Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2026 – 06:33 pm BST

PDB ID	:	9RG4 / pdb_00009rg4
Title	:	Unspecific peroxygenase from Psathyrella aberdarensis, Grogu variant, in complex with 5-formyl-2-furoic acid
Authors	:	Fernandez-Garcia, A.; Sanz-Aparicio, J.
Deposited on	:	2025-06-05
Resolution	:	1.70 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 (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:

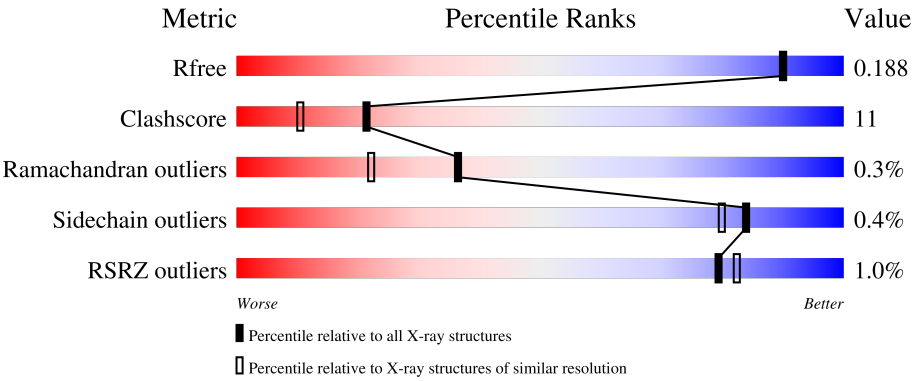
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	334	93% 7%
1	B	334	92% 8%
2	C	2	50% 50%
2	D	2	100%

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
12	A1JHS	B	401	-	X	-	-
3	NAG	A	407	-	-	X	-
3	NAG	B	413	-	-	X	-
5	PEG	A	406	-	-	X	-
5	PEG	A	409	-	-	X	-
6	GOL	A	404	-	-	X	-
6	GOL	A	405	-	-	X	-
6	GOL	B	411	-	-	X	-
6	GOL	B	412	-	-	X	-
8	MH0	A	412	X	-	-	-
8	MH0	B	414	X	-	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 6606 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 Heme-thiolate peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	5	0
			2613	1669	440	497	7			
1	B	334	Total	C	N	O	S	0	5	0
			2612	1669	439	497	7			

There are 6 discrepancies between the modelled and reference sequences:

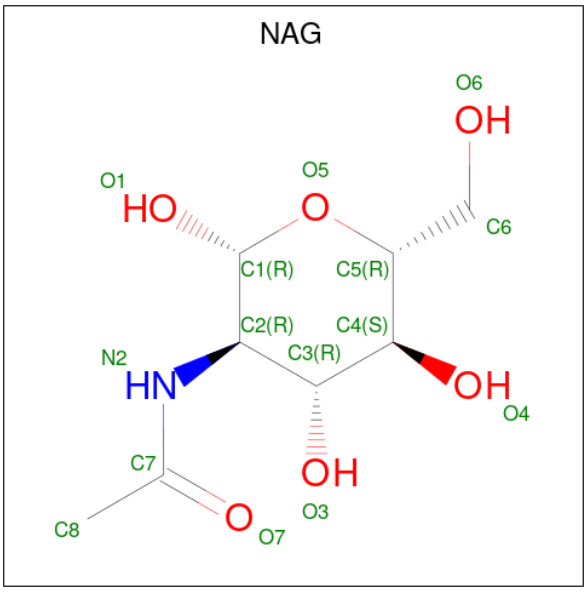
Chain	Residue	Modelled	Actual	Comment	Reference
A	61	ALA	SER	engineered mutation	UNP A0A4Q2DF39
A	79	ILE	LEU	engineered mutation	UNP A0A4Q2DF39
A	252	LEU	ALA	engineered mutation	UNP A0A4Q2DF39
B	61	ALA	SER	engineered mutation	UNP A0A4Q2DF39
B	79	ILE	LEU	engineered mutation	UNP A0A4Q2DF39
B	252	LEU	ALA	engineered mutation	UNP A0A4Q2DF39

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



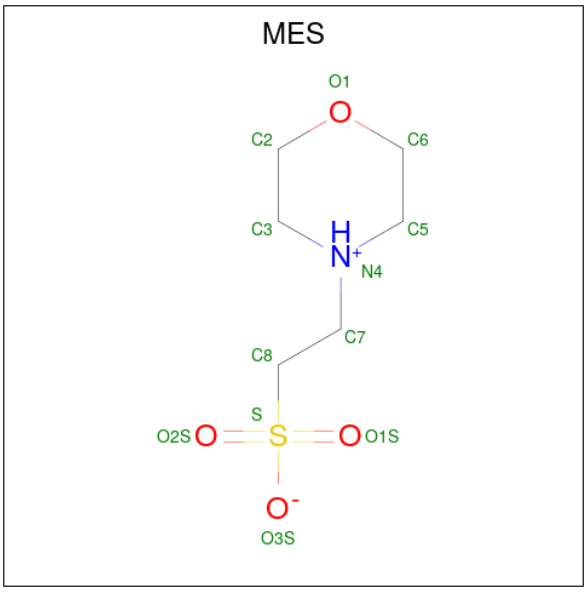
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



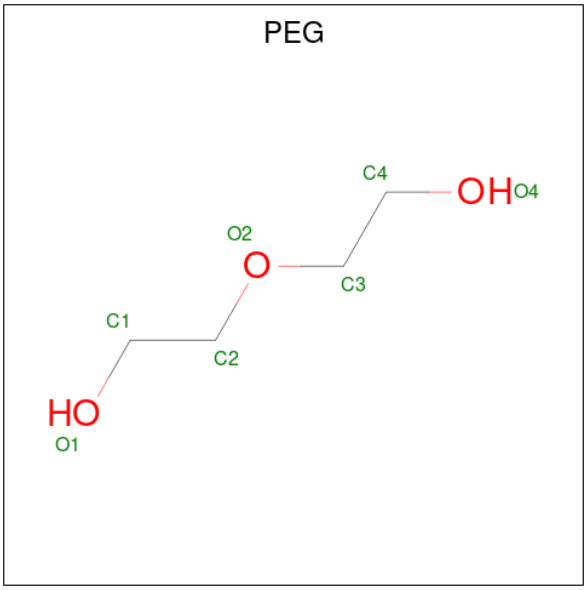
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



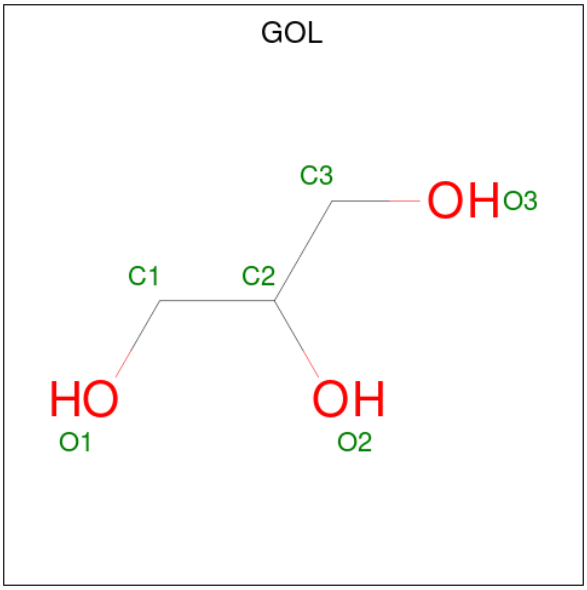
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

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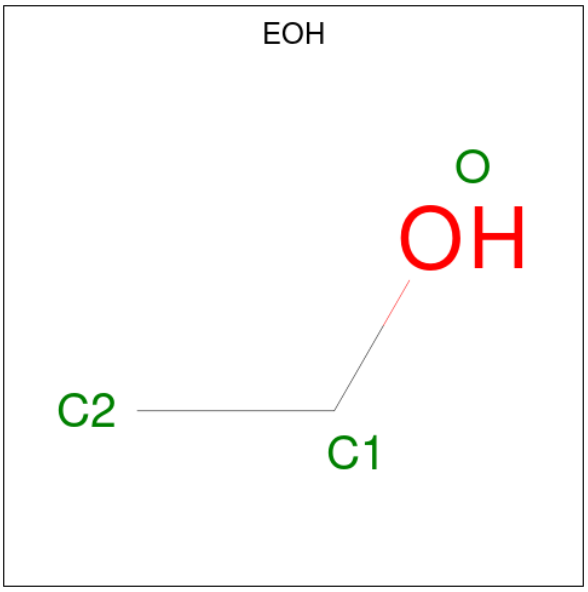
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



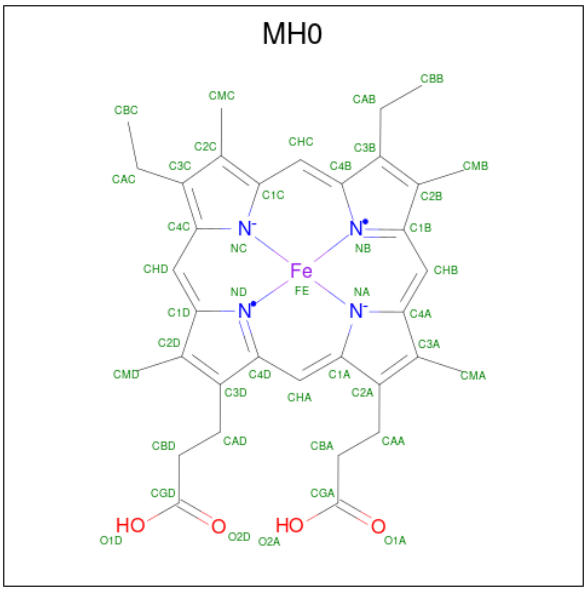
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 3 2 1	0	0
7	B	1	Total C O 3 2 1	0	0

- Molecule 8 is Mesoheme (CCD ID: MH0) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C Fe N O 43 34 1 4 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

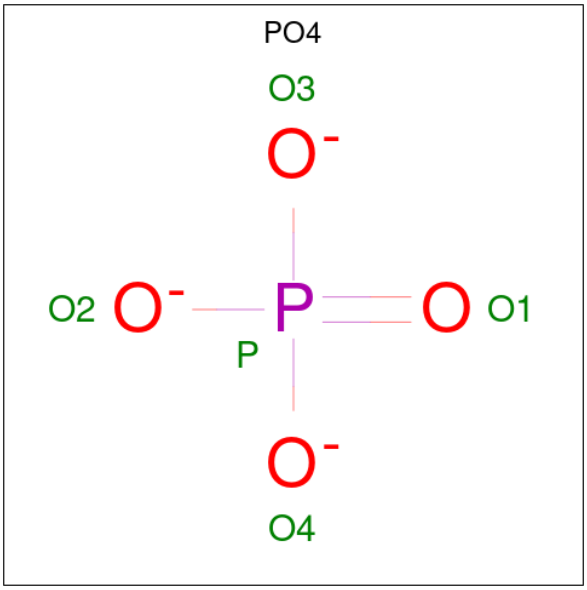
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		
9	B	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	10	Total	Zn	0	0
			10	10		
10	B	5	Total	Zn	0	0
			5	5		

- Molecule 11 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



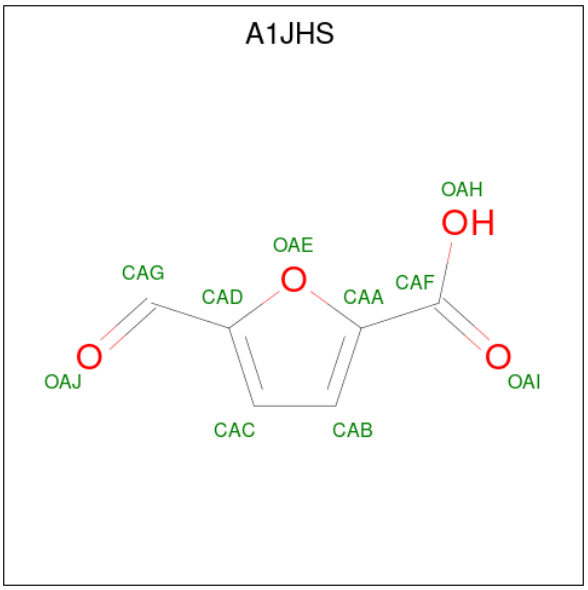
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	P	0	0
			5	4	1		

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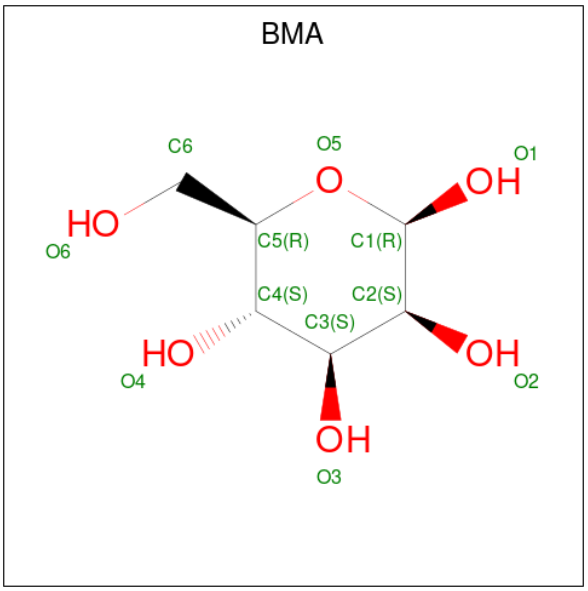
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total O P 5 4 1	0	0

- Molecule 12 is 5-Formyl-2-furancarboxylic Acid (CCD ID: A1JHS) (formula: $C_6H_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 13 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C O 11 6 5	0	0

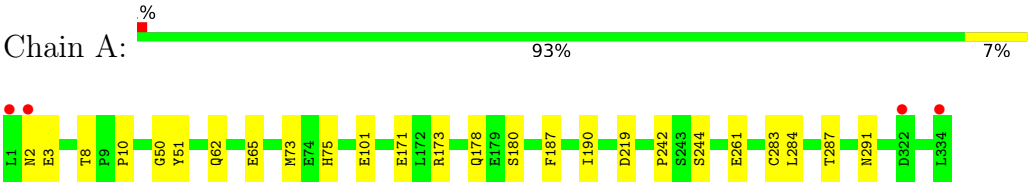
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	480	Total O 480 480	0	0
14	B	490	Total O 490 490	0	0

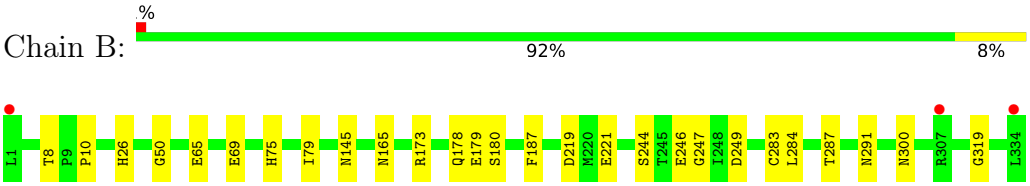
3 Residue-property plots (i)

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: Heme-thiolate peroxidase



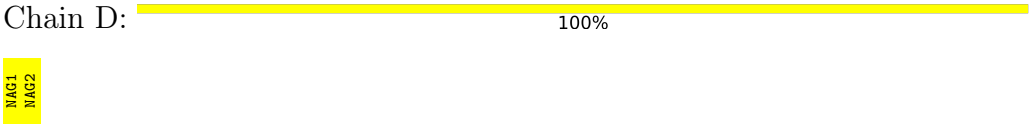
• Molecule 1: Heme-thiolate peroxidase



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	76.50Å 76.50Å 273.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.60 – 1.70 47.60 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.60-1.70) 98.5 (47.60-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.153 , 0.180 0.163 , 0.188	Depositor DCC
R_{free} test set	4772 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6606	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: ZN, MES, MG, EOH, A1JHS, PO4, MH0, BMA, GOL, NAG, PEG

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	0.54	0/2704	0.86	0/3687
1	B	0.53	0/2703	0.87	0/3687
All	All	0.53	0/5407	0.87	0/7374

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2613	0	2481	43	0
1	B	2612	0	2483	53	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	28	0	26	9	0
3	B	84	0	75	17	0
4	A	12	0	13	1	0
4	B	12	0	13	0	0
5	A	21	0	30	12	0
6	A	24	0	32	12	0
6	B	24	0	32	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	3	0	6	0	0
7	B	3	0	6	0	0
8	A	43	0	34	4	0
8	B	43	0	34	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	10	0	0	0	1
10	B	5	0	0	0	0
11	A	5	0	0	0	0
11	B	5	0	0	0	0
12	B	20	0	0	2	0
13	B	11	0	10	1	0
14	A	480	0	0	27	4
14	B	490	0	0	23	5
All	All	6606	0	5325	119	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 11.

