Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 10:20 AM JST

PDB ID	:	8Y0L / pdb_00008y0l
Title	:	beta-glucosidase from Thermoascus aurantiacus
Authors	:	Matsuzaki, C.; Katayama, T.
Deposited on	:	2024-01-22
Resolution	:	2.15 Å(reported)

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

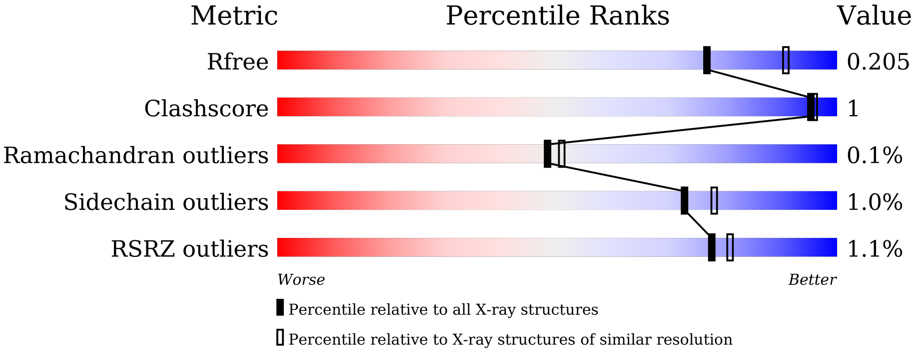
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

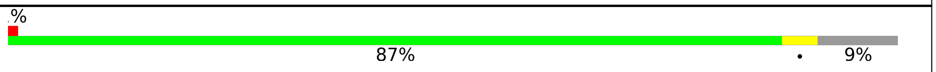
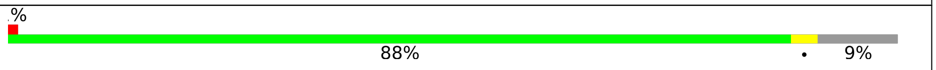
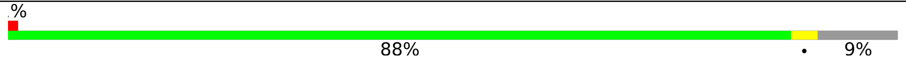
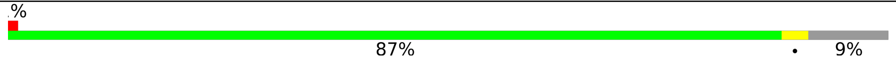
The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	861	
1	B	861	
1	C	861	
1	D	861	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27196 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.

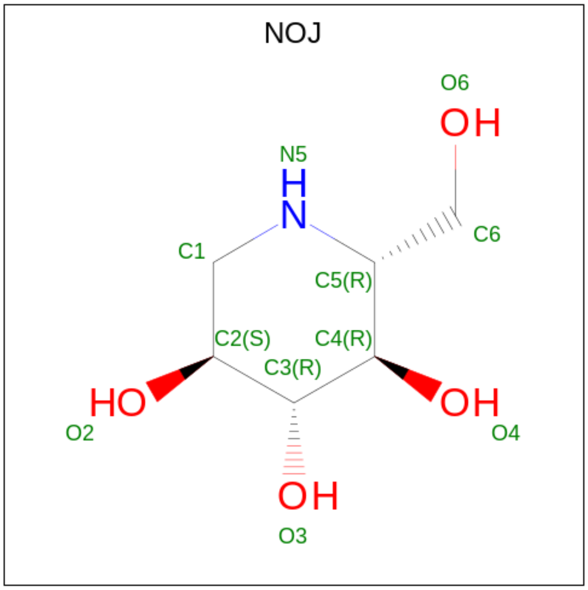
- Molecule 1 is a protein called beta-glucosidase.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	781	Total C N O S 5977 3784 1015 1154 24	0	0	0
1	B	781	Total C N O S 5977 3784 1015 1154 24	0	0	0
1	C	781	Total C N O S 5977 3784 1015 1154 24	0	0	0
1	D	781	Total C N O S 5977 3784 1015 1154 24	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 1-DEOXYNOJIRIMYCIN (CCD ID: NOJ) (formula: $C_6H_{13}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 11 6 1 4	0	0
3	B	1	Total C N O 11 6 1 4	0	0
3	C	1	Total C N O 11 6 1 4	0	0
3	D	1	Total C N O 11 6 1 4	0	0

- Molecule 4 is water.

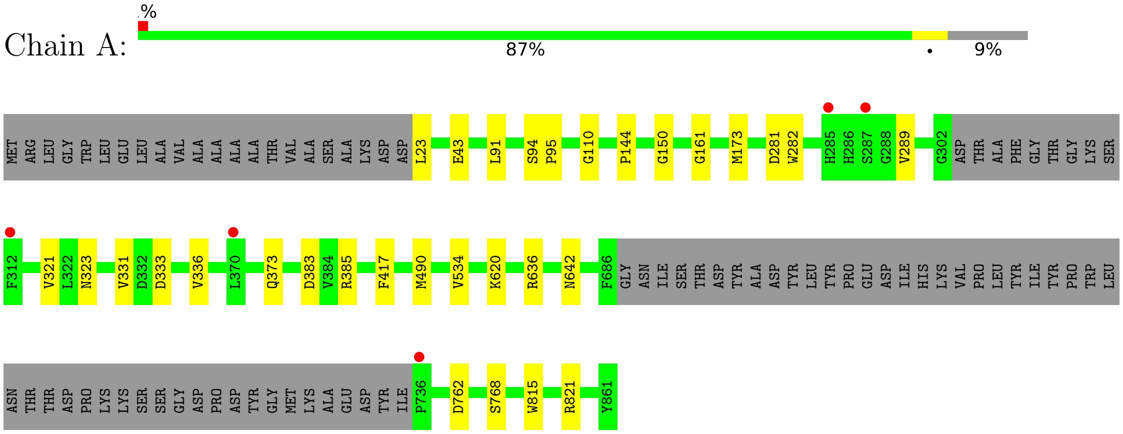
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	849	Total O 849 849	0	0
4	B	811	Total O 811 811	0	0
4	C	783	Total O 783 783	0	0
4	D	789	Total O 789 789	0	0

3 Residue-property plots

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.

