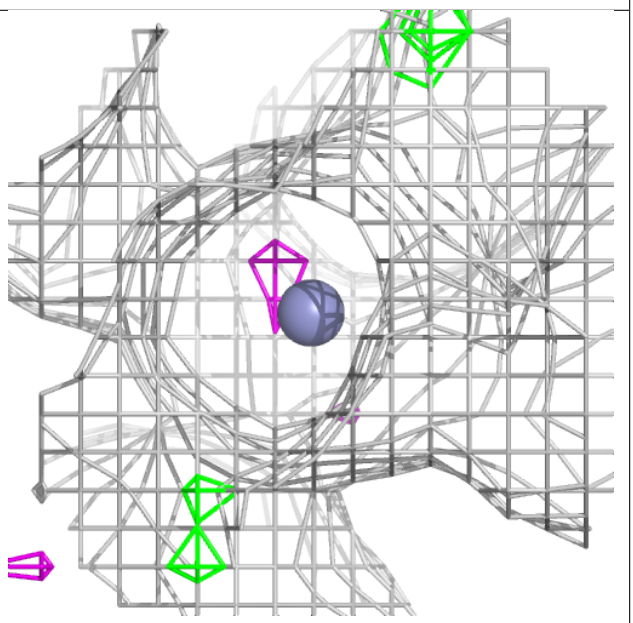


Electron density around ZN A 401:

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

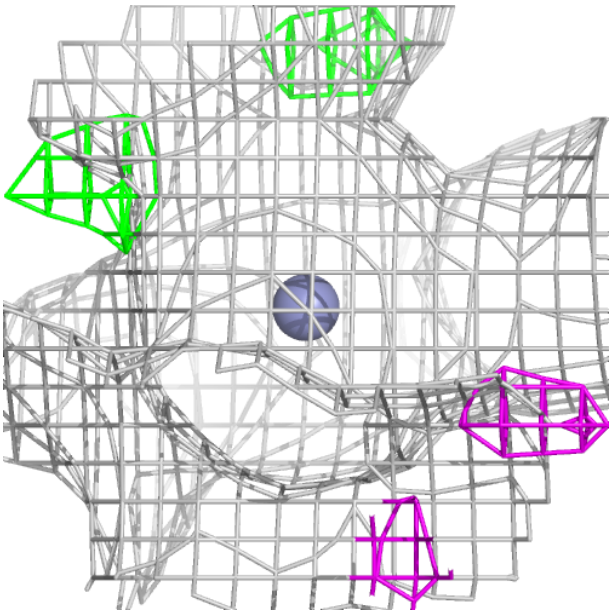


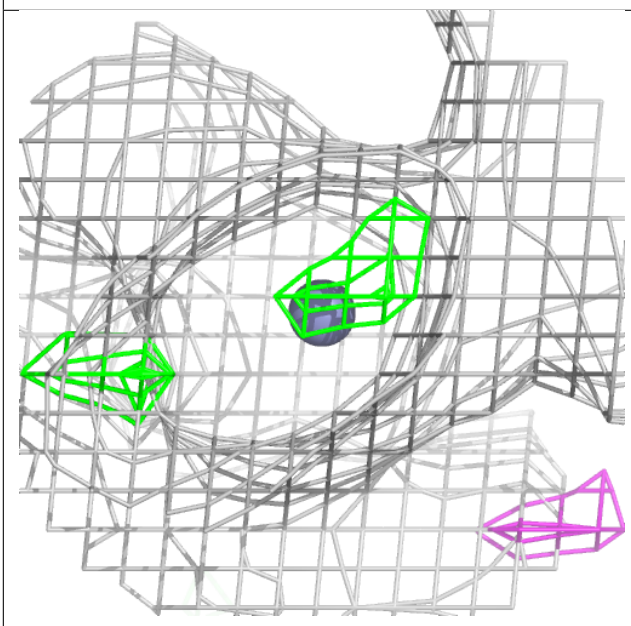


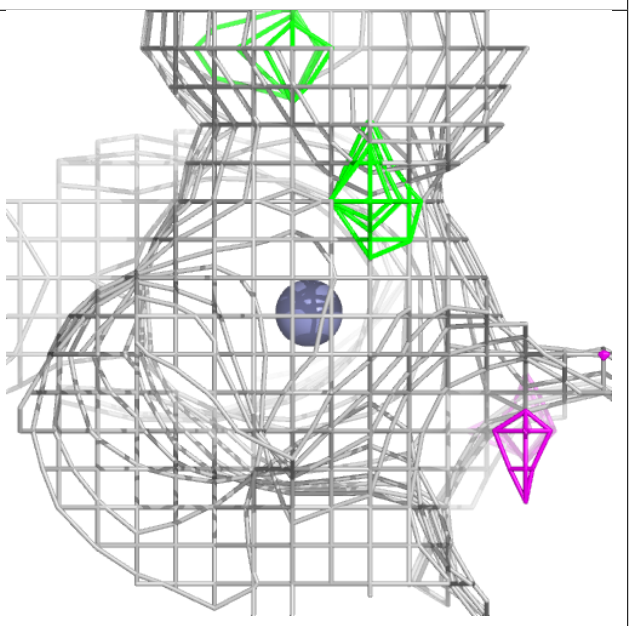


Electron density around ZN A 402:

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

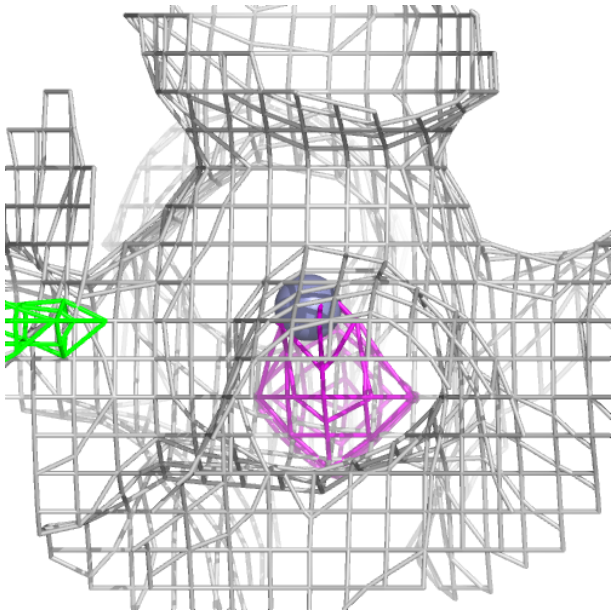


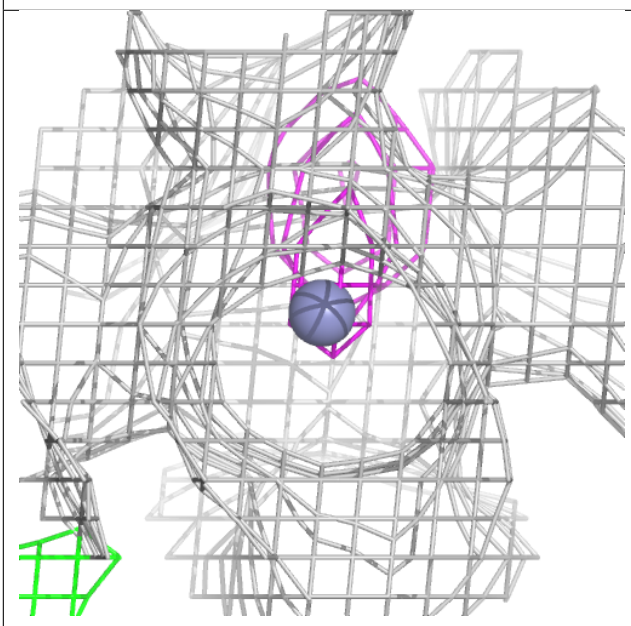


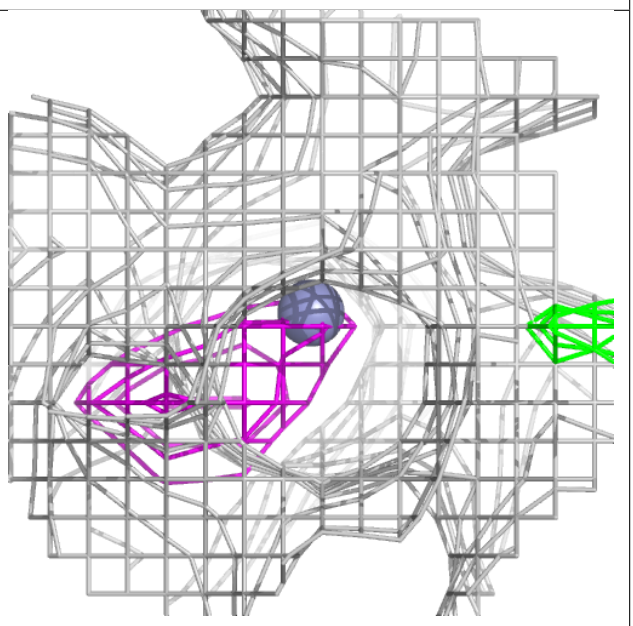


Electron density around ZN D 401:

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







Electron density around ZN D 402:

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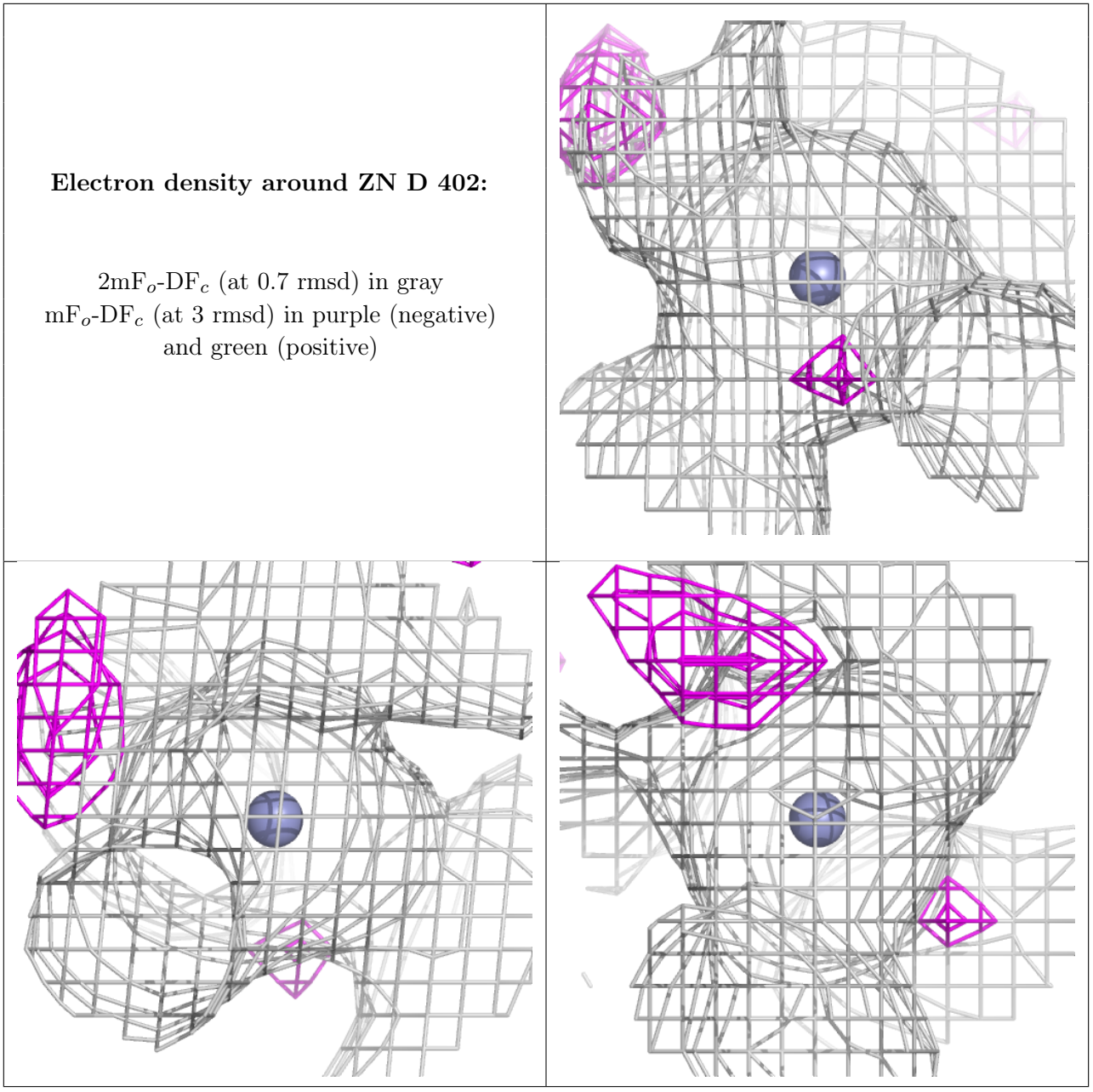
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.