All (119) 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:B:145:ASN:HD21	3:B:409:NAG:C1	0.92	1.51
1:B:165:ASN:ND2	3:B:406:NAG:C1	1.70	1.51
1:B:145:ASN:ND2	3:B:409:NAG:C1	1.77	1.47
1:A:291:ASN:HD21	3:A:407:NAG:C1	1.24	1.47
1:A:291:ASN:ND2	3:A:407:NAG:C1	1.90	1.31
1:B:291:ASN:ND2	3:B:413:NAG:C1	1.97	1.27
1:A:75:HIS:HD2	14:A:779:HOH:O	1.20	1.22
1:B:75:HIS:HD2	14:B:836:HOH:O	1.29	1.15
1:B:178:GLN:HG3	14:B:501:HOH:O	1.45	1.11
1:B:291:ASN:HD21	3:B:413:NAG:C1	1.60	1.11
6:A:404:GOL:H11	14:A:844:HOH:O	1.56	1.04
1:A:219:ASP:OD2	5:A:406:PEG:O2	1.78	1.02
1:A:65:GLU:OE1	6:A:405:GOL:H2	1.60	1.01
1:B:219:ASP:OD2	6:B:411:GOL:H12	1.60	1.01
1:A:261:GLU:OE2	14:A:501:HOH:O	1.79	0.99
1:B:291:ASN:CG	3:B:413:NAG:C1	2.38	0.97
1:B:219:ASP:CG	6:B:411:GOL:H12	1.87	0.97
1:A:178:GLN:HG3	14:A:510:HOH:O	1.68	0.93
1:B:8[B]:THR:HG22	14:B:589:HOH:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASN:CG	3:A:407:NAG:C1	2.47	0.87
1:A:219:ASP:OD2	5:A:406:PEG:C2	2.24	0.85
1:B:26:HIS:HE1	14:B:659:HOH:O	1.59	0.85
1:B:221:GLU:OE1	6:B:411:GOL:H32	1.75	0.84
6:A:404:GOL:C1	14:A:844:HOH:O	2.19	0.84
6:A:408:GOL:H31	14:A:872:HOH:O	1.80	0.82
1:B:249:ASP:H	6:B:412:GOL:H11	1.44	0.82
5:A:406:PEG:H12	14:A:840:HOH:O	1.80	0.81
1:A:101:GLU:OE1	14:A:502:HOH:O	1.97	0.81
1:A:284:LEU:HA	1:A:287[B]:THR:HG22	1.62	0.81
1:A:3:GLU:OE1	14:A:503:HOH:O	1.98	0.80
1:A:8:THR:HG22	14:A:951:HOH:O	1.80	0.79
1:B:284:LEU:HA	1:B:287[B]:THR:HG22	1.64	0.78
1:A:291:ASN:HD21	3:A:407:NAG:C2	1.95	0.78
1:B:26:HIS:CE1	14:B:659:HOH:O	2.33	0.78
5:A:409:PEG:O2	14:A:501:HOH:O	2.01	0.77
1:B:219:ASP:OD2	6:B:411:GOL:C1	2.32	0.77
1:B:179:GLU:OE2	14:B:502:HOH:O	2.03	0.77
1:B:178:GLN:NE2	14:B:501:HOH:O	1.93	0.76
1:B:145:ASN:CG	3:B:409:NAG:C1	2.60	0.75
1:B:287[A]:THR:HG22	14:B:673:HOH:O	1.86	0.73
1:B:69:GLU:OE2	14:B:504:HOH:O	2.05	0.73
4:A:402:MES:H52	14:A:856:HOH:O	1.89	0.73
1:B:291:ASN:ND2	3:B:413:NAG:O5	2.09	0.73
1:A:171:GLU:OE2	14:A:504:HOH:O	2.07	0.72
1:B:145:ASN:HD21	3:B:409:NAG:C2	1.96	0.72
1:A:2:ASN:HB3	14:A:851:HOH:O	1.89	0.71
8:B:414:MH0:H3	8:B:414:MH0:H20	1.71	0.71
6:A:411:GOL:H31	14:A:716:HOH:O	1.91	0.69
1:A:219:ASP:OD2	5:A:406:PEG:H21	1.91	0.69
8:A:412:MH0:H3	8:A:412:MH0:H20	1.75	0.68
1:B:178:GLN:CG	14:B:501:HOH:O	2.14	0.68
1:B:246:GLU:OE1	6:B:405:GOL:O3	2.10	0.68
1:B:65:GLU:OE1	14:B:505:HOH:O	2.14	0.66
1:A:219:ASP:CG	5:A:406:PEG:H21	2.21	0.66
1:A:219:ASP:CG	5:A:406:PEG:C2	2.71	0.64
6:A:408:GOL:C3	14:A:872:HOH:O	2.42	0.63
1:B:284:LEU:HD12	1:B:287[B]:THR:CG2	2.29	0.63
1:A:287[A]:THR:HG22	14:A:549:HOH:O	1.97	0.63
3:B:409:NAG:O3	3:B:410:NAG:C1	2.47	0.62
1:A:284:LEU:HD12	1:A:287[B]:THR:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASN:ND2	3:A:407:NAG:C2	2.59	0.61
1:B:249:ASP:HB2	6:B:412:GOL:C1	2.30	0.61
1:A:242:PRO:HB2	3:A:401:NAG:H82	1.83	0.61
1:B:291:ASN:OD1	3:B:413:NAG:C1	2.50	0.60
1:A:8:THR:CG2	14:A:951:HOH:O	2.44	0.59
1:A:73[B]:MET:HE3	8:A:412:MH0:H23	1.86	0.58
1:B:50:GLY:HA2	14:B:522:HOH:O	2.05	0.57
1:A:178:GLN:CG	14:A:510:HOH:O	2.40	0.56
1:B:75:HIS:CE1	1:B:79:ILE:HD11	2.42	0.55
1:A:219:ASP:OD1	5:A:406:PEG:H21	2.07	0.54
1:B:249:ASP:HB2	6:B:412:GOL:H11	1.88	0.54
1:B:287[A]:THR:HG21	14:B:842:HOH:O	2.08	0.54
1:A:51:TYR:O	6:A:405:GOL:H32	2.07	0.54
1:A:261:GLU:OE1	5:A:409:PEG:H42	2.08	0.54
1:A:50:GLY:HA2	14:A:517:HOH:O	2.07	0.53
1:B:247:GLY:H	6:B:412:GOL:C2	2.21	0.53
1:B:249:ASP:N	6:B:412:GOL:H11	2.21	0.53
1:B:249:ASP:CB	6:B:412:GOL:H11	2.39	0.52
1:A:291:ASN:OD1	3:A:407:NAG:C1	2.57	0.52
1:A:219:ASP:OD1	5:A:406:PEG:C2	2.58	0.51
1:B:75:HIS:NE2	1:B:79:ILE:HD11	2.26	0.51
1:B:219:ASP:OD1	6:B:411:GOL:H2	2.11	0.50
1:A:287[A]:THR:HG21	14:A:828:HOH:O	2.11	0.49
12:B:402:A1JHS:CAF	14:B:512:HOH:O	2.59	0.49
6:A:404:GOL:C3	14:A:844:HOH:O	2.60	0.49
6:A:404:GOL:H31	14:A:844:HOH:O	2.13	0.49
1:B:300:ASN:HB2	14:B:624:HOH:O	2.12	0.48
3:B:410:NAG:H2	14:B:611:HOH:O	2.14	0.48
3:B:413:NAG:C8	14:B:767:HOH:O	2.61	0.48
1:A:75:HIS:CD2	14:A:779:HOH:O	2.12	0.48
1:B:283:CYS:O	1:B:287[A]:THR:HG23	2.15	0.47
1:A:178:GLN:NE2	14:A:518:HOH:O	2.48	0.47
1:A:283:CYS:O	1:A:287[A]:THR:HG23	2.14	0.47
1:B:10:PRO:O	1:B:75:HIS:HE1	1.96	0.46
1:A:10:PRO:O	1:A:75:HIS:HE1	1.99	0.46
1:A:62:GLN:O	6:A:405:GOL:O3	2.32	0.46
1:B:319:GLY:O	12:B:402:A1JHS:CAB	2.63	0.46
1:A:291:ASN:ND2	3:A:407:NAG:O5	2.25	0.46
3:B:410:NAG:HO3	13:B:415:BMA:C1	2.28	0.46
3:A:401:NAG:H81	14:A:519:HOH:O	2.16	0.45
1:B:221:GLU:CD	6:B:411:GOL:H32	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASN:CG	14:B:624:HOH:O	2.60	0.45
3:B:413:NAG:H81	14:B:767:HOH:O	2.16	0.45
6:A:404:GOL:H2	14:A:765:HOH:O	2.17	0.45
5:A:409:PEG:H41	5:A:409:PEG:H22	1.81	0.45
1:B:287[A]:THR:CG2	14:B:673:HOH:O	2.58	0.44
1:B:247:GLY:H	6:B:412:GOL:H2	1.81	0.44
1:A:73[B]:MET:HE3	8:A:412:MH0:CMC	2.48	0.43
1:B:165:ASN:ND2	3:B:406:NAG:C2	2.67	0.43
1:A:180:SER:HB3	1:A:187:PHE:CD1	2.54	0.43
1:A:65:GLU:CD	6:A:405:GOL:H2	2.38	0.43
6:B:411:GOL:O3	14:B:503:HOH:O	2.03	0.42
1:B:75:HIS:CD2	14:B:836:HOH:O	2.21	0.42
1:A:190:ILE:CD1	5:A:409:PEG:H31	2.49	0.42
8:A:412:MH0:H21	8:A:412:MH0:H28	2.02	0.41
1:B:247:GLY:N	6:B:412:GOL:H2	2.35	0.41
1:B:300:ASN:CB	14:B:624:HOH:O	2.69	0.41
1:B:145:ASN:ND2	3:B:409:NAG:C2	2.71	0.40
1:B:180:SER:HB3	1:B:187:PHE:CD1	2.56	0.40

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)
10:A:423:ZN:ZN	14:B:532:HOH:O[5_545]	1.49	0.71
14:A:649:HOH:O	14:B:915:HOH:O[5_545]	1.69	0.51
14:A:777:HOH:O	14:B:532:HOH:O[5_545]	1.74	0.46
14:A:872:HOH:O	14:B:915:HOH:O[5_545]	2.12	0.08
14:A:576:HOH:O	14:B:577:HOH:O[5_555]	2.15	0.05

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	337/334 (101%)	324 (96%)	12 (4%)	1 (0%)	36	22
1	B	337/334 (101%)	322 (96%)	14 (4%)	1 (0%)	36	22
All	All	674/668 (101%)	646 (96%)	26 (4%)	2 (0%)	36	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	SER
1	B	244	SER

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	279/274 (102%)	278 (100%)	1 (0%)	84	80
1	B	279/274 (102%)	278 (100%)	1 (0%)	84	80
All	All	558/548 (102%)	556 (100%)	2 (0%)	84	80

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	B	173	ARG

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	241	GLN
1	A	291	ASN
1	B	145	ASN
1	B	241	GLN

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)

4 monosaccharides 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	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.30	0	17,19,21	0.81	0
2	NAG	C	2	2	14,14,15	0.37	0	17,19,21	1.30	2 (11%)
2	NAG	D	1	2,1	14,14,15	0.36	0	17,19,21	1.09	2 (11%)
2	NAG	D	2	2	14,14,15	0.35	0	17,19,21	1.03	2 (11%)

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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C2-N2-C7	3.65	128.09	122.90
2	C	2	NAG	C1-O5-C5	-2.91	108.25	112.19
2	D	2	NAG	C1-C2-N2	2.64	114.99	110.49
2	D	2	NAG	O4-C4-C3	-2.49	104.58	110.35
2	D	1	NAG	O5-C1-C2	2.36	115.01	111.29
2	D	1	NAG	C1-C2-N2	2.12	114.11	110.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

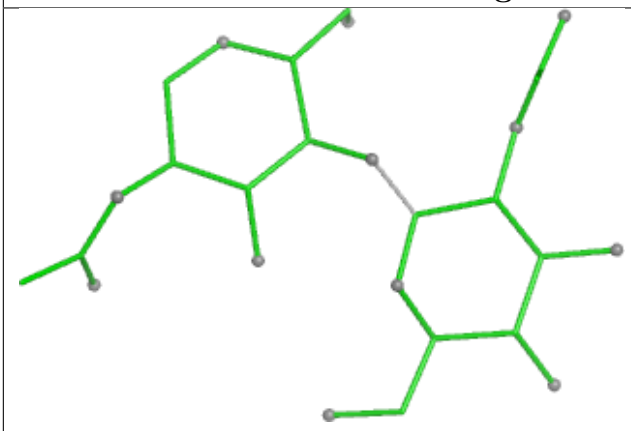
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2

There are no ring outliers.

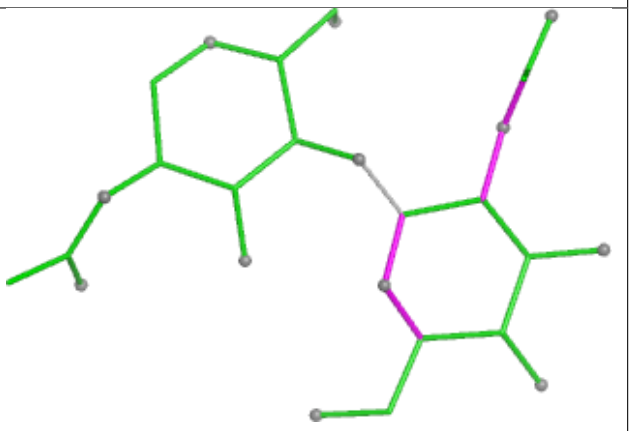
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

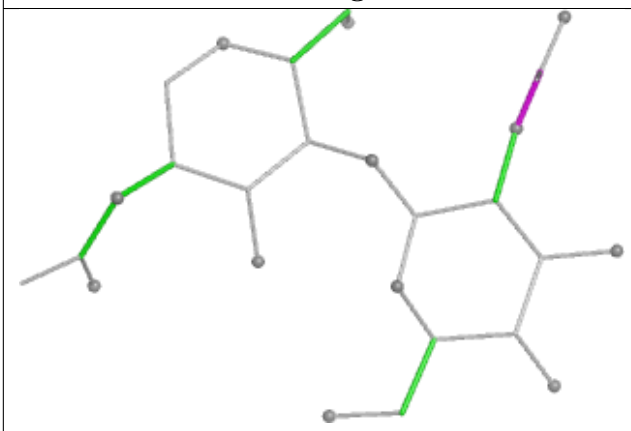
Oligosaccharide Chain C



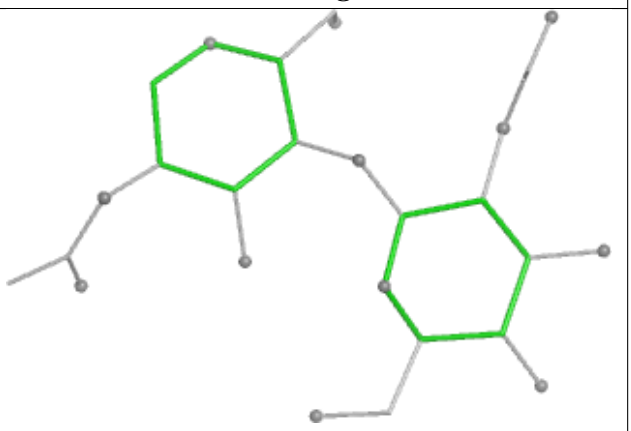
Bond lengths



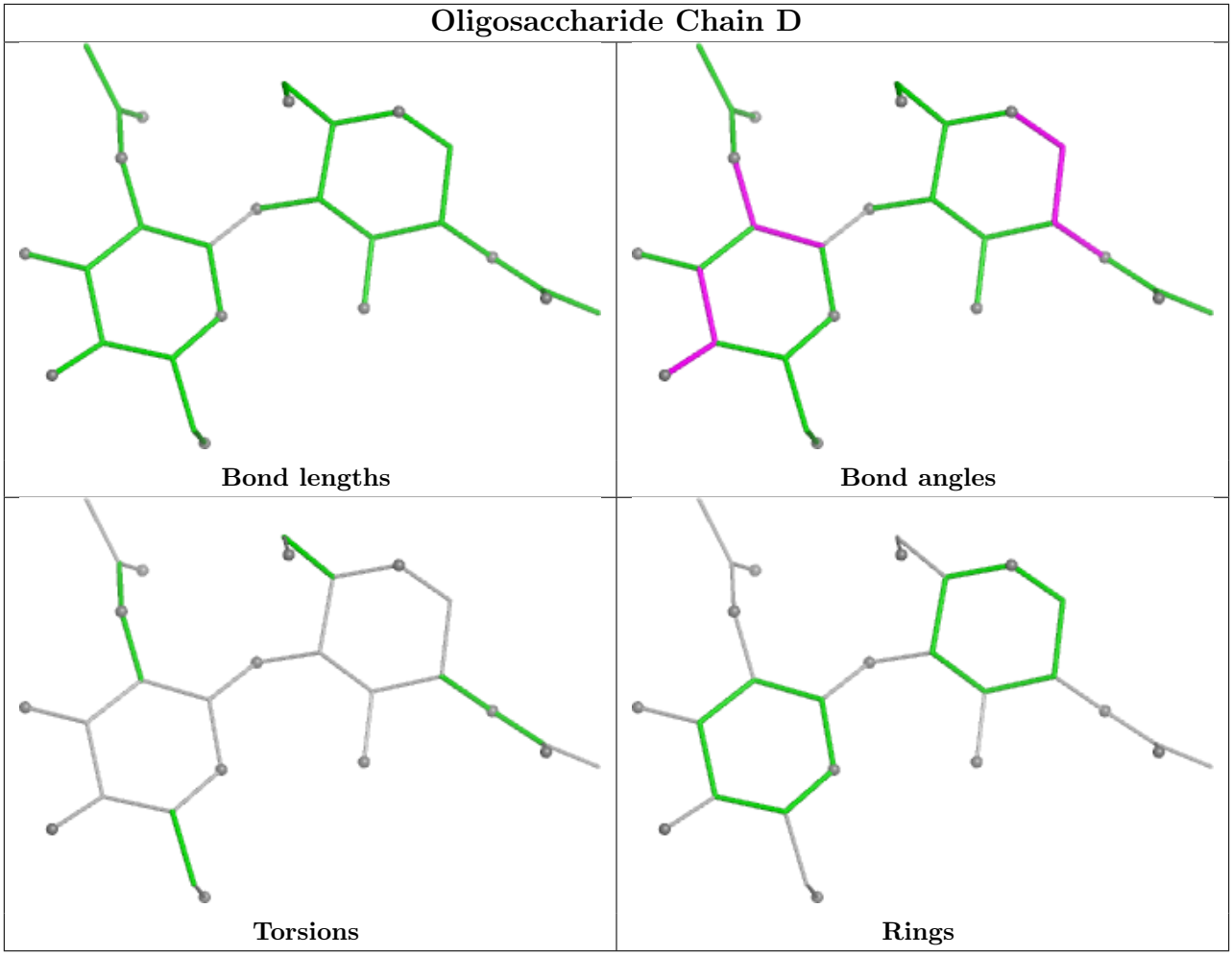
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 17 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
5	PEG	A	409	-	6,6,6	0.31	0	5,5,5	0.12	0
11	PO4	B	423	-	4,4,4	1.00	0	6,6,6	0.45	0
11	PO4	A	424	-	4,4,4	1.09	0	6,6,6	0.49	0
8	MH0	A	412	9,14,1	50,50,50	1.67	8 (16%)	68,82,82	1.94	22 (32%)
13	BMA	B	415	3	11,11,12	0.62	0	15,15,17	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	B	408	-	5,5,5	0.21	0	5,5,5	0.47	0
3	NAG	B	406	3	14,14,15	0.51	0	17,19,21	1.70	4 (23%)
6	GOL	A	405	-	5,5,5	0.18	0	5,5,5	0.31	0
8	MH0	B	414	9,14,1	50,50,50	1.75	12 (24%)	68,82,82	2.04	23 (33%)
6	GOL	B	412	-	5,5,5	0.22	0	5,5,5	0.57	0
3	NAG	B	413	-	14,14,15	0.31	0	17,19,21	0.74	0
6	GOL	B	411	-	5,5,5	0.12	0	5,5,5	0.43	0
5	PEG	A	403	-	6,6,6	0.19	0	5,5,5	0.14	0
3	NAG	B	407	3	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	B	410	13,3	14,14,15	0.36	0	17,19,21	1.43	4 (23%)
3	NAG	A	407	-	14,14,15	0.33	0	17,19,21	1.39	3 (17%)
12	A1JHS	B	401	-	10,10,10	1.80	2 (20%)	12,13,13	3.19	6 (50%)
6	GOL	B	405	-	5,5,5	0.17	0	5,5,5	0.30	0
3	NAG	B	409	3	14,14,15	0.55	0	17,19,21	1.05	1 (5%)
7	EOH	B	417	-	2,2,2	0.01	0	1,1,1	0.08	0
12	A1JHS	B	402	-	10,10,10	1.39	2 (20%)	12,13,13	3.13	7 (58%)
4	MES	B	404	-	12,12,12	0.91	0	14,16,16	0.72	1 (7%)
5	PEG	A	406	-	6,6,6	0.43	0	5,5,5	0.37	0
4	MES	A	402	-	12,12,12	0.81	0	14,16,16	1.67	1 (7%)
6	GOL	A	408	-	5,5,5	0.18	0	5,5,5	0.47	0
3	NAG	A	401	-	14,14,15	0.35	0	17,19,21	1.30	3 (17%)
7	EOH	A	410	-	2,2,2	0.23	0	1,1,1	0.19	0
6	GOL	A	404	-	5,5,5	0.17	0	5,5,5	0.46	0
6	GOL	A	411	-	5,5,5	0.17	0	5,5,5	0.35	0
3	NAG	B	403	-	14,14,15	0.44	0	17,19,21	2.01	2 (11%)