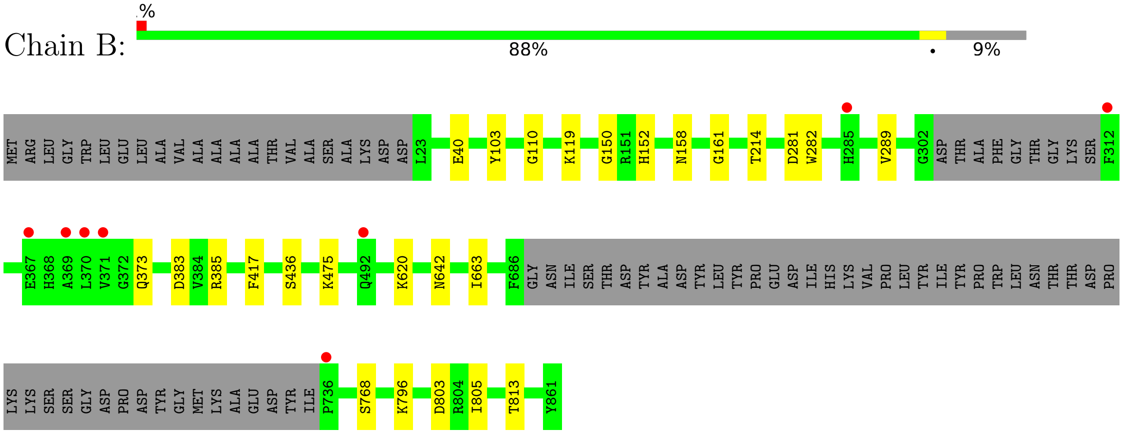
- Molecule 1: beta-glucosidase

Chain A:



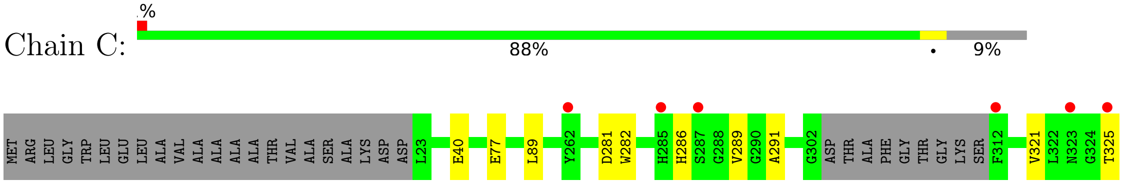
- Molecule 1: beta-glucosidase

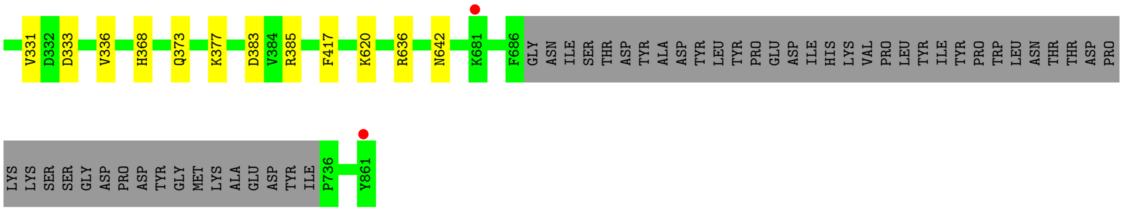
Chain B:



- Molecule 1: beta-glucosidase

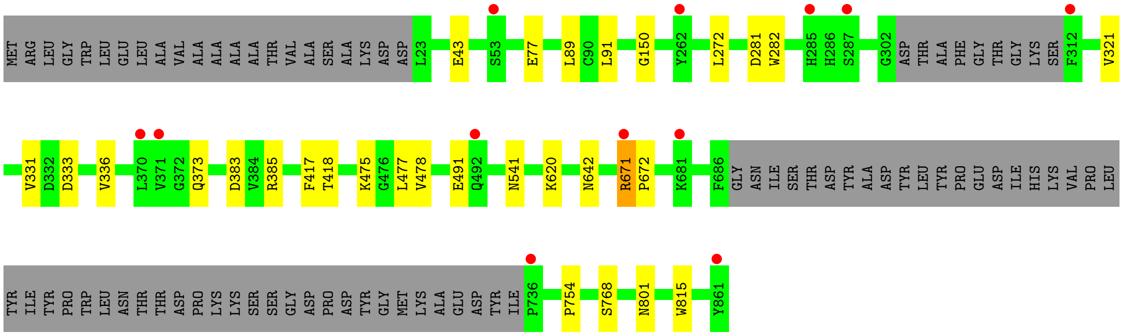
Chain C:





- Molecule 1: beta-glucosidase

Chain D:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	138.94Å 149.75Å 175.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.13 – 2.15 37.13 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.13-2.15) 99.8 (37.13-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.168 , 0.201 0.175 , 0.205	Depositor DCC
R_{free} test set	9982 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.2	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	0.96	EDS
Total number of atoms	27196	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0823e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.30	0/6134	0.56	0/8357
1	B	0.30	0/6134	0.55	0/8357
1	C	0.30	0/6134	0.56	0/8357
1	D	0.30	0/6134	0.56	0/8357
All	All	0.30	0/24536	0.56	0/33428