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
5	PEG	A	409	-	-	3/4/4/4	-
8	MH0	A	412	9,14,1	1/1/3/7	6/14/54/54	-
13	BMA	B	415	3	-	0/2/19/22	0/1/1/1
6	GOL	B	408	-	-	3/4/4/4	-
3	NAG	B	406	3	-	0/6/23/26	0/1/1/1
8	MH0	B	414	9,14,1	1/1/3/7	6/14/54/54	-
6	GOL	A	405	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	412	-	-	1/4/4/4	-
3	NAG	B	413	-	-	2/6/23/26	0/1/1/1
6	GOL	B	411	-	-	2/4/4/4	-
5	PEG	A	403	-	-	0/4/4/4	-
3	NAG	B	407	3	-	2/6/23/26	0/1/1/1
3	NAG	B	410	13,3	-	2/6/23/26	0/1/1/1
3	NAG	A	407	-	-	0/6/23/26	0/1/1/1
12	A1JHS	B	401	-	-	6/6/6/6	0/1/1/1
6	GOL	B	405	-	-	0/4/4/4	-
3	NAG	B	409	3	-	0/6/23/26	0/1/1/1
12	A1JHS	B	402	-	-	2/6/6/6	0/1/1/1
4	MES	B	404	-	-	1/6/14/14	0/1/1/1
5	PEG	A	406	-	-	2/4/4/4	-
4	MES	A	402	-	-	0/6/14/14	0/1/1/1
6	GOL	A	408	-	-	2/4/4/4	-
3	NAG	A	401	-	-	0/6/23/26	0/1/1/1
6	GOL	A	404	-	-	0/4/4/4	-
6	GOL	A	411	-	-	1/4/4/4	-
3	NAG	B	403	-	-	0/6/23/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	412	MH0	CBC-CAC	-4.71	1.30	1.51
8	B	414	MH0	CBC-CAC	-4.53	1.31	1.51
8	A	412	MH0	CBB-CAB	-4.51	1.31	1.51
12	B	401	A1JHS	CAG-CAD	4.23	1.53	1.44
8	B	414	MH0	CBB-CAB	-4.06	1.33	1.51
8	B	414	MH0	C4B-NB	-3.99	1.33	1.40
8	B	414	MH0	FE-NB	3.90	2.06	1.94
8	B	414	MH0	FE-NC	3.84	2.08	1.95
8	A	412	MH0	FE-NB	3.71	2.06	1.94
8	A	412	MH0	FE-NC	3.43	2.06	1.95
8	A	412	MH0	C4B-NB	-3.41	1.34	1.40
8	A	412	MH0	C1D-ND	-3.00	1.35	1.40
12	B	402	A1JHS	CAG-CAD	2.60	1.50	1.44
8	B	414	MH0	C1D-ND	-2.55	1.35	1.40
8	B	414	MH0	FE-NA	2.52	2.03	1.95
8	B	414	MH0	C4B-C3B	2.49	1.49	1.45
8	B	414	MH0	C1C-NC	-2.47	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	414	MH0	C4D-C3D	2.32	1.49	1.45
12	B	401	A1JHS	OAI-CAF	2.30	1.28	1.22
8	B	414	MH0	C4C-NC	-2.20	1.35	1.39
8	A	412	MH0	C1D-C2D	2.20	1.48	1.44
8	A	412	MH0	C4D-C3D	2.07	1.48	1.45
12	B	402	A1JHS	OAI-CAF	2.06	1.28	1.22
8	B	414	MH0	C1B-NB	-2.00	1.34	1.38

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	403	NAG	O5-C1-C2	7.36	122.91	111.29
12	B	401	A1JHS	OAE-CAD-CAG	6.84	127.54	118.33
12	B	402	A1JHS	OAE-CAD-CAG	6.83	127.52	118.33
8	B	414	MH0	C4C-NC-C1C	5.71	110.94	105.35
4	A	402	MES	O2S-S-C8	-5.48	100.32	106.92
12	B	402	A1JHS	OAE-CAA-CAB	-5.07	103.71	109.69
12	B	401	A1JHS	OAE-CAA-CAB	-4.97	103.83	109.69
8	A	412	MH0	C4C-NC-C1C	4.61	109.86	105.35
8	B	414	MH0	C4B-NB-C1B	4.53	109.75	105.07
8	A	412	MH0	CAB-C3B-C4B	4.23	130.30	124.81
8	B	414	MH0	CHC-C4B-NB	4.13	129.47	124.37
8	B	414	MH0	CMB-C2B-C1B	4.13	131.33	125.04
8	A	412	MH0	CHC-C4B-NB	4.06	129.38	124.37
3	B	406	NAG	O5-C1-C2	4.00	117.61	111.29
8	A	412	MH0	C4B-NB-C1B	3.79	108.98	105.07
3	B	406	NAG	O3-C3-C2	-3.77	101.67	109.47
12	B	402	A1JHS	CAC-CAB-CAA	3.70	110.27	106.95
12	B	401	A1JHS	CAC-CAB-CAA	3.68	110.25	106.95
8	B	414	MH0	CAB-C3B-C4B	3.66	129.55	124.81
3	B	410	NAG	C1-O5-C5	3.57	117.03	112.19
3	A	407	NAG	C1-C2-N2	3.55	116.55	110.49
8	A	412	MH0	C4A-NA-C1A	3.44	108.71	105.35
12	B	401	A1JHS	CAA-OAE-CAD	3.39	113.94	106.59
8	B	414	MH0	CHA-C4D-ND	3.37	128.07	124.42
8	A	412	MH0	CAC-C3C-C4C	-3.33	120.30	124.92
8	A	412	MH0	CHA-C1A-NA	3.28	127.98	124.44
8	A	412	MH0	CHA-C4D-ND	3.21	127.90	124.42
8	B	414	MH0	CAC-C3C-C2C	3.15	131.90	126.86
3	A	401	NAG	O5-C1-C2	-3.13	106.34	111.29
12	B	401	A1JHS	OAE-CAD-CAC	-3.11	104.96	109.75
8	B	414	MH0	C3C-C4C-NC	-3.09	106.70	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	414	MH0	CHA-C4D-C3D	-3.06	120.35	124.84
12	B	402	A1JHS	CAA-OAE-CAD	3.05	113.21	106.59
8	A	412	MH0	CHA-C4D-C3D	-2.98	120.47	124.84
3	A	407	NAG	O5-C1-C2	-2.95	106.63	111.29
8	B	414	MH0	CBC-CAC-C3C	2.94	120.54	112.43
8	B	414	MH0	CAC-C3C-C4C	-2.93	120.85	124.92
8	B	414	MH0	CHA-C1A-NA	2.91	127.59	124.44
8	A	412	MH0	CHB-C4A-NA	2.88	127.55	124.44
8	B	414	MH0	CHB-C1B-NB	2.84	127.50	124.42
12	B	401	A1JHS	OAH-CAF-CAA	2.83	121.27	114.20
3	B	410	NAG	O4-C4-C5	2.81	116.28	109.30
3	A	407	NAG	C1-O5-C5	-2.80	108.40	112.19
12	B	402	A1JHS	OAH-CAF-CAA	2.73	121.00	114.20
3	A	401	NAG	C1-O5-C5	2.72	115.88	112.19
8	B	414	MH0	CAB-C3B-C2B	-2.69	122.92	127.53
8	A	412	MH0	CHD-C4C-NC	2.69	128.79	123.85
3	B	410	NAG	O4-C4-C3	-2.68	104.16	110.35
8	B	414	MH0	O1D-CGD-CBD	2.63	122.48	114.03
8	B	414	MH0	CHD-C4C-NC	2.61	128.66	123.85
8	A	412	MH0	C3C-C4C-NC	-2.58	107.27	110.15
8	A	412	MH0	CBB-CAB-C3B	2.57	119.52	112.43
3	B	409	NAG	O5-C1-C2	-2.57	107.23	111.29
8	A	412	MH0	C2A-C1A-NA	-2.56	107.83	110.32
8	B	414	MH0	C3B-C4B-NB	-2.56	107.32	110.17
8	A	412	MH0	CBC-CAC-C3C	2.54	119.43	112.43
3	B	403	NAG	C1-O5-C5	2.52	115.60	112.19
8	A	412	MH0	CAC-C3C-C2C	2.50	130.86	126.86
3	A	401	NAG	C1-C2-N2	2.50	114.75	110.49
12	B	402	A1JHS	OAE-CAD-CAC	-2.49	105.91	109.75
8	A	412	MH0	CHB-C1B-NB	2.47	127.10	124.42
8	A	412	MH0	CAB-C3B-C2B	-2.47	123.31	127.53
13	B	415	BMA	O2-C2-C3	2.43	115.00	110.14
8	A	412	MH0	O1D-CGD-CBD	2.41	121.77	114.03
3	B	406	NAG	O5-C5-C6	-2.37	103.49	107.20
8	A	412	MH0	C3B-C4B-NB	-2.37	107.53	110.17
8	A	412	MH0	CMB-C2B-C1B	2.34	128.60	125.04
8	B	414	MH0	CBB-CAB-C3B	2.30	118.77	112.43
3	B	406	NAG	C1-O5-C5	2.27	115.27	112.19
8	B	414	MH0	C1A-CHA-C4D	-2.27	121.17	126.06
8	B	414	MH0	CHB-C4A-NA	2.21	126.83	124.44
8	A	412	MH0	CAD-CBD-CGD	-2.20	108.88	113.60
8	B	414	MH0	C4A-NA-C1A	2.10	107.41	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	402	A1JHS	CAB-CAA-CAF	-2.10	127.20	132.19
8	B	414	MH0	CHD-C1D-ND	2.07	126.93	124.37
8	B	414	MH0	CAD-CBD-CGD	-2.05	109.18	113.60
4	B	404	MES	O1S-S-C8	-2.05	104.45	106.92
3	B	410	NAG	O5-C5-C6	-2.02	104.05	107.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	412	MH0	NA
8	B	414	MH0	NA

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	407	NAG	C8-C7-N2-C2
3	B	407	NAG	O7-C7-N2-C2
3	B	413	NAG	C8-C7-N2-C2
4	B	404	MES	C8-C7-N4-C5
6	A	405	GOL	O1-C1-C2-C3
6	A	405	GOL	C1-C2-C3-O3
6	A	408	GOL	C1-C2-C3-O3
6	A	408	GOL	O2-C2-C3-O3
8	A	412	MH0	C2C-C3C-CAC-CBC
12	B	401	A1JHS	OAE-CAA-CAF-OAH
12	B	401	A1JHS	OAE-CAA-CAF-OAI
12	B	401	A1JHS	OAE-CAD-CAG-OAJ
12	B	401	A1JHS	CAC-CAD-CAG-OAJ
12	B	402	A1JHS	OAE-CAD-CAG-OAJ
12	B	402	A1JHS	CAC-CAD-CAG-OAJ
8	B	414	MH0	C4B-C3B-CAB-CBB
8	B	414	MH0	C2C-C3C-CAC-CBC
8	A	412	MH0	C4C-C3C-CAC-CBC
8	A	412	MH0	C4B-C3B-CAB-CBB
8	A	412	MH0	C2B-C3B-CAB-CBB
8	B	414	MH0	C2B-C3B-CAB-CBB
8	B	414	MH0	C4C-C3C-CAC-CBC
3	B	413	NAG	O7-C7-N2-C2
3	B	410	NAG	O5-C5-C6-O6
6	A	405	GOL	O2-C2-C3-O3
5	A	406	PEG	O1-C1-C2-O2
5	A	409	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	408	GOL	C1-C2-C3-O3
6	B	411	GOL	O1-C1-C2-C3
6	A	405	GOL	O1-C1-C2-O2
6	B	408	GOL	O2-C2-C3-O3
6	B	411	GOL	O1-C1-C2-O2
3	B	410	NAG	C4-C5-C6-O6
12	B	401	A1JHS	CAB-CAA-CAF-OAH
12	B	401	A1JHS	CAB-CAA-CAF-OAI
6	A	411	GOL	O2-C2-C3-O3
6	B	408	GOL	O1-C1-C2-O2
5	A	409	PEG	C4-C3-O2-C2
5	A	409	PEG	C1-C2-O2-C3
8	A	412	MH0	CAA-CBA-CGA-O2A
8	B	414	MH0	CAA-CBA-CGA-O2A
8	B	414	MH0	CAA-CBA-CGA-O1A
8	A	412	MH0	CAA-CBA-CGA-O1A
6	B	412	GOL	O1-C1-C2-O2
5	A	406	PEG	C1-C2-O2-C3

There are no ring outliers.

20 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	409	PEG	4	0
8	A	412	MH0	4	0
13	B	415	BMA	1	0
3	B	406	NAG	2	0
6	A	405	GOL	4	0
8	B	414	MH0	1	0
6	B	412	GOL	8	0
3	B	413	NAG	7	0
6	B	411	GOL	7	0
3	B	410	NAG	3	0
3	A	407	NAG	7	0
6	B	405	GOL	1	0
3	B	409	NAG	6	0
12	B	402	A1JHS	2	0
5	A	406	PEG	8	0
4	A	402	MES	1	0
6	A	408	GOL	2	0
3	A	401	NAG	2	0
6	A	404	GOL	5	0

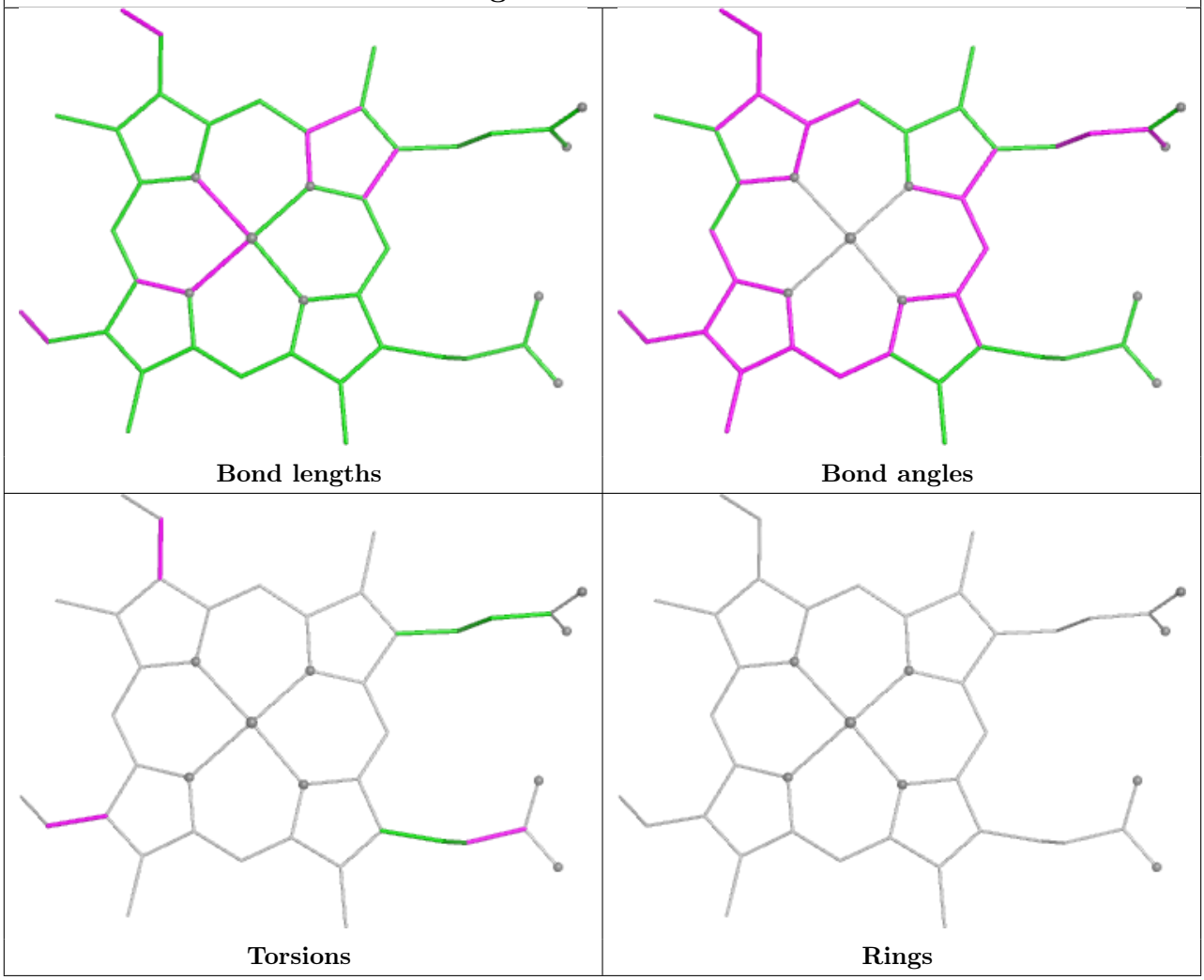
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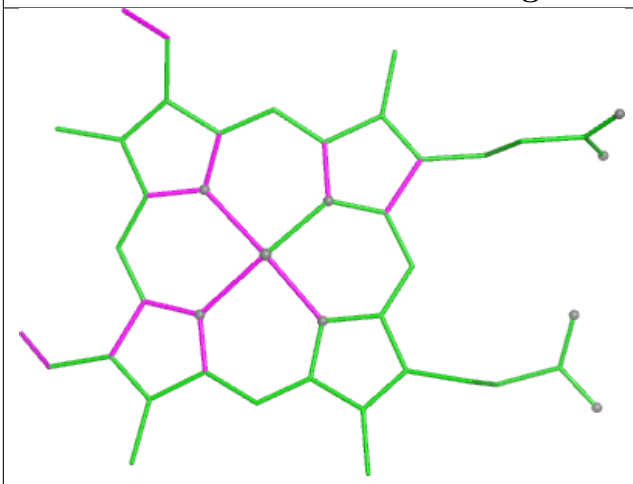
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	411	GOL	1	0

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.

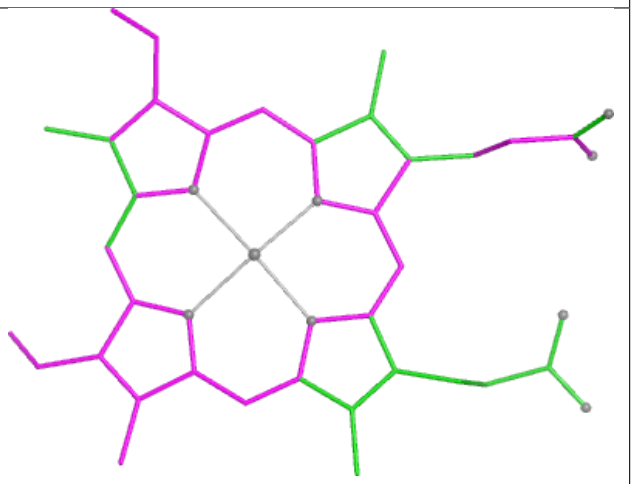
Ligand MH0 A 412



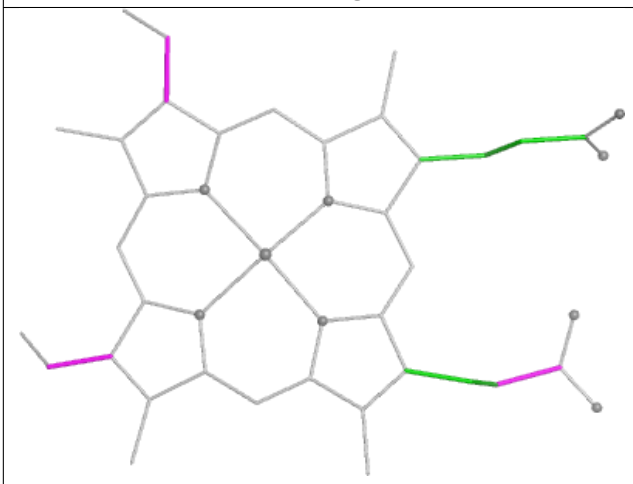
Ligand MH0 B 414



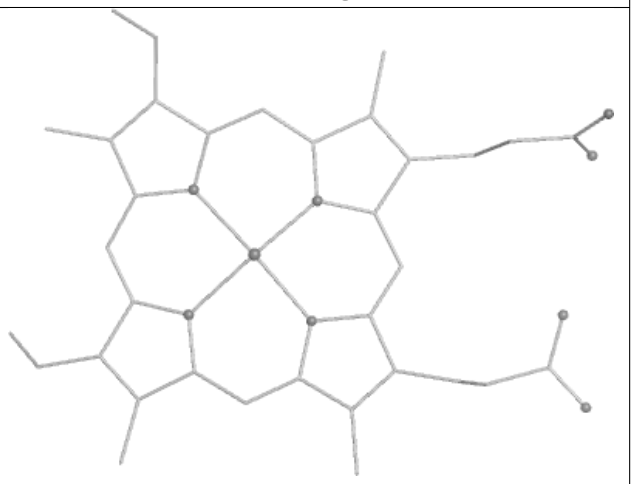
Bond lengths



Bond angles

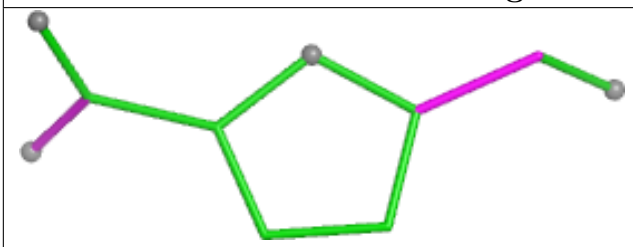


Torsions

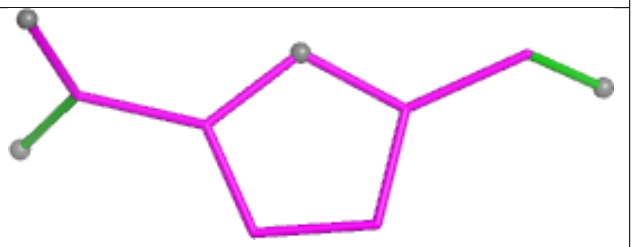


Rings

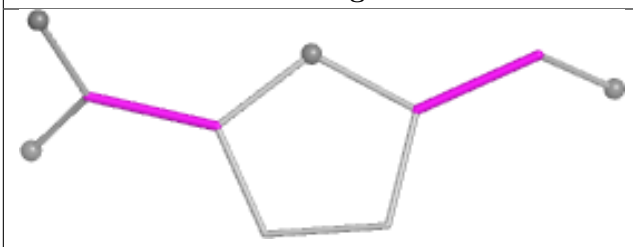
Ligand A1JHS B 401



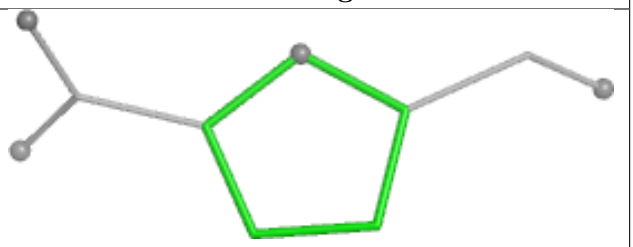
Bond lengths



Bond angles

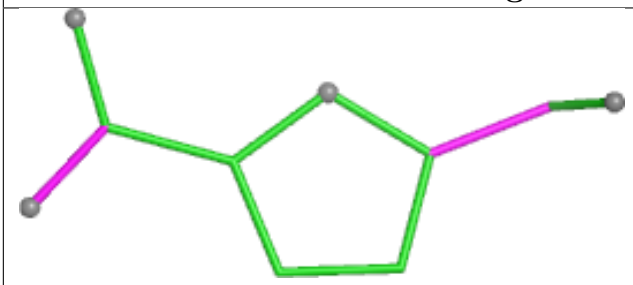


Torsions

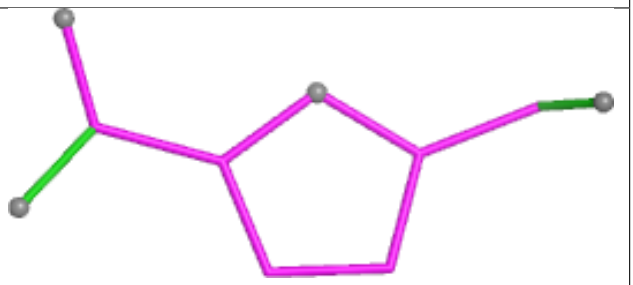


Rings

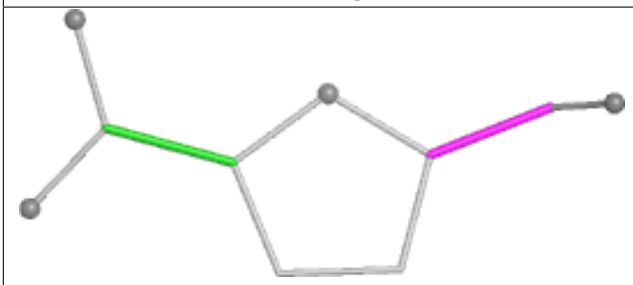
Ligand A1JHS B 402



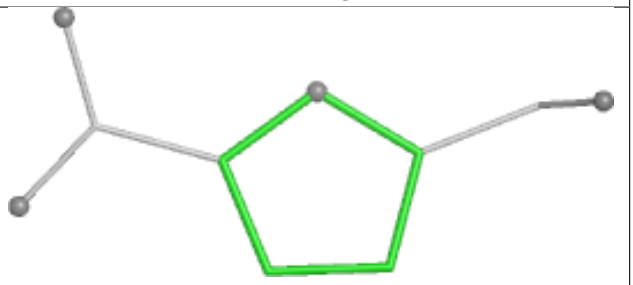
Bond lengths



Bond angles



Torsions



Rings

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	334/334 (100%)	-0.17	4 (1%)	76	80	12, 22, 34, 83	5 (1%)
1	B	334/334 (100%)	-0.07	3 (0%)	81	83	12, 23, 35, 76	5 (1%)
All	All	668/668 (100%)	-0.12	7 (1%)	79	82	12, 23, 35, 83	10 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	LEU	6.7
1	A	1	LEU	5.8
1	B	334	LEU	4.1
1	A	2	ASN	3.6
1	A	334	LEU	2.6
1	B	307	ARG	2.2
1	A	322	ASP	2.1

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

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
2	NAG	D	2	14/15	0.71	0.17	44,51,57,57	0
2	NAG	C	2	14/15	0.73	0.14	38,43,48,48	0

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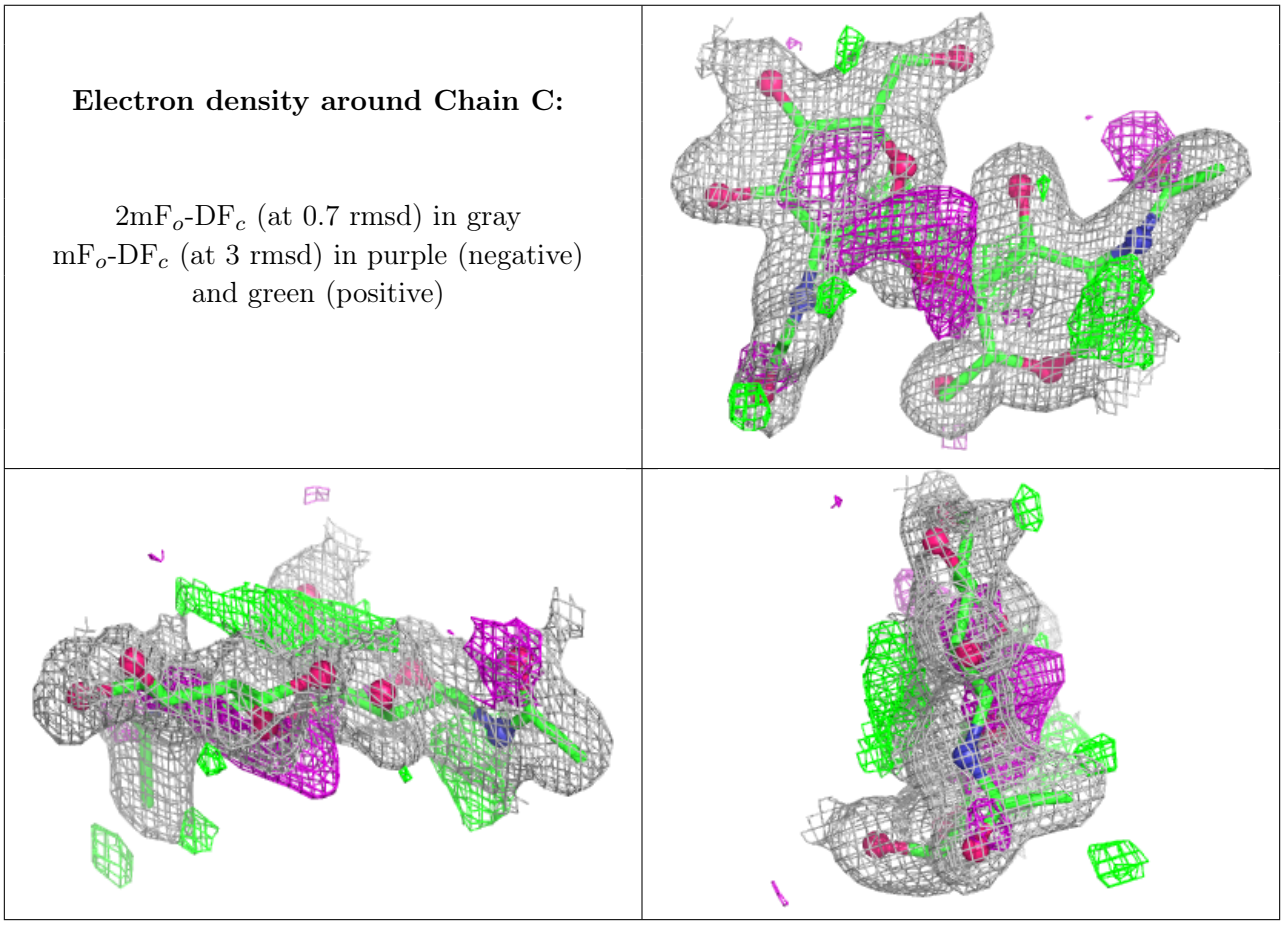
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	1	14/15	0.83	0.13	30,32,40,44	0
2	NAG	D	1	14/15	0.94	0.08	26,29,34,36	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

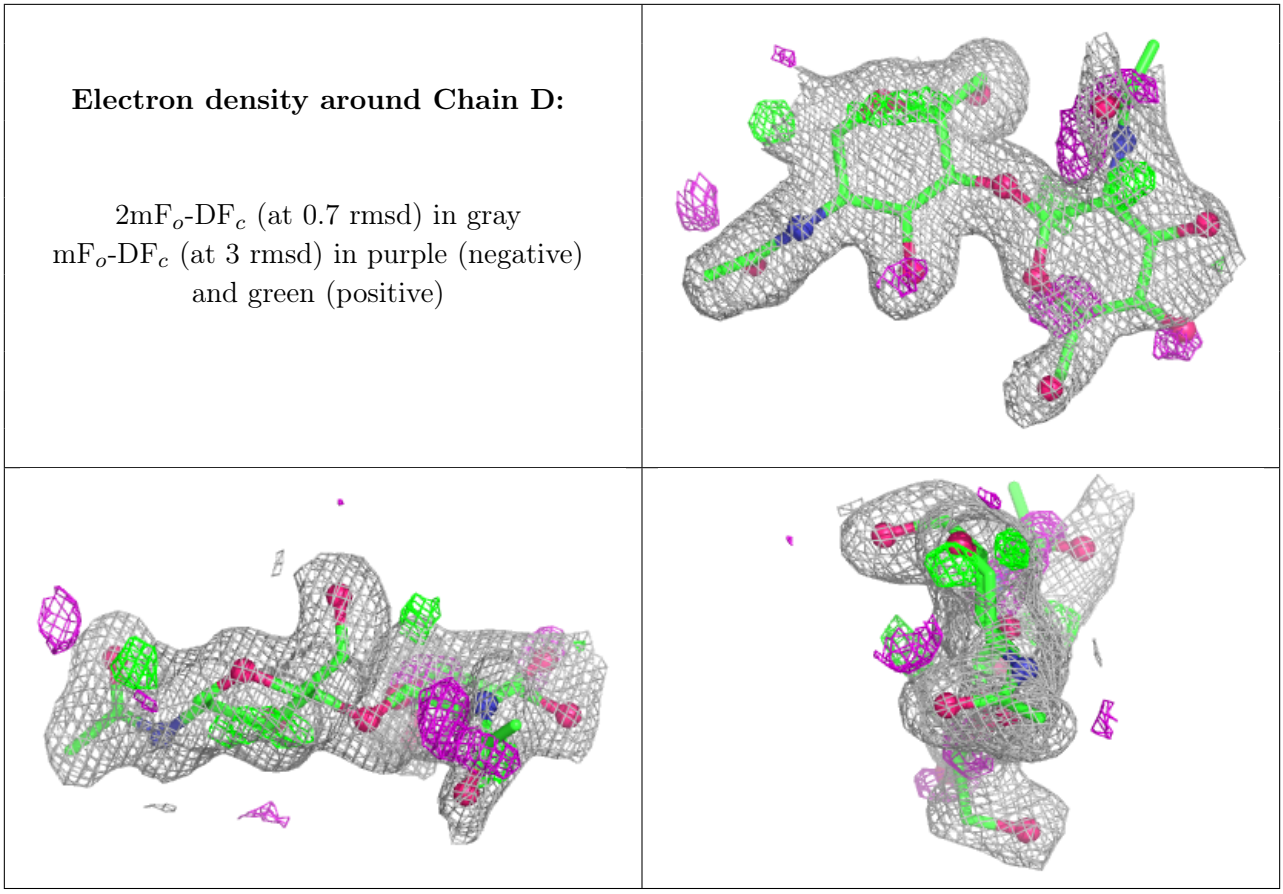
Electron density around Chain C:

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



Electron density around Chain D:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
13	BMA	B	415	11/12	0.44	0.17	52,54,56,57	0
3	NAG	B	413	14/15	0.55	0.17	48,52,56,62	0
3	NAG	A	401	14/15	0.55	0.21	55,57,62,62	0
12	A1JHS	B	402	10/10	0.56	0.19	35,38,42,44	0
3	NAG	B	407	14/15	0.61	0.17	43,50,55,56	0
7	EOH	B	417	3/3	0.61	0.24	36,36,38,38	0
5	PEG	A	409	7/7	0.62	0.19	34,36,37,41	0
3	NAG	B	410	14/15	0.63	0.18	43,49,58,63	0
6	GOL	B	408	6/6	0.68	0.16	38,39,41,41	0
11	PO4	A	424	5/5	0.69	0.15	42,43,49,50	0
6	GOL	A	411	6/6	0.70	0.16	41,41,42,43	0
3	NAG	B	409	14/15	0.73	0.17	34,37,43,45	0
6	GOL	B	405	6/6	0.75	0.15	36,38,41,42	0

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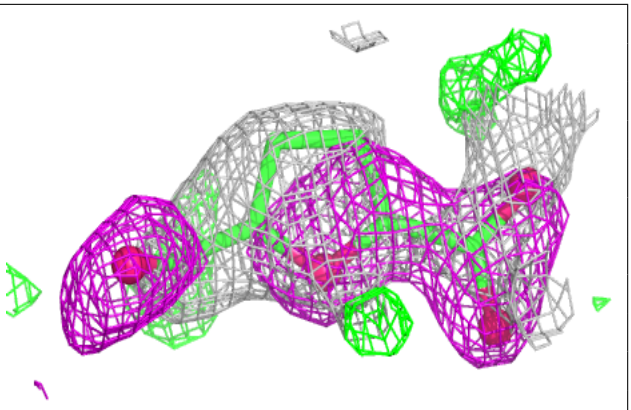
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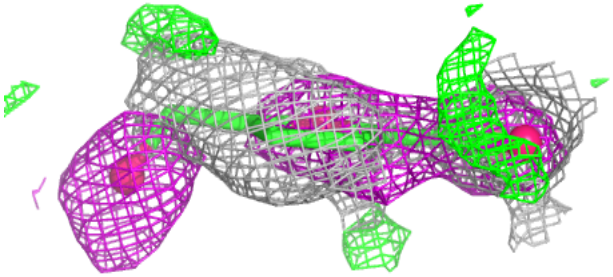
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EOH	A	410	3/3	0.75	0.19	37,37,37,39	0
11	PO4	B	423	5/5	0.76	0.16	42,45,50,50	0
12	A1JHS	B	401	10/10	0.76	0.16	36,39,41,43	0
6	GOL	A	405	6/6	0.77	0.18	24,32,35,41	0
6	GOL	B	411	6/6	0.77	0.14	35,39,41,42	0
6	GOL	A	408	6/6	0.77	0.14	35,37,39,40	0
6	GOL	A	404	6/6	0.79	0.13	36,38,40,42	0
6	GOL	B	412	6/6	0.80	0.15	33,36,37,39	0
3	NAG	A	407	14/15	0.80	0.13	45,49,54,54	0
5	PEG	A	403	7/7	0.82	0.15	34,36,39,42	0
3	NAG	B	403	14/15	0.83	0.12	33,38,43,47	0
5	PEG	A	406	7/7	0.86	0.14	31,32,38,39	0
10	ZN	B	421	1/1	0.90	0.37	57,57,57,57	0
3	NAG	B	406	14/15	0.90	0.10	31,33,35,38	0
10	ZN	A	416	1/1	0.91	0.09	41,41,41,41	0
10	ZN	A	419	1/1	0.93	0.07	32,32,32,32	0
10	ZN	A	421	1/1	0.93	0.34	53,53,53,53	0
4	MES	A	402	12/12	0.95	0.12	23,32,35,35	0
4	MES	B	404	12/12	0.95	0.12	21,33,38,38	0
10	ZN	A	414	1/1	0.96	0.10	41,41,41,41	0
10	ZN	A	417	1/1	0.96	0.06	36,36,36,36	0
10	ZN	A	418	1/1	0.97	0.04	30,30,30,30	0
10	ZN	A	415	1/1	0.98	0.04	27,27,27,27	0
8	MH0	B	414	43/43	0.98	0.06	18,20,24,31	0
10	ZN	A	420	1/1	0.98	0.07	37,37,37,37	0
8	MH0	A	412	43/43	0.98	0.06	16,18,22,26	0
10	ZN	B	418	1/1	0.98	0.23	43,43,43,43	0
10	ZN	B	420	1/1	0.98	0.07	41,41,41,41	0
10	ZN	B	419	1/1	0.99	0.07	36,36,36,36	0
10	ZN	A	422	1/1	0.99	0.02	22,22,22,22	0
10	ZN	A	423	1/1	0.99	0.04	33,33,33,33	0
9	MG	A	413	1/1	0.99	0.16	10,10,10,10	0
10	ZN	B	422	1/1	1.00	0.02	23,23,23,23	0
9	MG	B	416	1/1	1.00	0.13	10,10,10,10	0