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 (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	5977	0	5717	16	0
1	B	5977	0	5717	15	0
1	C	5977	0	5717	12	0
1	D	5977	0	5717	17	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	11	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	13	1	0
3	C	11	0	13	1	0
3	D	11	0	13	1	0
4	A	849	0	0	1	0
4	B	811	0	0	1	0
4	C	783	0	0	1	0
4	D	789	0	0	0	0
All	All	27196	0	22920	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (50) 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:373:GLN:HE22	1:C:620:LYS:H	1.30	0.79
1:A:620:LYS:H	1:D:373:GLN:HE22	1.36	0.72
1:A:373:GLN:HE22	1:D:620:LYS:H	1.46	0.63
1:B:620:LYS:H	1:C:373:GLN:HE22	1.45	0.63
1:A:23:LEU:N	4:A:1001:HOH:O	2.31	0.62
1:A:383:ASP:OD1	1:A:385:ARG:HD3	2.03	0.58
1:B:383:ASP:OD1	1:B:385:ARG:HD3	2.05	0.56
1:C:377:LYS:NZ	4:C:1001:HOH:O	2.38	0.56
1:C:383:ASP:OD1	1:C:385:ARG:HD3	2.08	0.54
1:D:383:ASP:OD1	1:D:385:ARG:HD3	2.08	0.52
1:D:281:ASP:OD1	3:D:904:NOJ:H11	2.11	0.50
1:B:620:LYS:H	1:C:373:GLN:NE2	2.10	0.49
1:C:281:ASP:OD1	3:C:904:NOJ:H11	2.11	0.49
1:A:373:GLN:NE2	1:D:620:LYS:H	2.11	0.48
1:D:333:ASP:HA	1:D:336:VAL:HG12	1.95	0.47
1:B:281:ASP:OD1	3:B:904:NOJ:H11	2.15	0.47
1:D:671:ARG:HD3	1:D:672:PRO:O	2.15	0.46
1:A:144:PRO:HG2	1:A:173:MET:SD	2.56	0.46
1:B:214:THR:OG1	1:C:368:HIS:HE1	1.99	0.45
1:A:321:VAL:HG21	1:A:331:VAL:HG21	1.99	0.45
1:D:321:VAL:HG21	1:D:331:VAL:HG21	1.99	0.45
1:D:491:GLU:HG2	1:D:541:ASN:ND2	2.32	0.44
1:A:762:ASP:OD2	1:A:821:ARG:NH2	2.50	0.44
1:D:272:LEU:O	1:D:754:PRO:HA	2.18	0.44
1:C:77:GLU:HA	1:C:89:LEU:O	2.17	0.44
1:B:103:TYR:CE1	1:D:477:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASP:HA	1:A:336:VAL:HG12	2.00	0.43
1:A:323:ASN:OD1	1:A:323:ASN:C	2.56	0.43
1:B:373:GLN:NE2	1:C:620:LYS:H	2.07	0.43
1:B:385:ARG:NH2	1:D:475:LYS:O	2.42	0.43
1:A:91:LEU:HD12	1:A:91:LEU:N	2.34	0.43
1:C:333:ASP:HA	1:C:336:VAL:HG12	2.01	0.43
1:A:94:SER:HB2	1:A:95:PRO:CD	2.48	0.42
1:D:77:GLU:HA	1:D:89:LEU:O	2.19	0.42
1:D:768:SER:HA	1:D:815:TRP:O	2.20	0.42
1:B:796:LYS:HG2	4:B:1587:HOH:O	2.19	0.42
1:D:91:LEU:N	1:D:91:LEU:HD12	2.34	0.42
1:A:281:ASP:OD1	3:A:904:NOJ:H11	2.19	0.42
1:C:286:HIS:HB2	1:C:291:ALA:HB2	2.03	0.41
1:A:768:SER:HA	1:A:815:TRP:O	2.19	0.41
1:B:119:LYS:NZ	1:B:803:ASP:OD1	2.54	0.41
1:B:110:GLY:HA3	1:B:161:GLY:O	2.21	0.41
1:B:805:ILE:HG21	1:B:813:THR:HG21	2.03	0.41
1:A:110:GLY:HA3	1:A:161:GLY:O	2.21	0.40
1:B:663:ILE:HA	1:B:768:SER:O	2.22	0.40
1:D:321:VAL:CG2	1:D:331:VAL:HG21	2.51	0.40
1:B:152:HIS:O	1:B:158:ASN:ND2	2.53	0.40
1:D:418:THR:O	1:D:478:VAL:HA	2.21	0.40
1:A:490:MET:SD	1:A:534:VAL:HG13	2.61	0.40
1:C:321:VAL:CG2	1:C:331:VAL:HG21	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	775/861 (90%)	752 (97%)	22 (3%)	1 (0%)	48	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	775/861 (90%)	750 (97%)	24 (3%)	1 (0%)	48	51
1	C	775/861 (90%)	749 (97%)	26 (3%)	0	100	100
1	D	775/861 (90%)	752 (97%)	22 (3%)	1 (0%)	48	51
All	All	3100/3444 (90%)	3003 (97%)	94 (3%)	3 (0%)	48	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	GLY
1	D	150	GLY
1	A	150	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	631/695 (91%)	625 (99%)	6 (1%)	73	78
1	B	631/695 (91%)	624 (99%)	7 (1%)	70	75
1	C	631/695 (91%)	624 (99%)	7 (1%)	70	75
1	D	631/695 (91%)	625 (99%)	6 (1%)	73	78
All	All	2524/2780 (91%)	2498 (99%)	26 (1%)	73	78

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	282	TRP
1	A	289	VAL
1	A	417	PHE
1	A	636	ARG
1	A	642	ASN
1	B	40	GLU
1	B	282	TRP

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Mol	Chain	Res	Type
1	B	289	VAL
1	B	417	PHE
1	B	436	SER
1	B	475	LYS
1	B	642	ASN
1	C	40	GLU
1	C	282	TRP
1	C	289	VAL
1	C	325	THR
1	C	417	PHE
1	C	636	ARG
1	C	642	ASN
1	D	43	GLU
1	D	282	TRP
1	D	417	PHE
1	D	642	ASN
1	D	671	ARG
1	D	801	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	368	HIS
1	A	373	GLN
1	A	468	ASN
1	A	492	GLN
1	A	541	ASN
1	A	669	ASN
1	B	368	HIS
1	B	373	GLN
1	B	468	ASN
1	B	492	GLN
1	B	642	ASN
1	C	368	HIS
1	C	373	GLN
1	C	468	ASN
1	C	492	GLN
1	D	38	ASN
1	D	368	HIS
1	D	373	GLN
1	D	468	ASN

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Mol	Chain	Res	Type
1	D	496	GLN
1	D	541	ASN
1	D	642	ASN
1	D	808	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 12 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	NOJ	A	904	-	11,11,11	0.21	0	13,15,15	0.79	0
3	NOJ	C	904	-	11,11,11	0.24	0	13,15,15	0.80	1 (7%)
3	NOJ	D	904	-	11,11,11	0.23	0	13,15,15	0.67	0
3	NOJ	B	904	-	11,11,11	0.23	0	13,15,15	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NOJ	A	904	-	-	0/2/19/19	0/1/1/1
3	NOJ	C	904	-	-	0/2/19/19	0/1/1/1
3	NOJ	D	904	-	-	0/2/19/19	0/1/1/1
3	NOJ	B	904	-	-	0/2/19/19	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	904	NOJ	C1-N5-C5	2.07	114.09	109.61

There are no chirality outliers.

There are no torsion outliers.

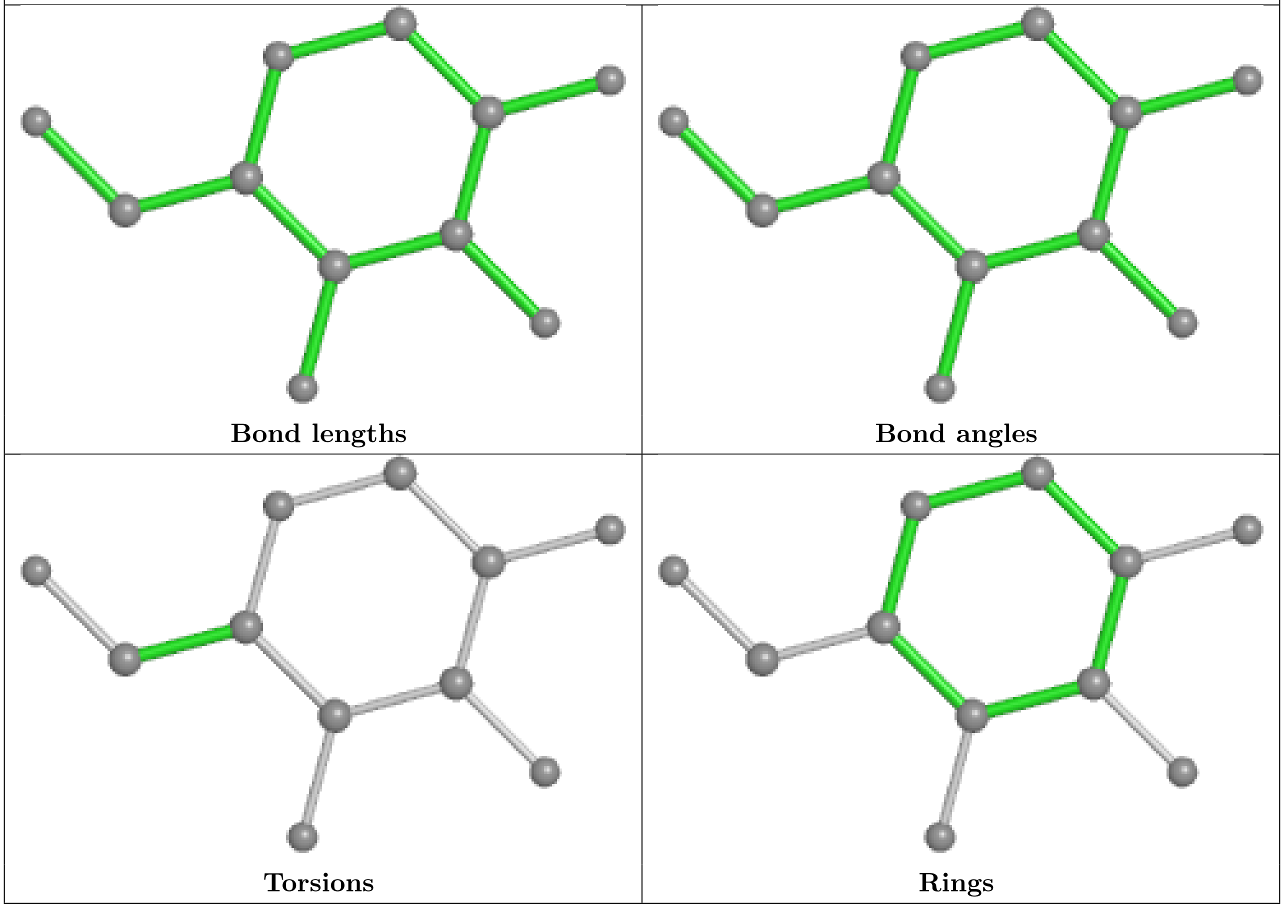
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	904	NOJ	1	0
3	C	904	NOJ	1	0
3	D	904	NOJ	1	0
3	B	904	NOJ	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 NOJ A 904