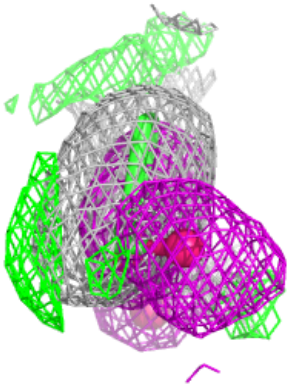
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1JHS 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)

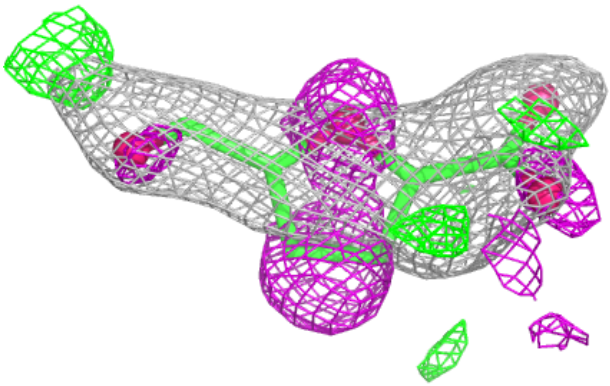


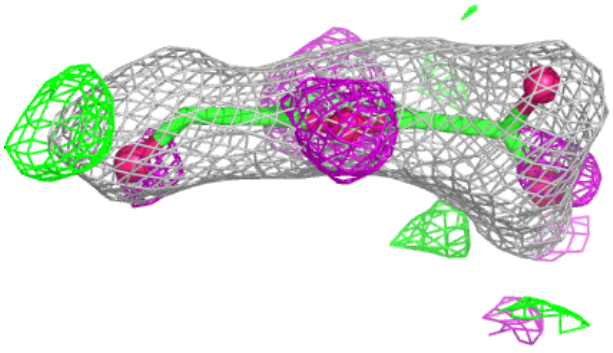


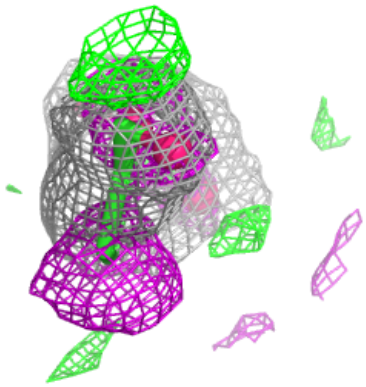


Electron density around A1JHS B 401:

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

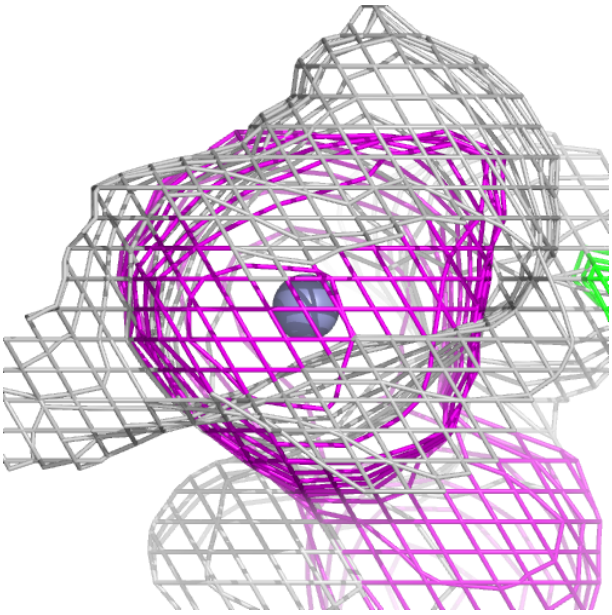


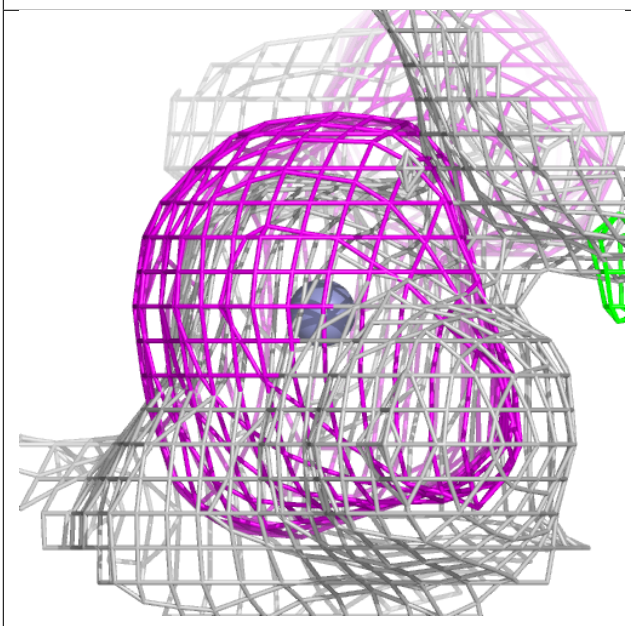


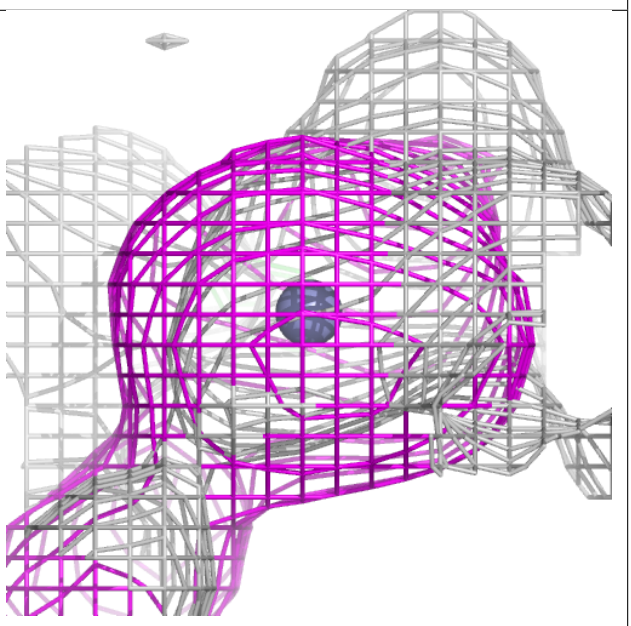


Electron density around ZN B 421:

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

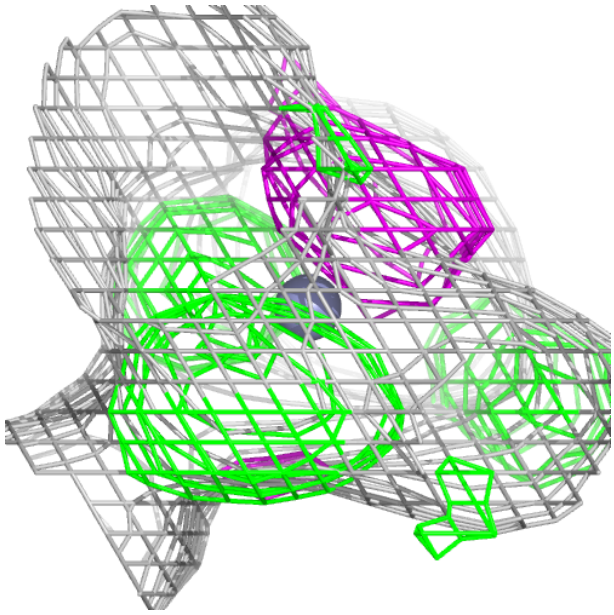


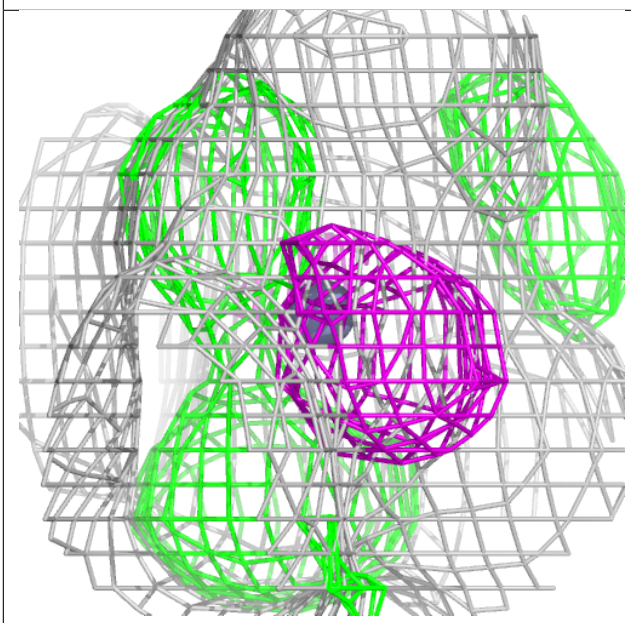


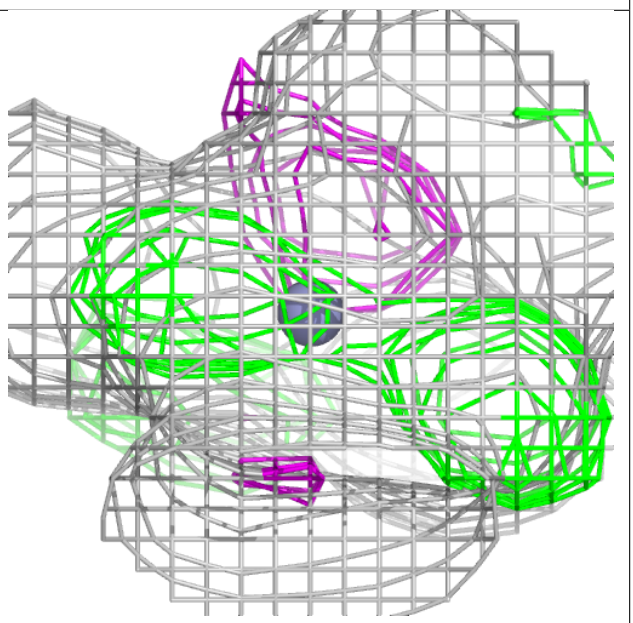


Electron density around ZN A 416:

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

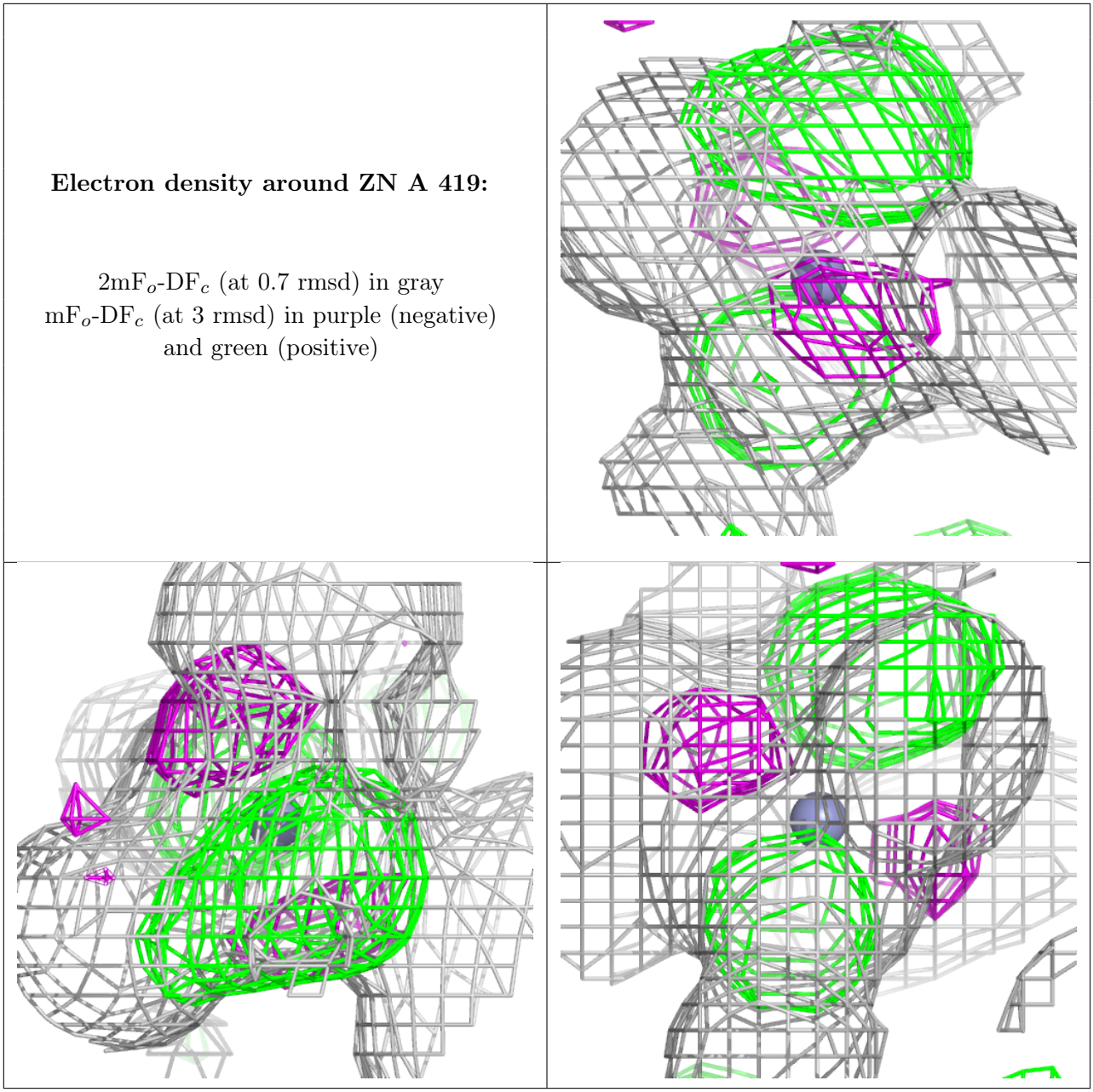






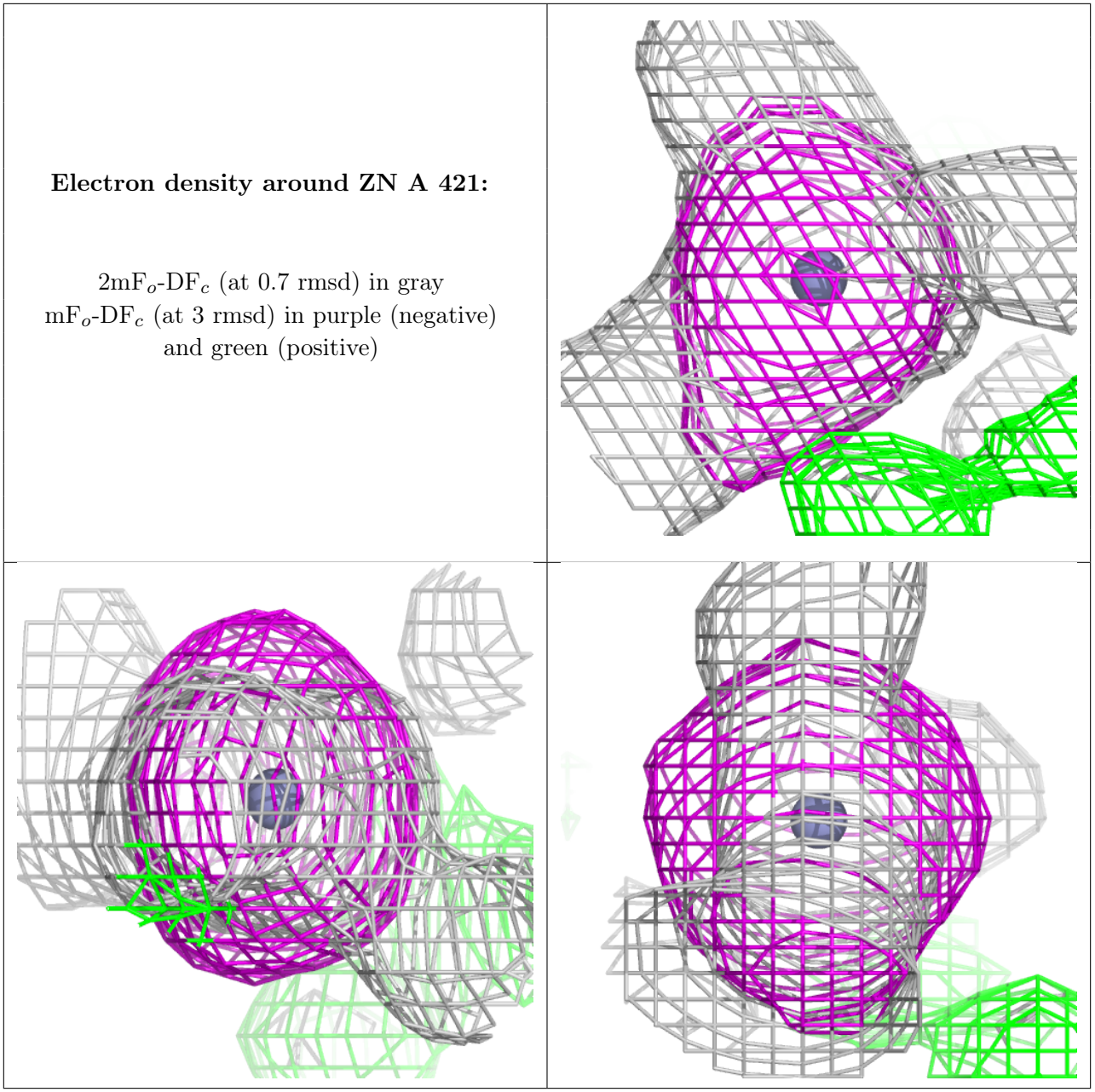
Electron density around ZN A 419:

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



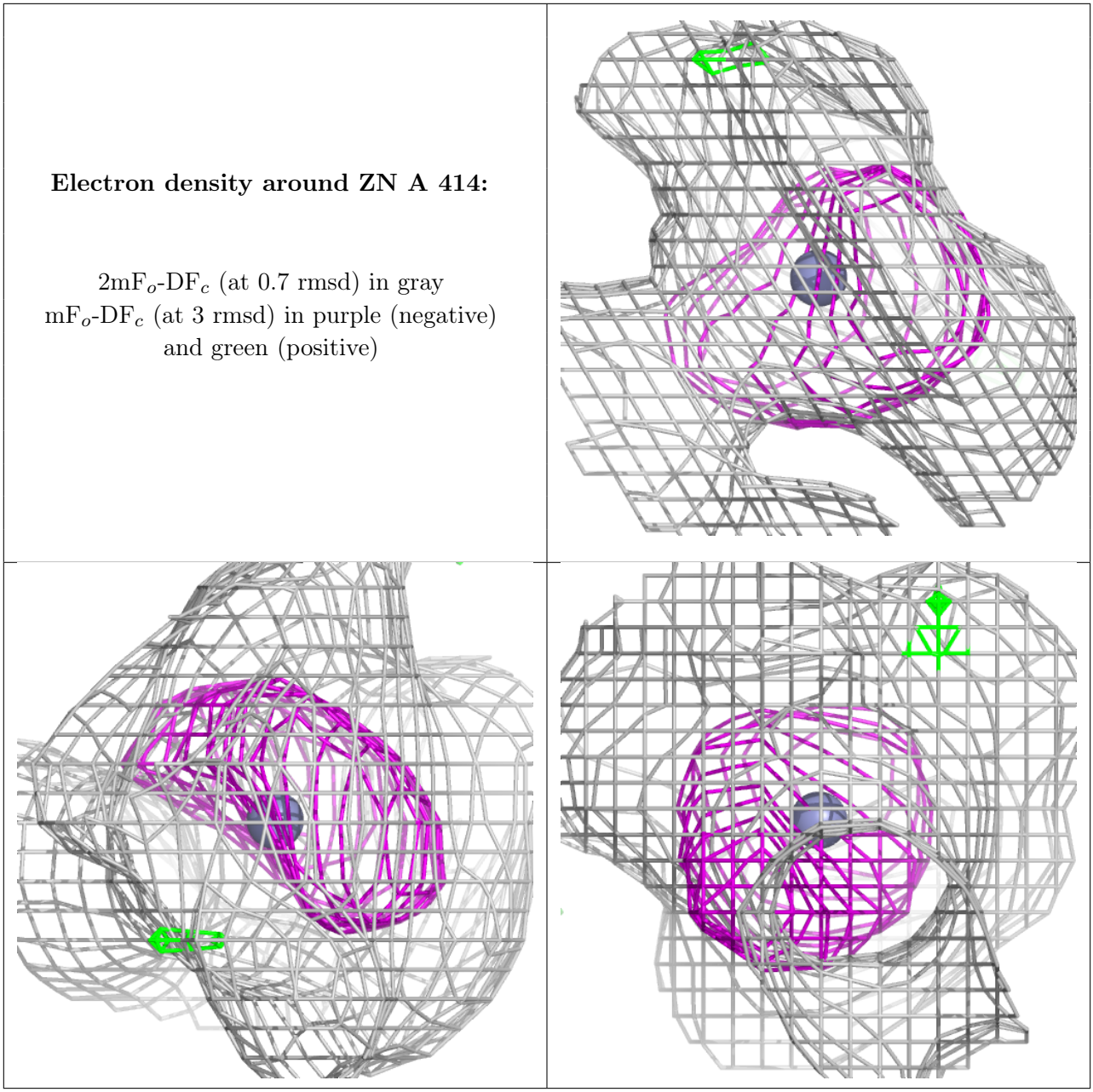
Electron density around ZN A 421:

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



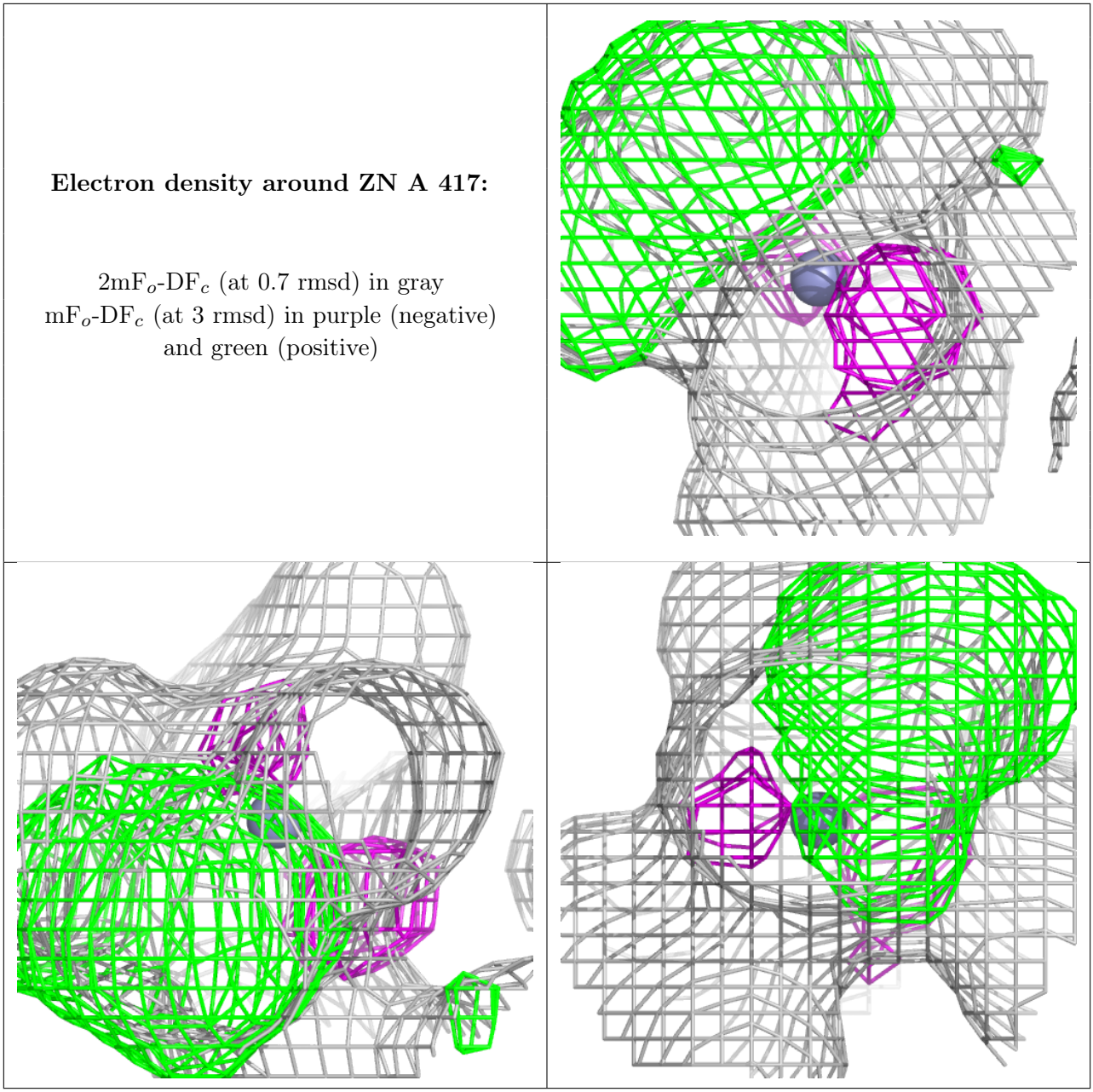
Electron density around ZN A 414:

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



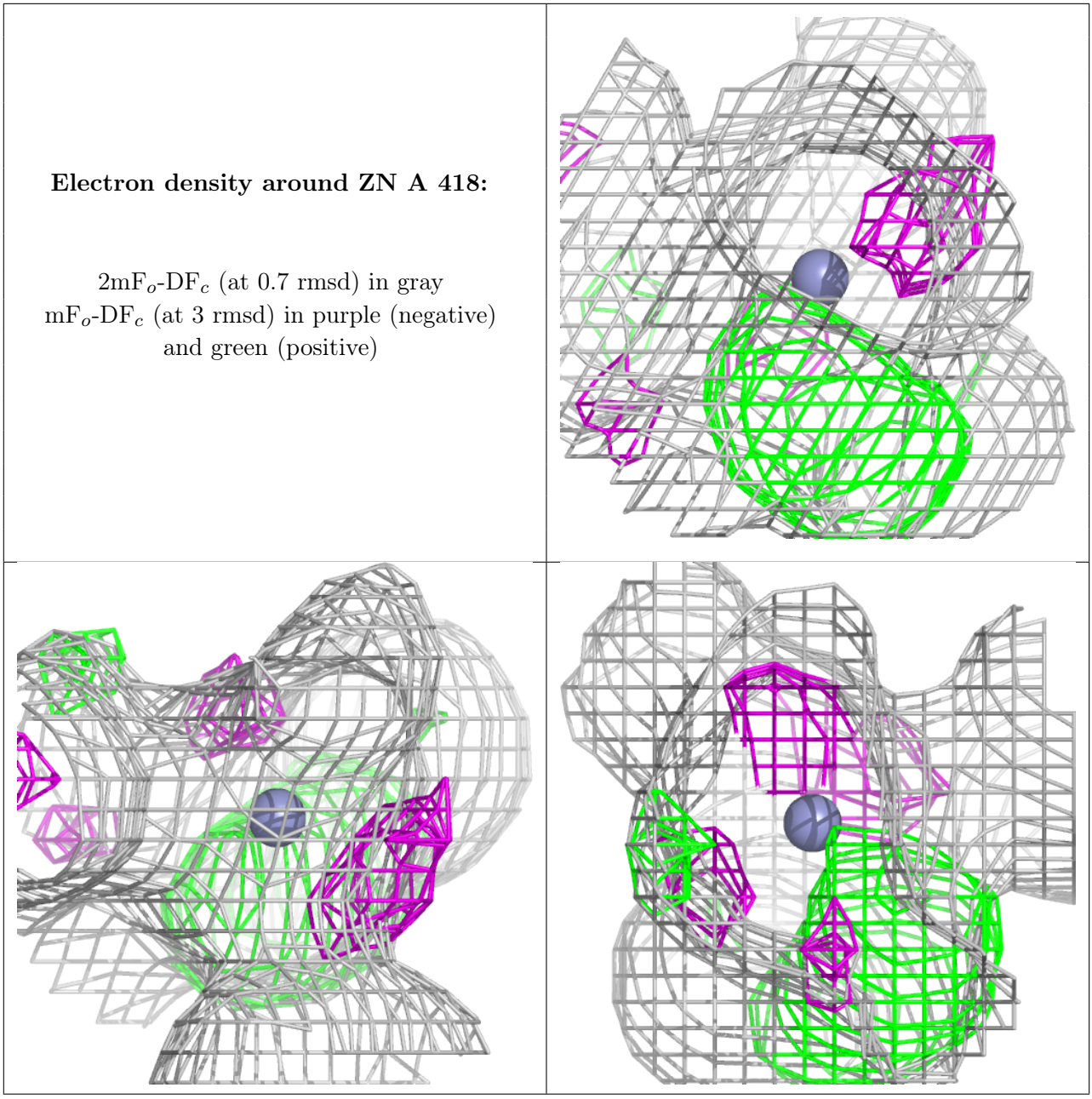
Electron density around ZN A 417:

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



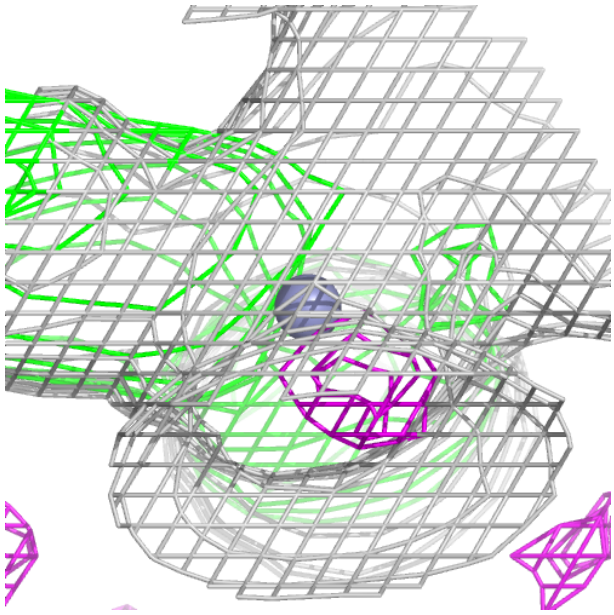
Electron density around ZN A 418:

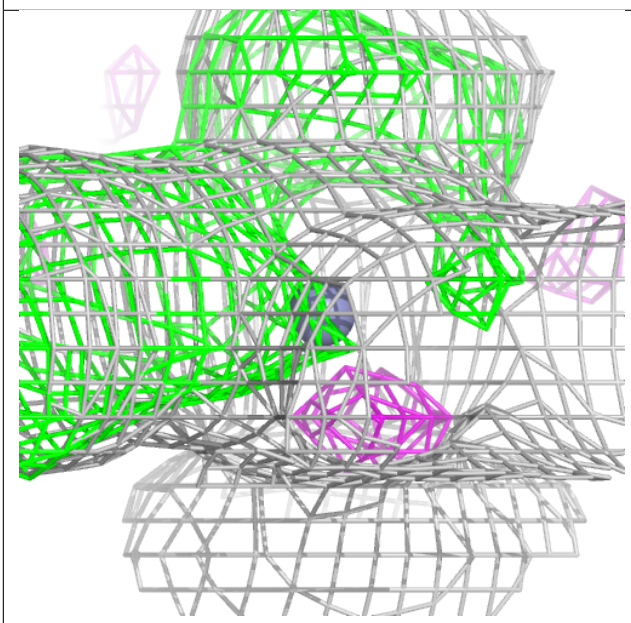
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

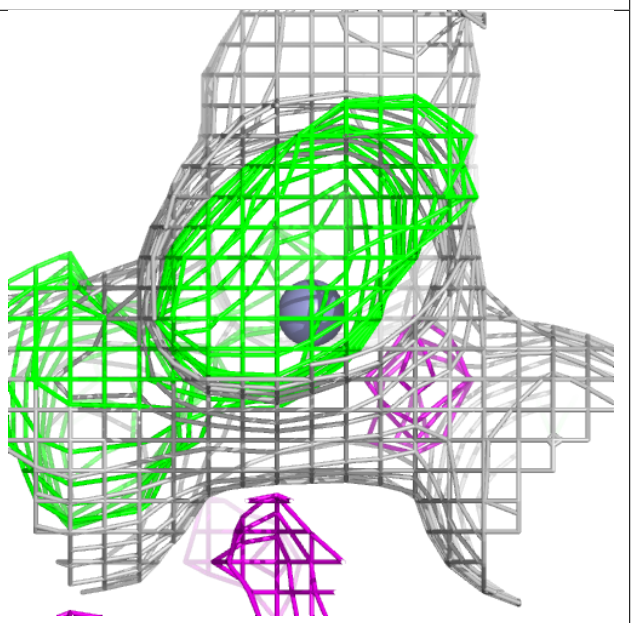


Electron density around ZN A 415:

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

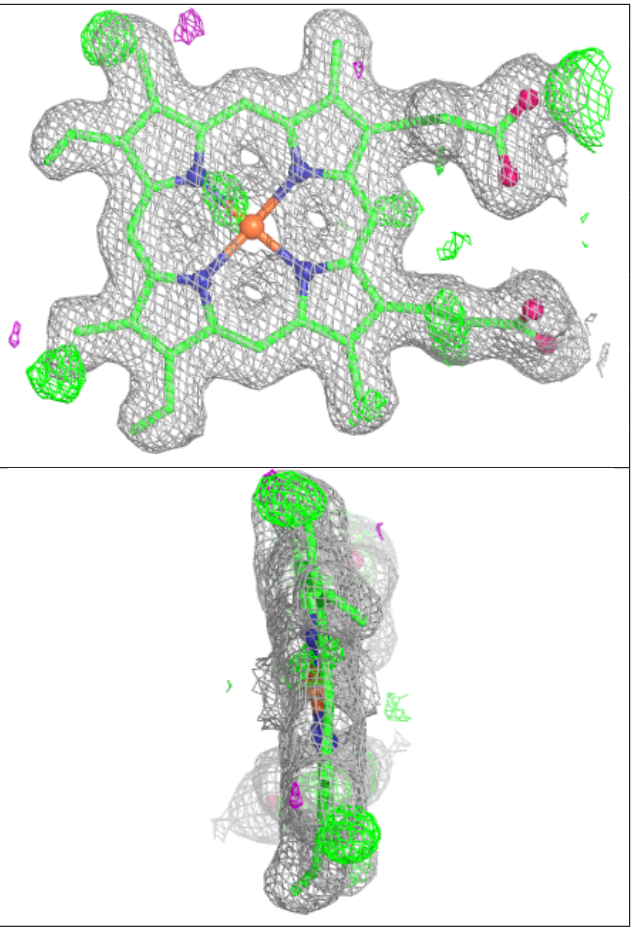


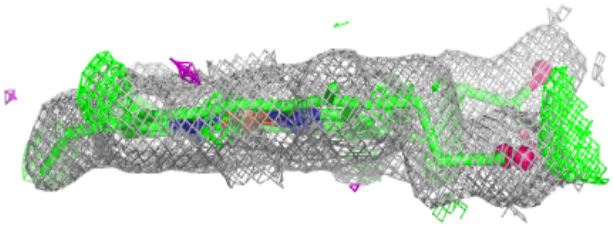




Electron density around MH0 B 414:

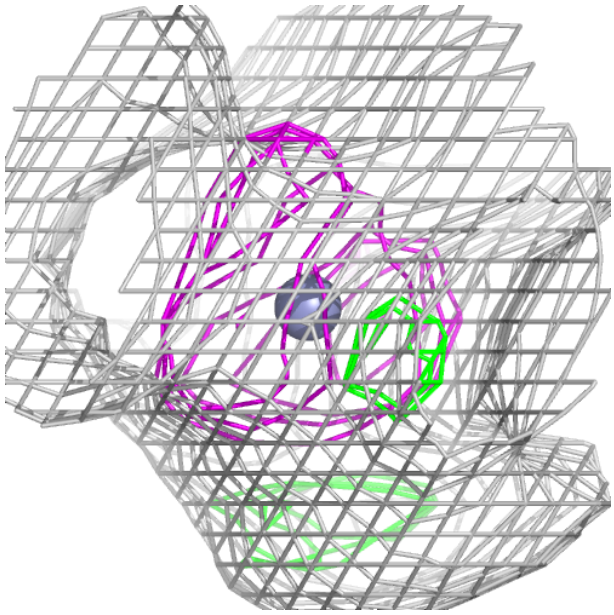
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