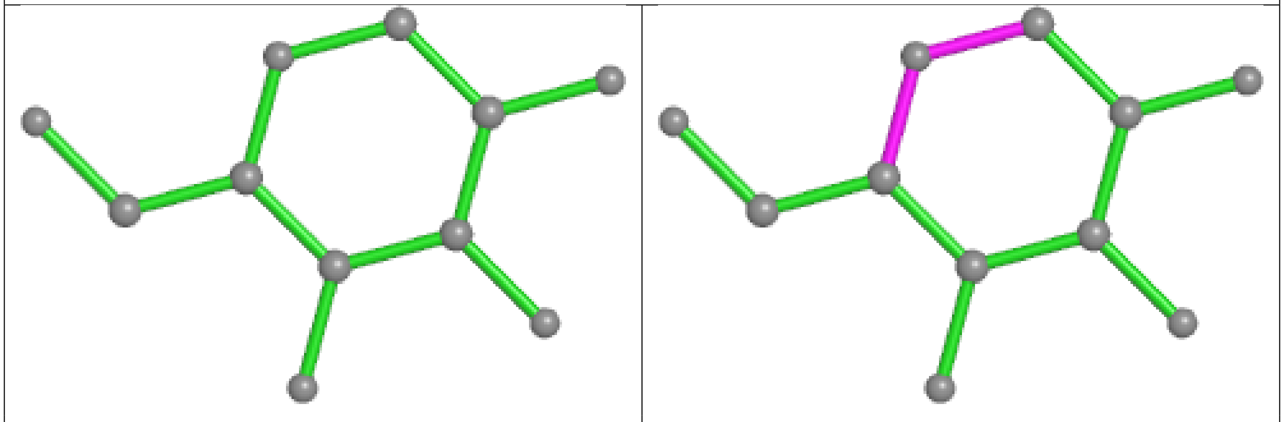
Bond lengths

Bond angles

Torsions

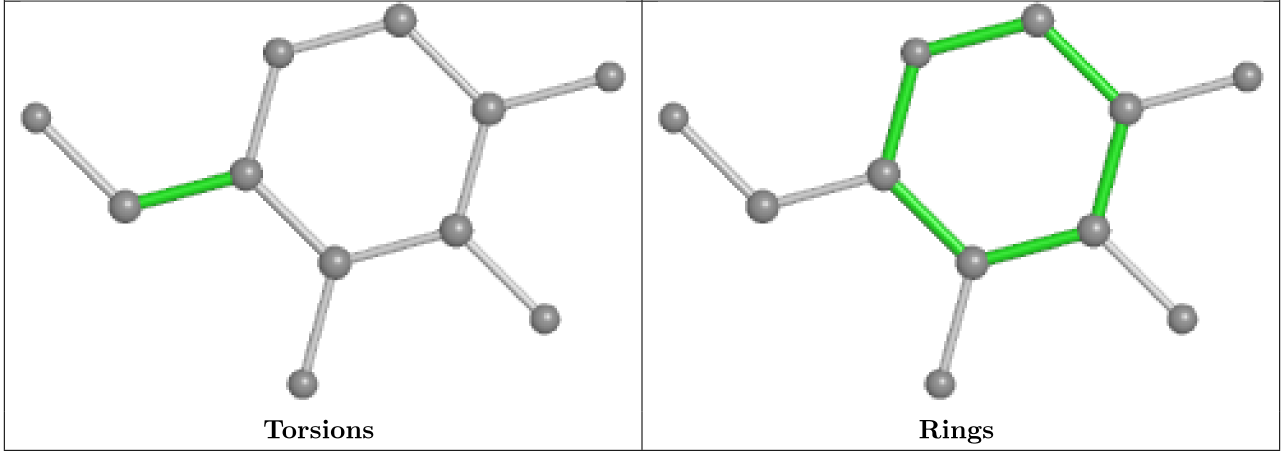
Rings

Ligand NOJ C 904



Bond lengths

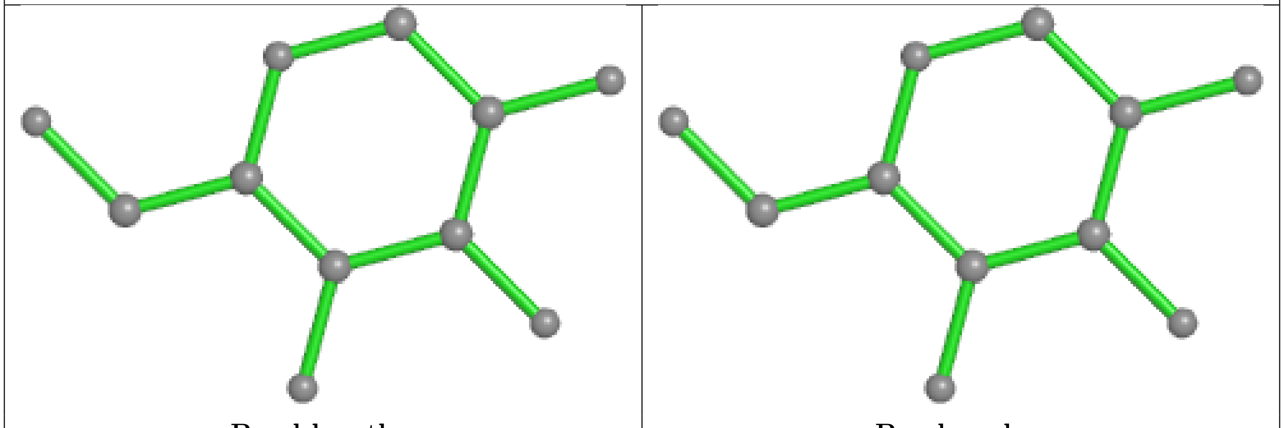
Bond angles



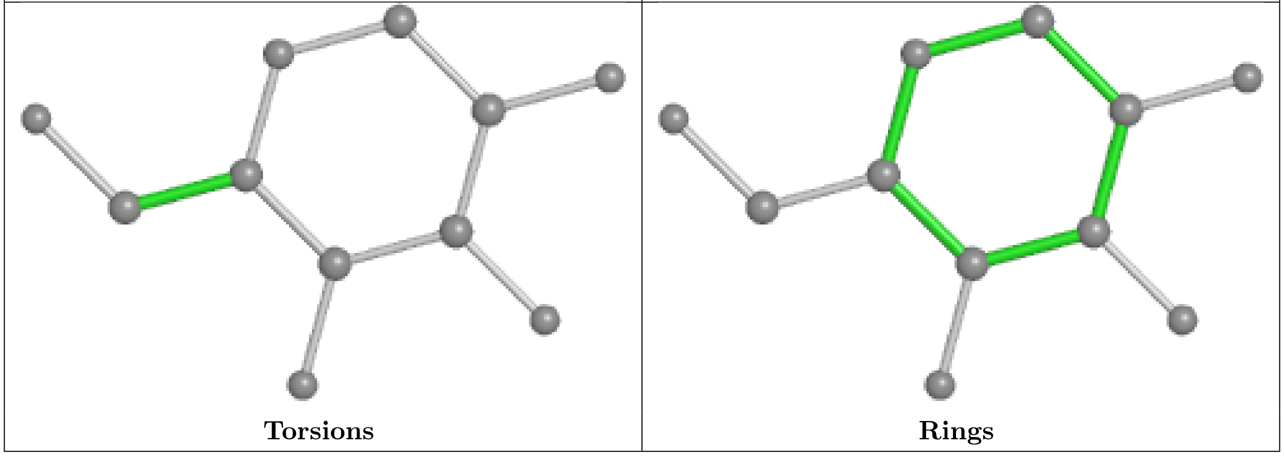
Torsions

Rings

Ligand NOJ D 904

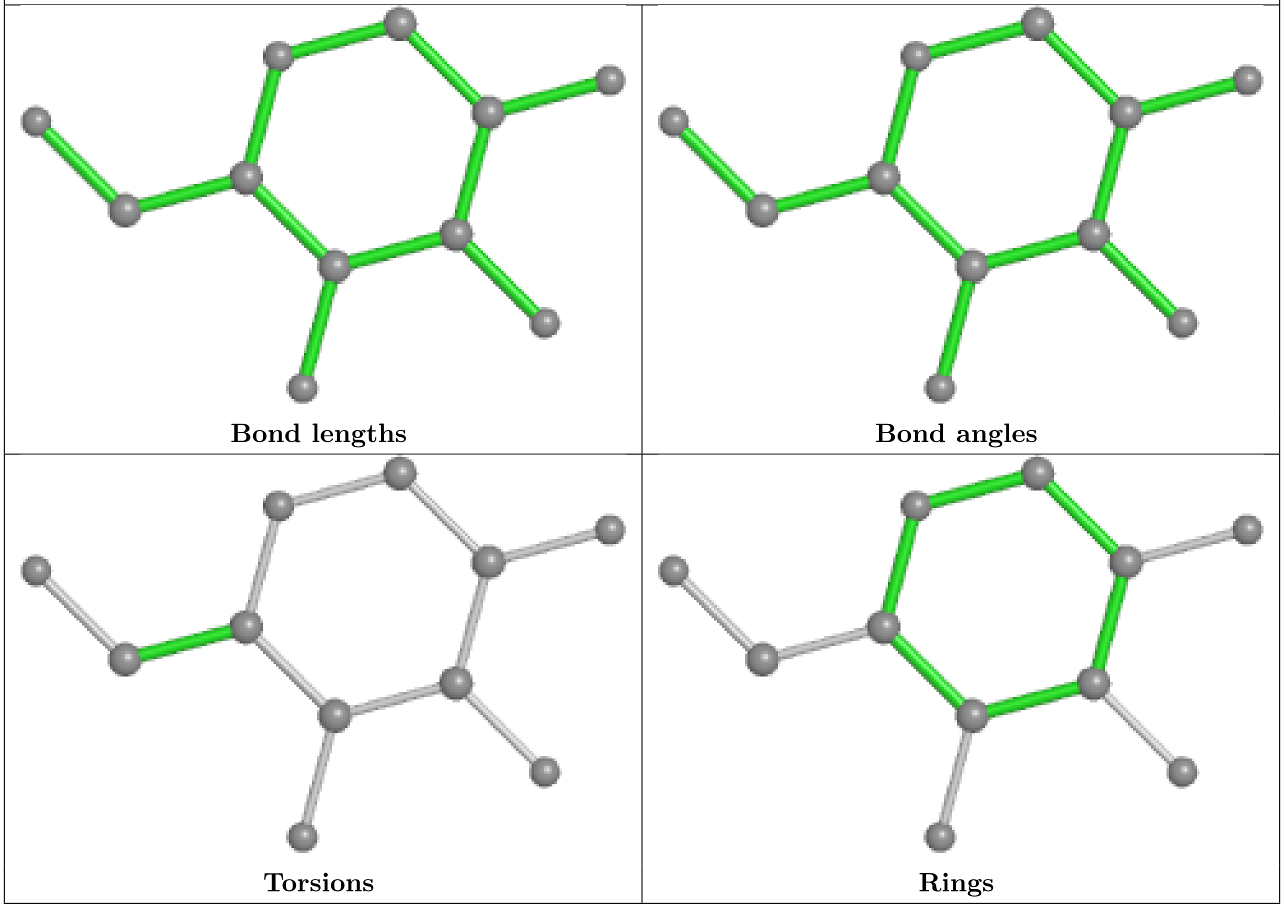


Bond lengths Bond angles



Torsions Rings

Ligand NOJ B 904



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	781/861 (90%)	-0.40	5 (0%)	85	87	10, 15, 27, 46	0
1	B	781/861 (90%)	-0.33	8 (1%)	79	82	11, 16, 28, 52	0
1	C	781/861 (90%)	-0.31	8 (1%)	79	82	11, 17, 34, 55	0
1	D	781/861 (90%)	-0.28	12 (1%)	71	75	11, 17, 36, 58	0
All	All	3124/3444 (90%)	-0.33	33 (1%)	77	81	10, 16, 32, 58	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	312	PHE	5.9
1	B	312	PHE	5.1
1	A	312	PHE	4.7
1	C	312	PHE	4.3
1	C	323	ASN	3.6
1	B	370	LEU	3.5
1	D	370	LEU	3.5
1	D	262	TYR	3.4
1	B	371	VAL	3.4
1	A	285	HIS	3.4
1	D	285	HIS	3.4
1	A	287	SER	3.3
1	C	285	HIS	3.2
1	D	671	ARG	3.1
1	C	287	SER	3.1
1	A	736	PRO	3.0
1	A	370	LEU	2.8
1	D	736	PRO	2.8
1	D	861	TYR	2.8
1	D	371	VAL	2.8
1	B	492	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	861	TYR	2.6
1	D	681	LYS	2.6
1	B	736	PRO	2.6
1	D	492	GLN	2.5
1	D	287	SER	2.5
1	C	681	LYS	2.5
1	B	369	ALA	2.3
1	B	285	HIS	2.2
1	B	367	GLU	2.2
1	C	262	TYR	2.2
1	C	325	THR	2.1
1	D	53	SER	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 ⓘ

There are no monosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	MG	A	903	1/1	0.87	0.10	39,39,39,39	0
2	MG	C	902	1/1	0.91	0.10	36,36,36,36	0
2	MG	D	902	1/1	0.91	0.06	33,33,33,33	0
2	MG	B	902	1/1	0.93	0.05	29,29,29,29	0
3	NOJ	B	904	11/11	0.95	0.06	12,12,12,12	0
3	NOJ	C	904	11/11	0.95	0.07	12,13,13,13	0
3	NOJ	A	904	11/11	0.96	0.05	10,10,10,10	0
2	MG	D	901	1/1	0.96	0.04	26,26,26,26	0
2	MG	D	903	1/1	0.96	0.04	37,37,37,37	0
2	MG	A	902	1/1	0.97	0.03	15,15,15,15	0
2	MG	C	903	1/1	0.97	0.03	25,25,25,25	0