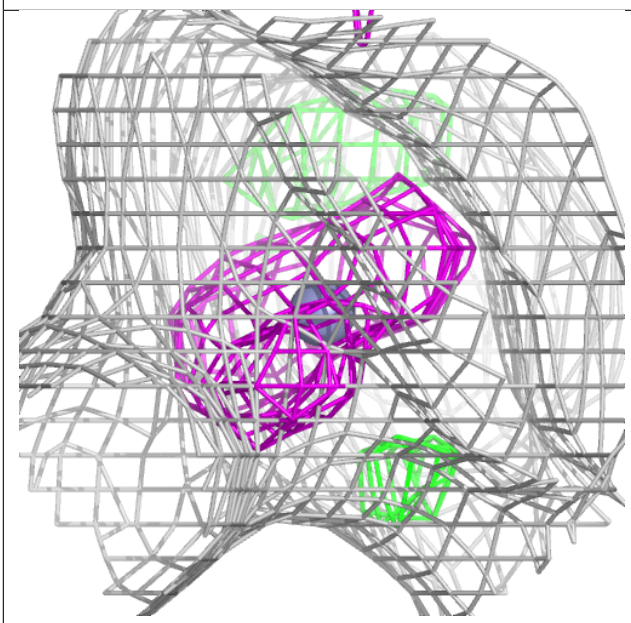


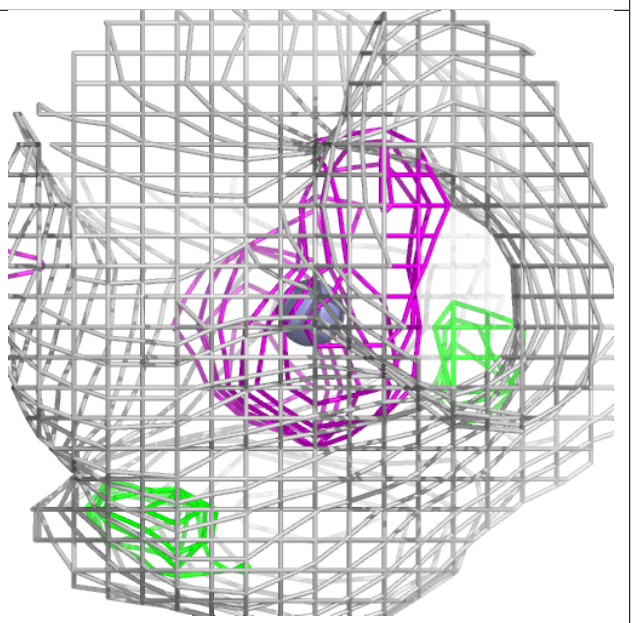


Electron density around ZN A 420:

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

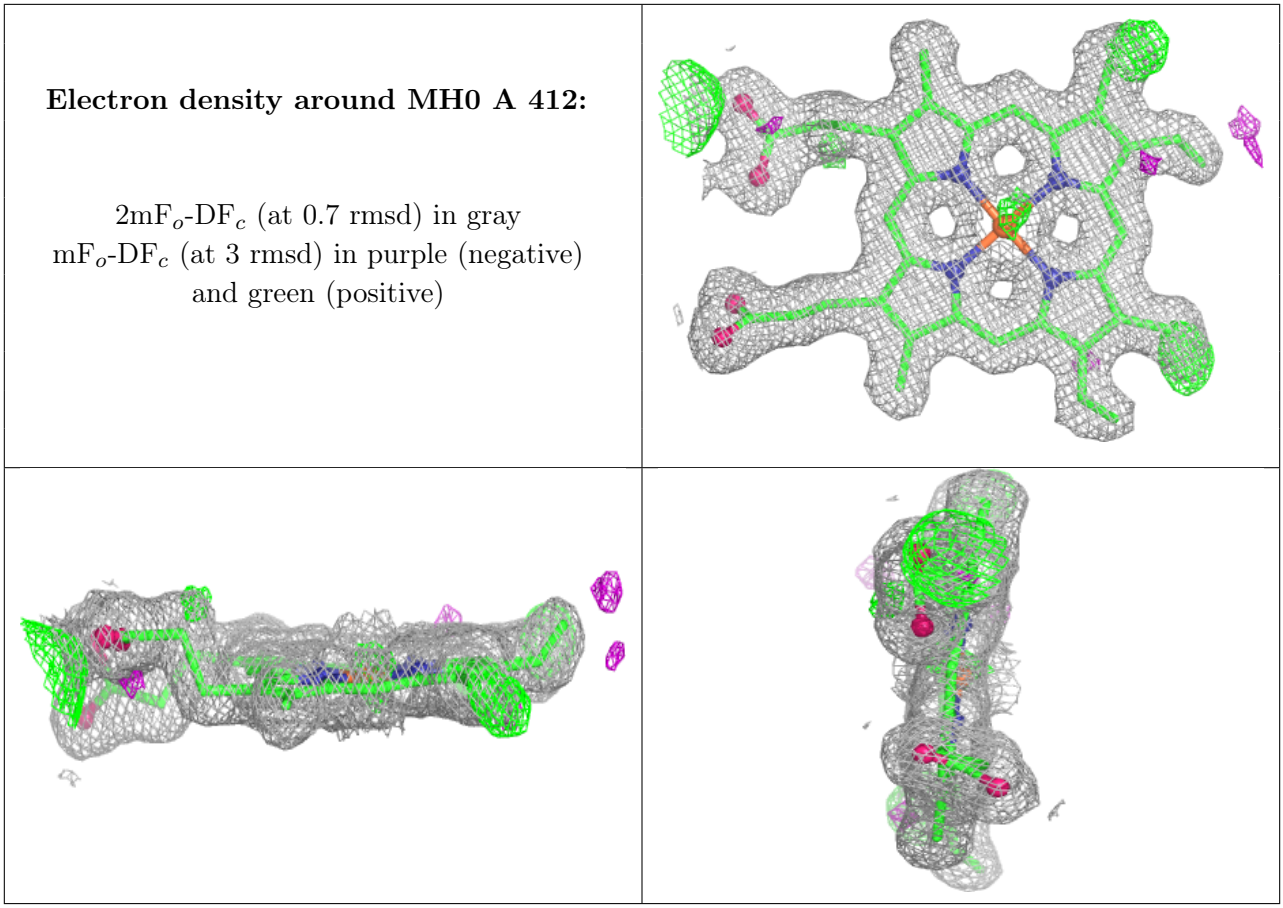






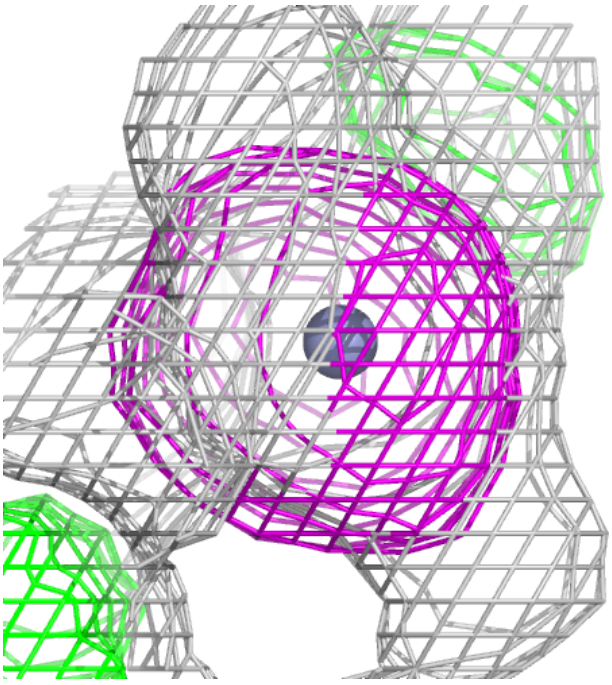
Electron density around MH0 A 412:

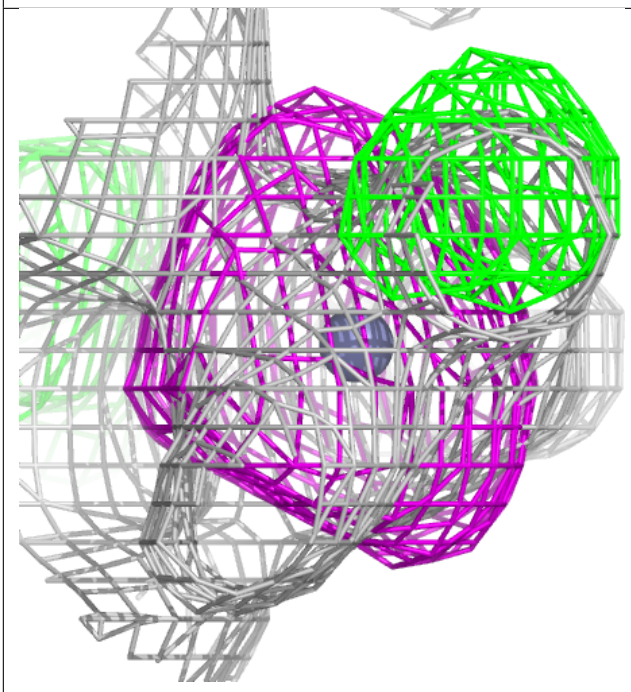
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

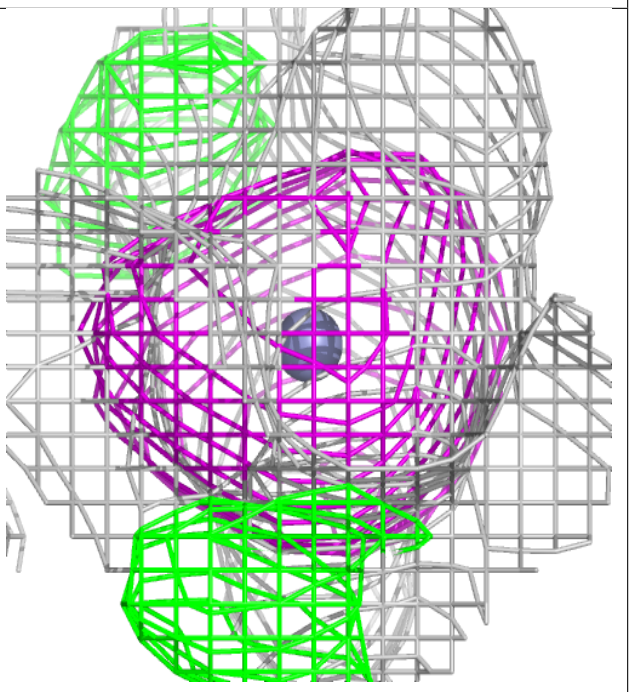


Electron density around ZN B 418:

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

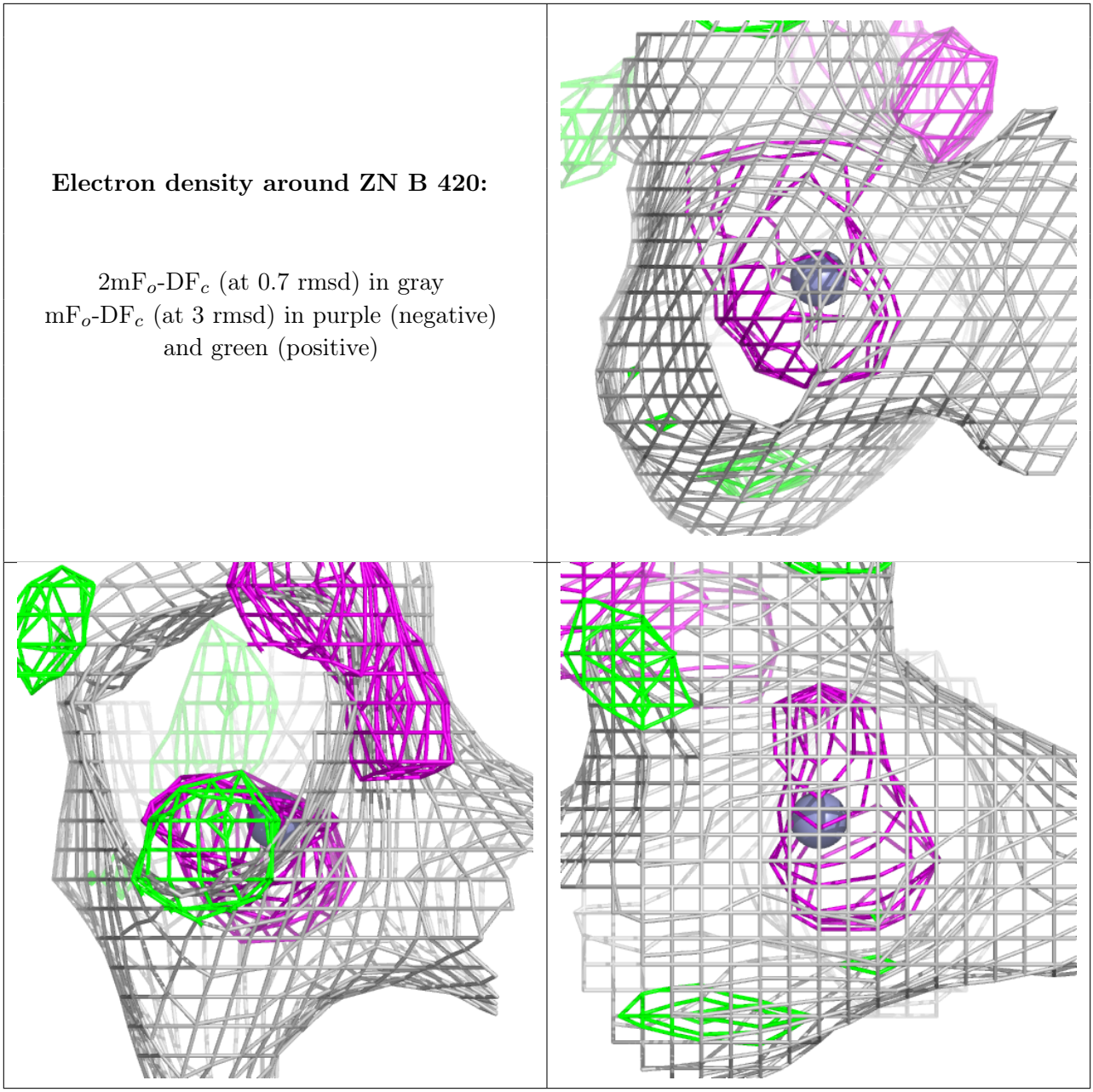






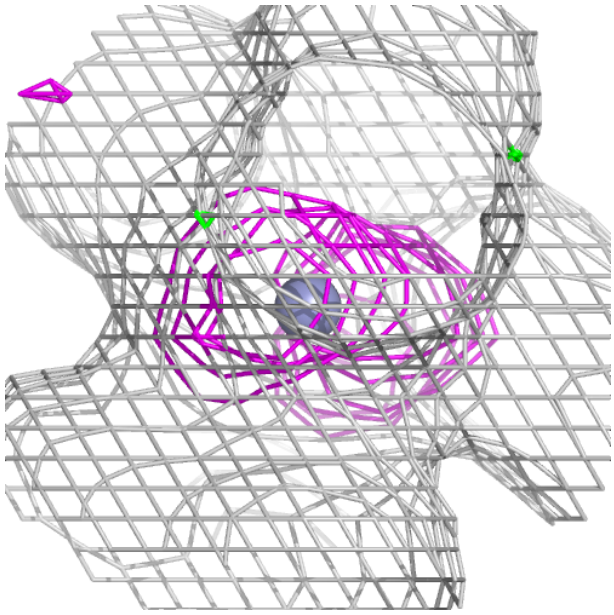
Electron density around ZN B 420:

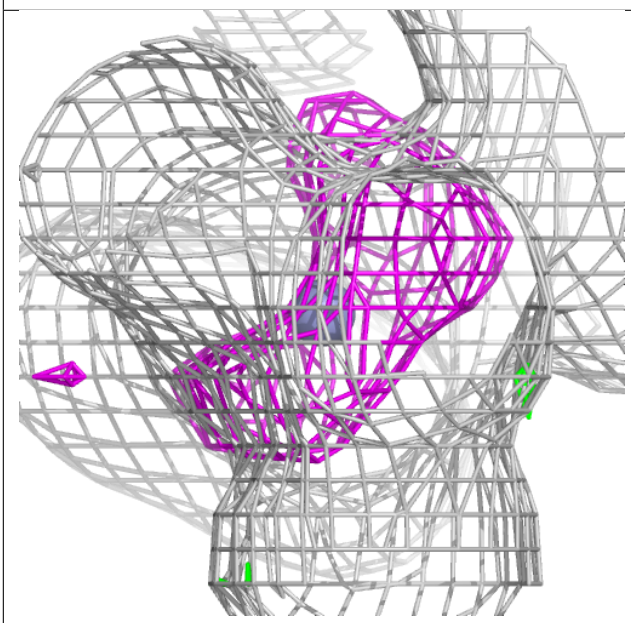
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

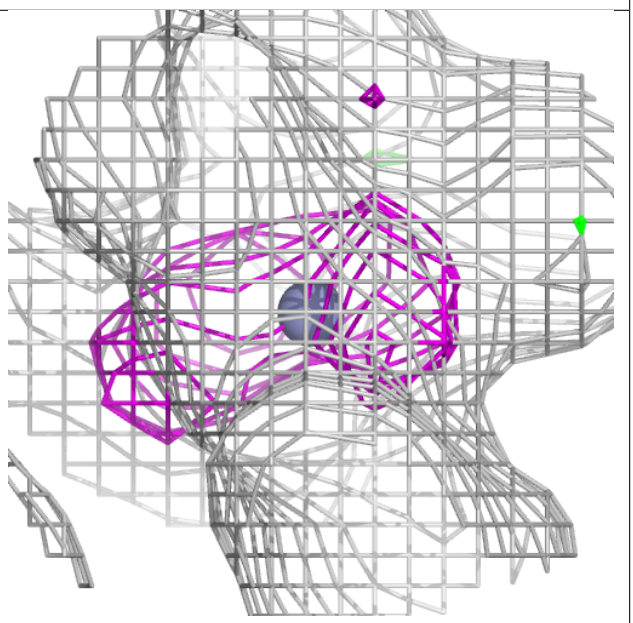


Electron density around ZN B 419:

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

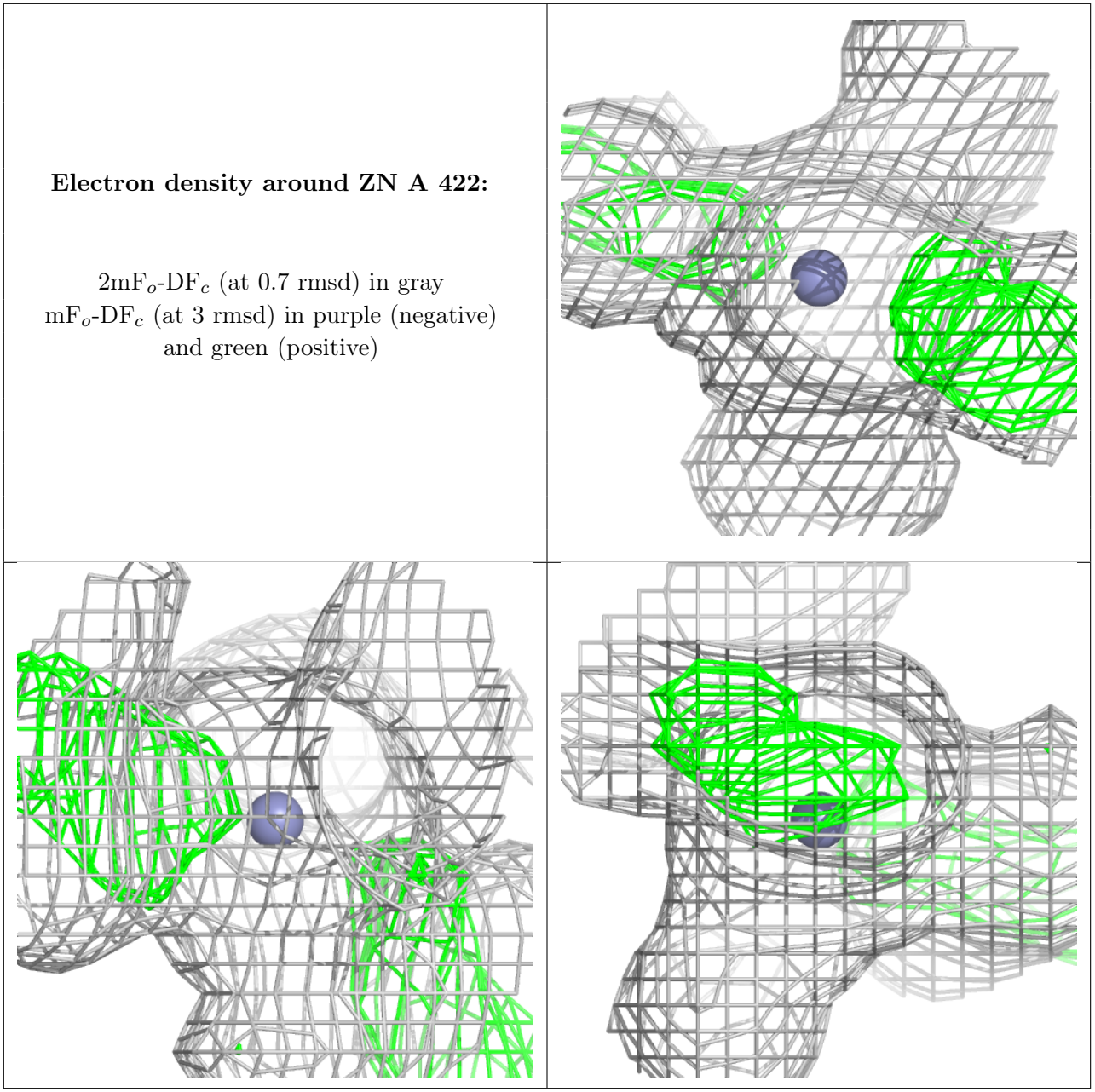






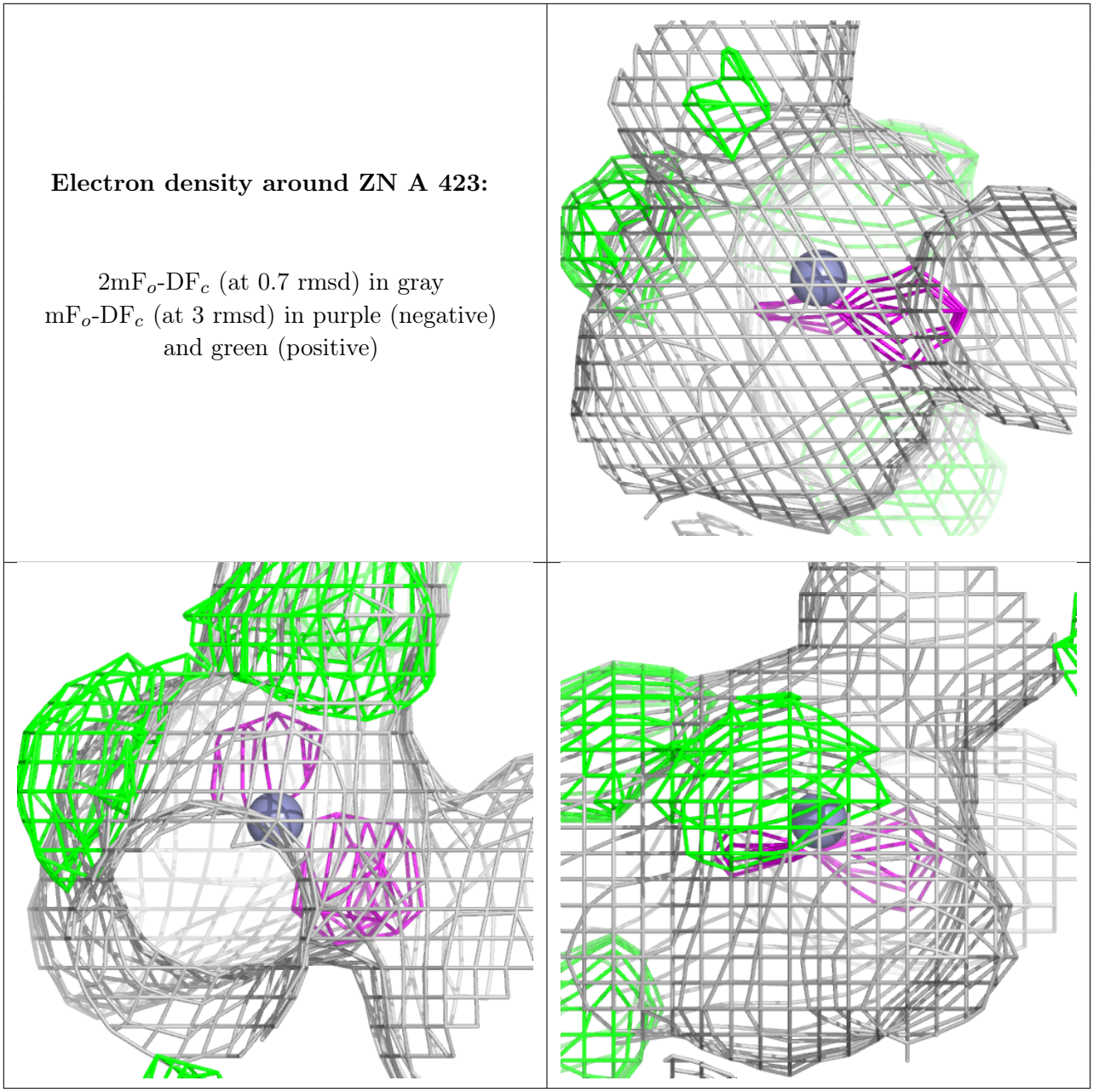
Electron density around ZN A 422:

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



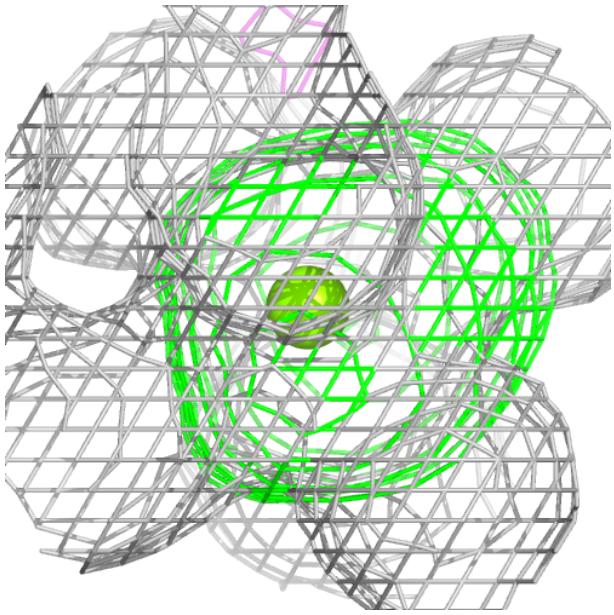
Electron density around ZN A 423:

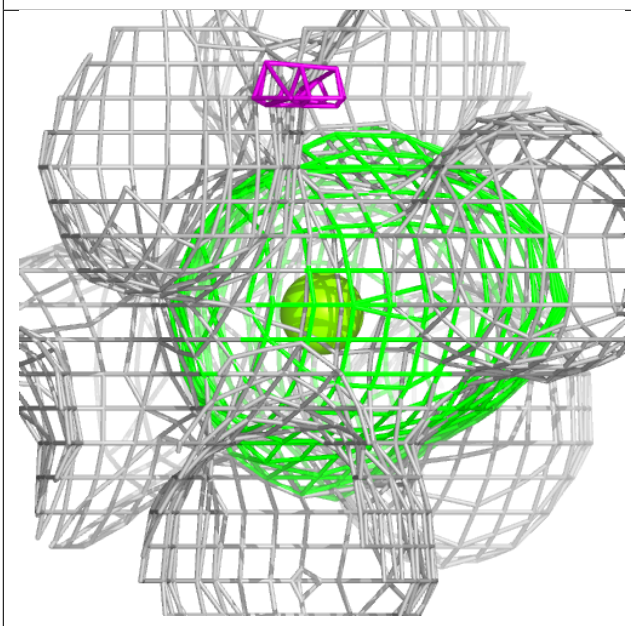
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

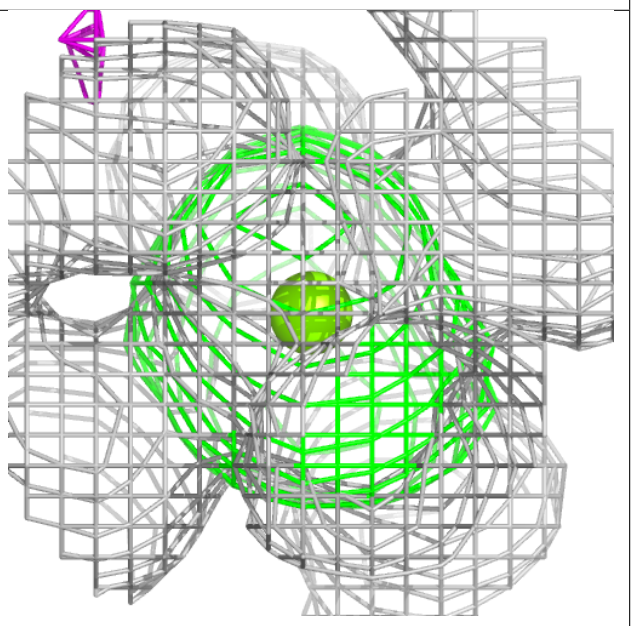


Electron density around MG A 413:

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

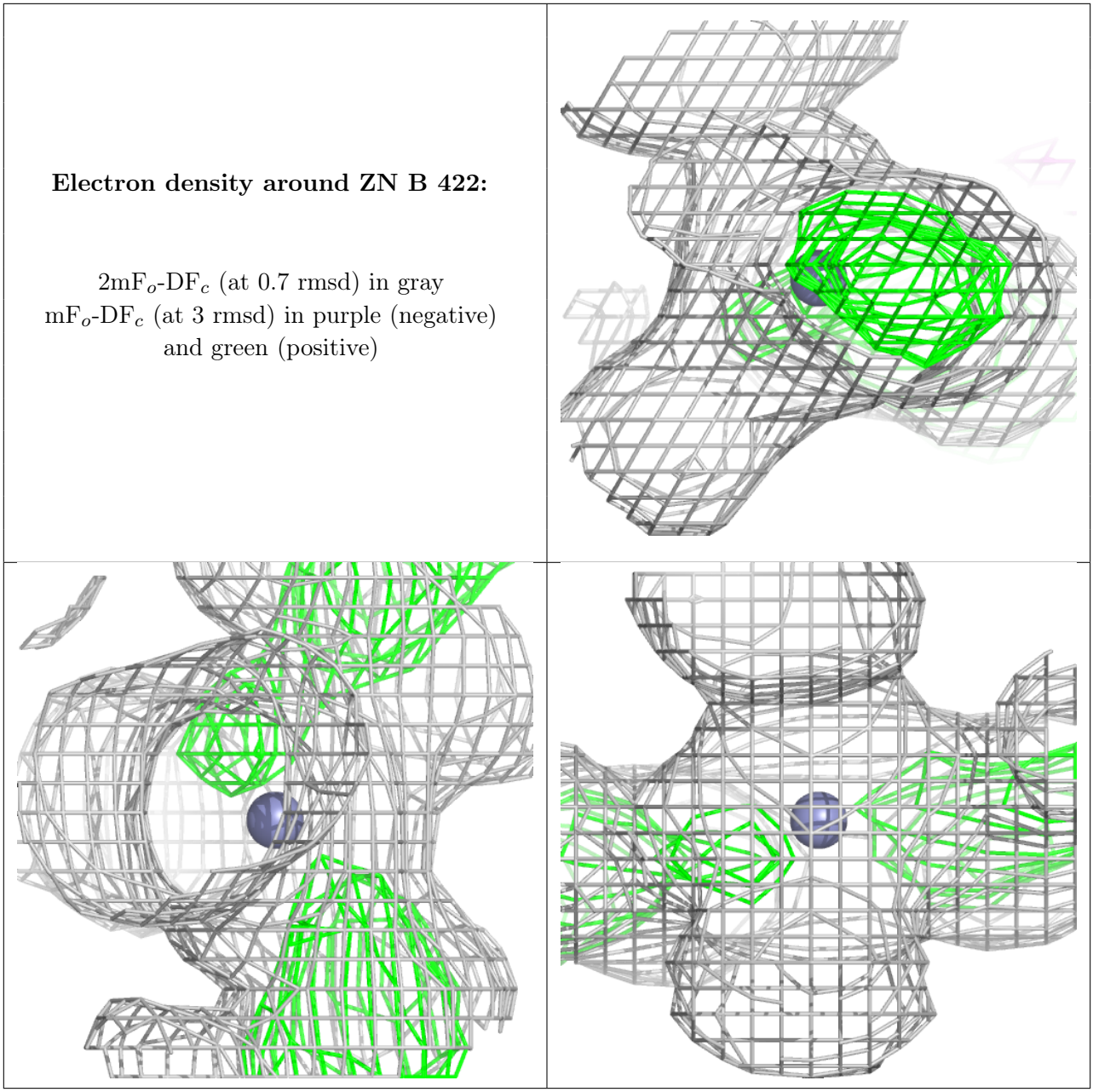






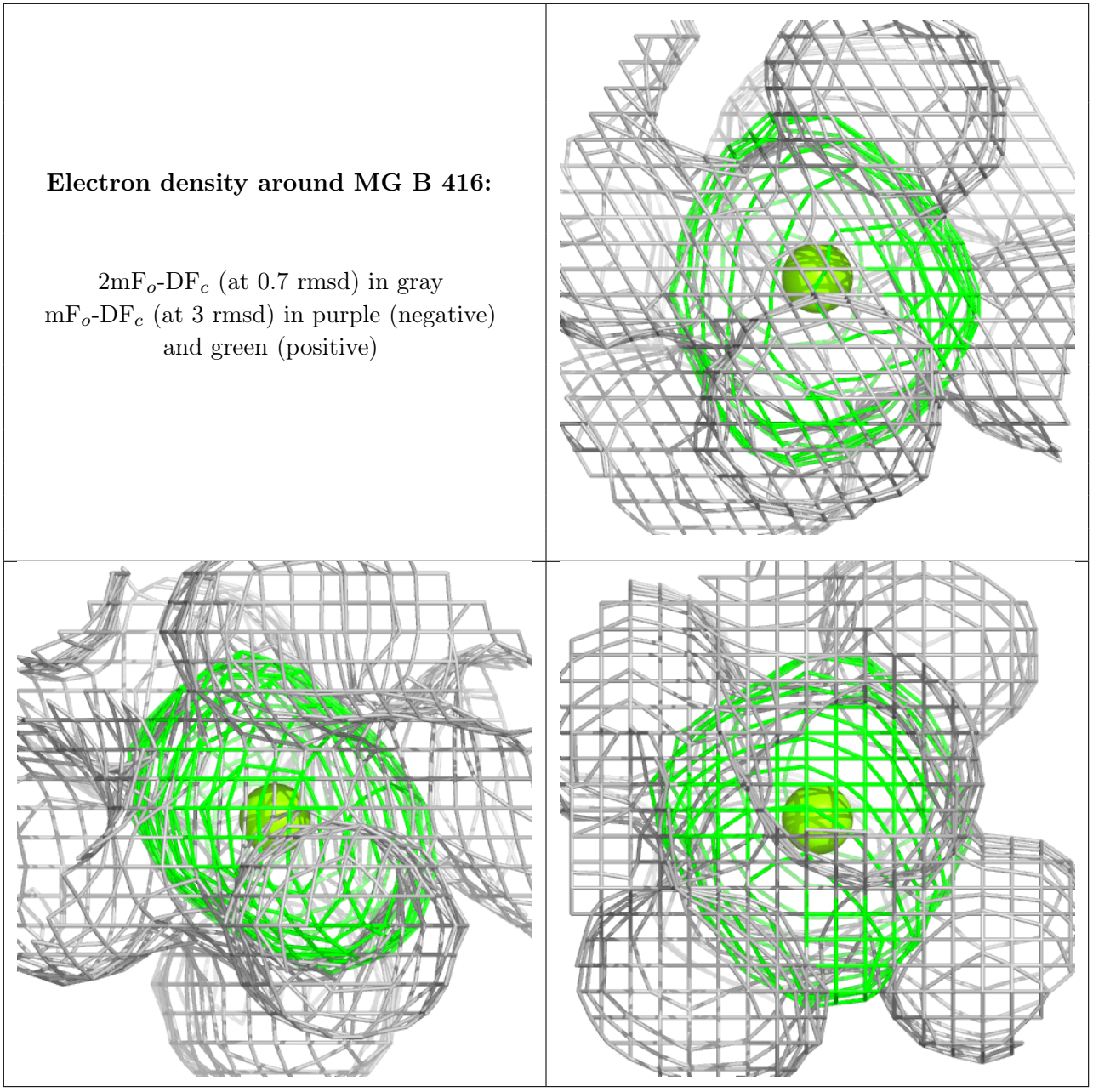
Electron density around ZN B 422:

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



Electron density around MG B 416:

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



6.5 Other polymers (i)

There are no such residues in this entry.