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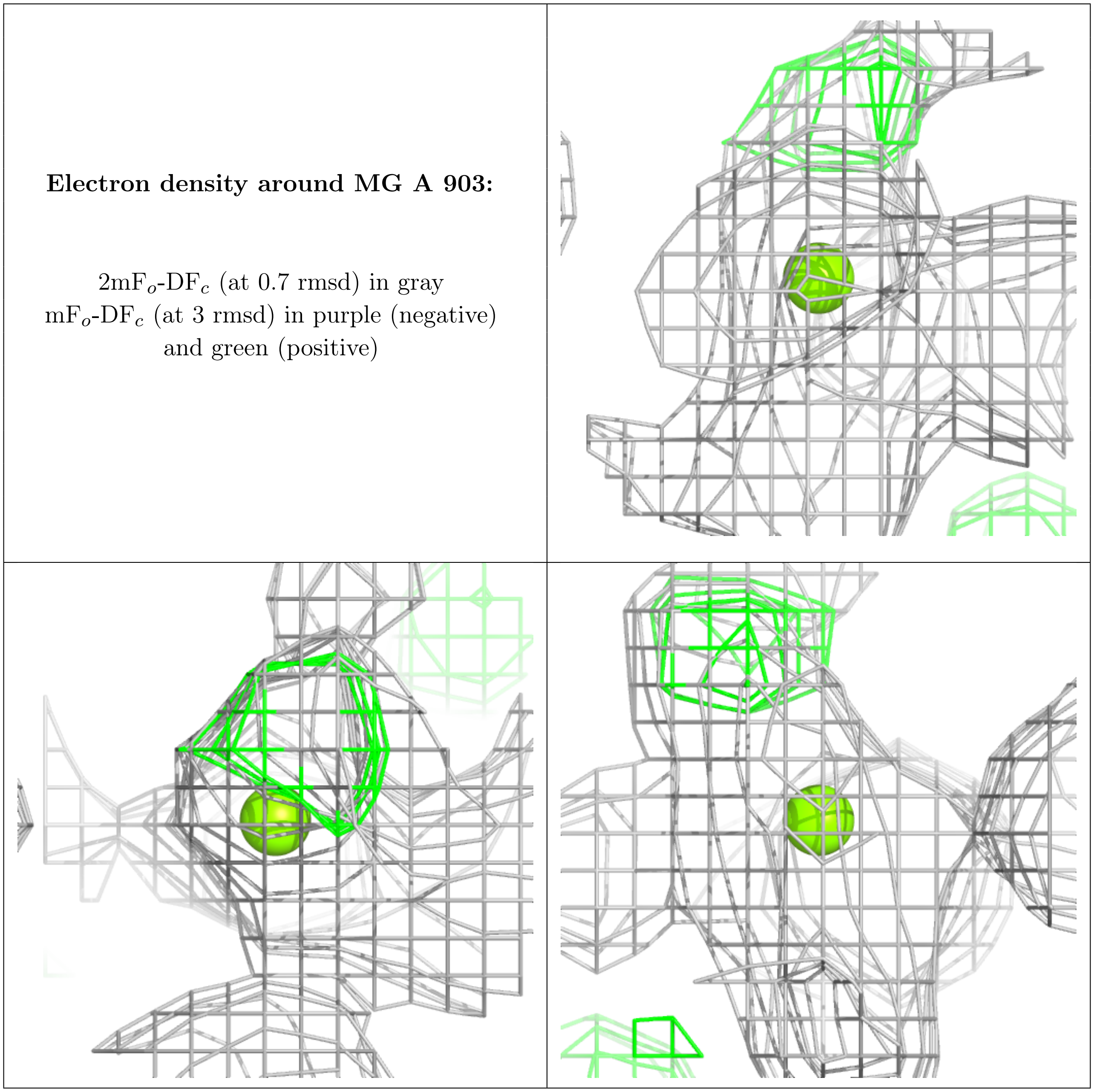
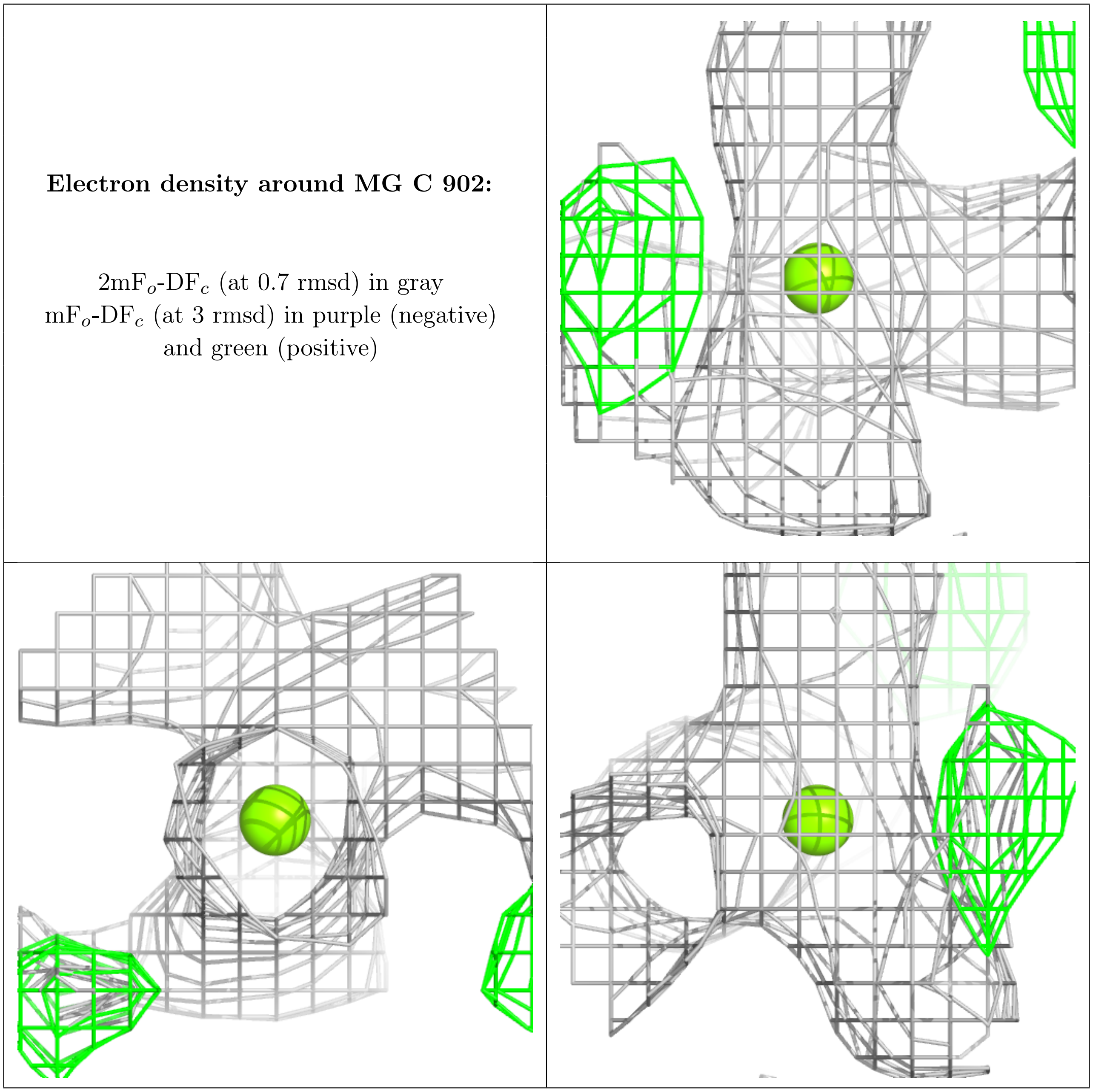
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	NOJ	D	904	11/11	0.97	0.05	14,14,14,14	0
2	MG	A	901	1/1	0.98	0.03	21,21,21,21	0
2	MG	B	903	1/1	0.98	0.03	29,29,29,29	0
2	MG	C	901	1/1	0.98	0.04	23,23,23,23	0
2	MG	B	901	1/1	0.98	0.04	17,17,17,17	0

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.



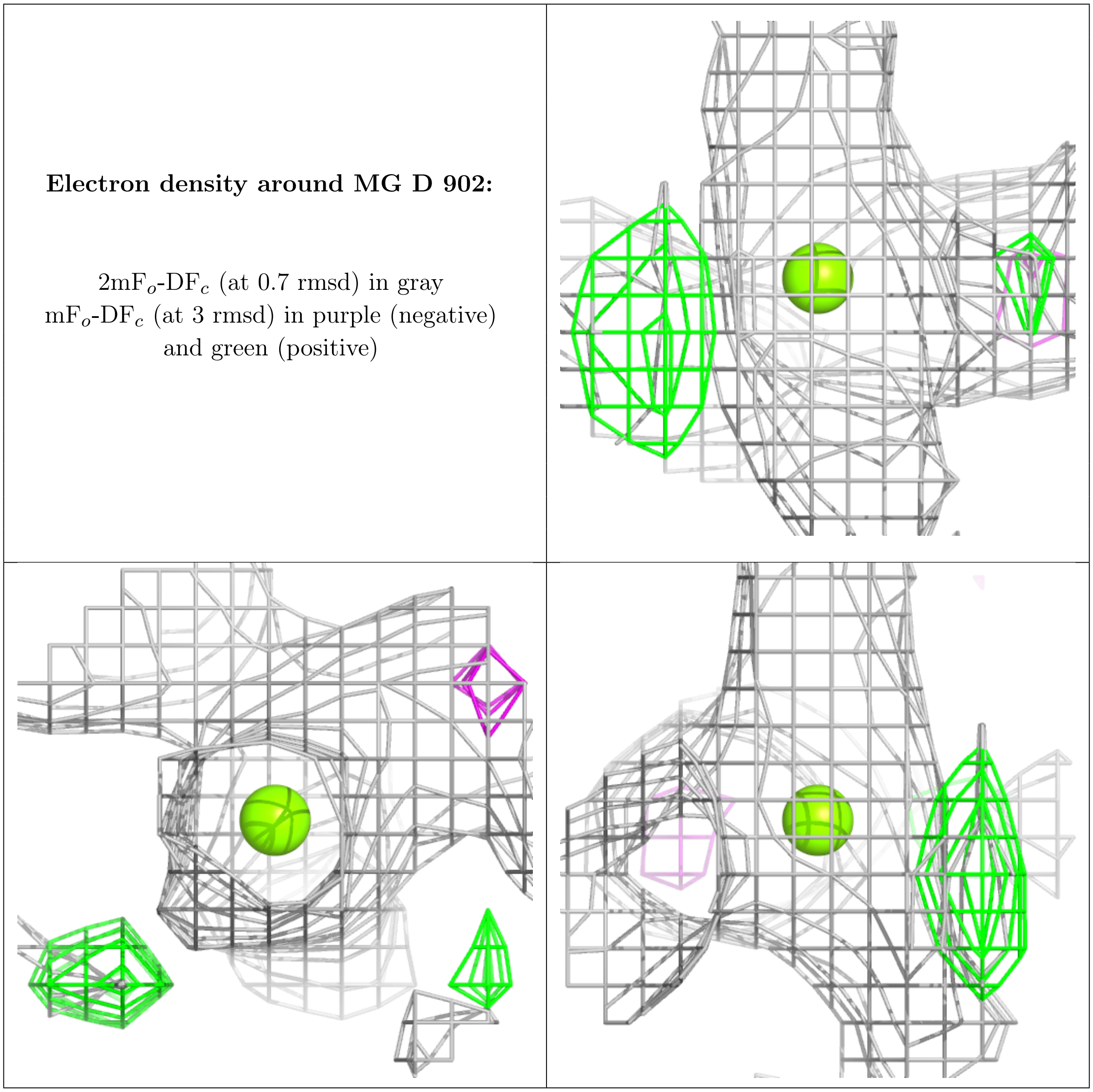
Electron density around MG A 903:

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 C 902:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

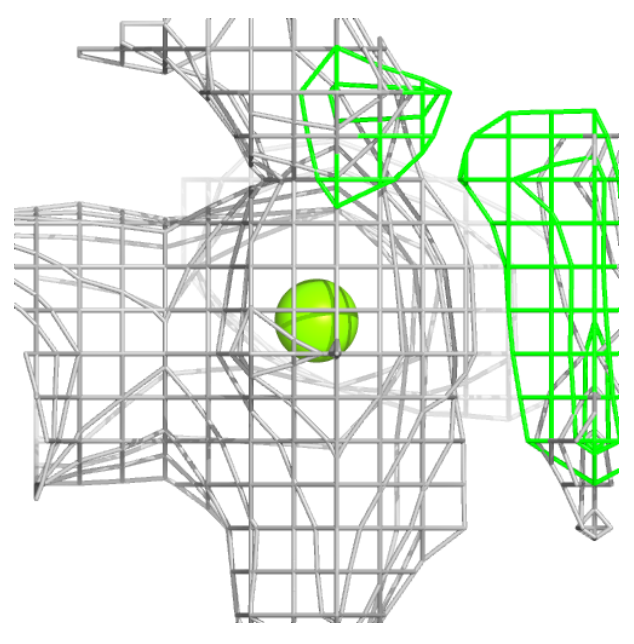


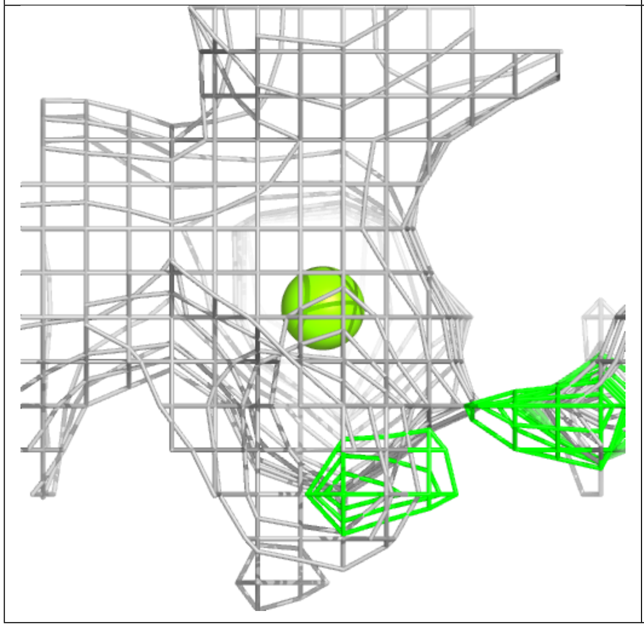
Electron density around MG D 902:

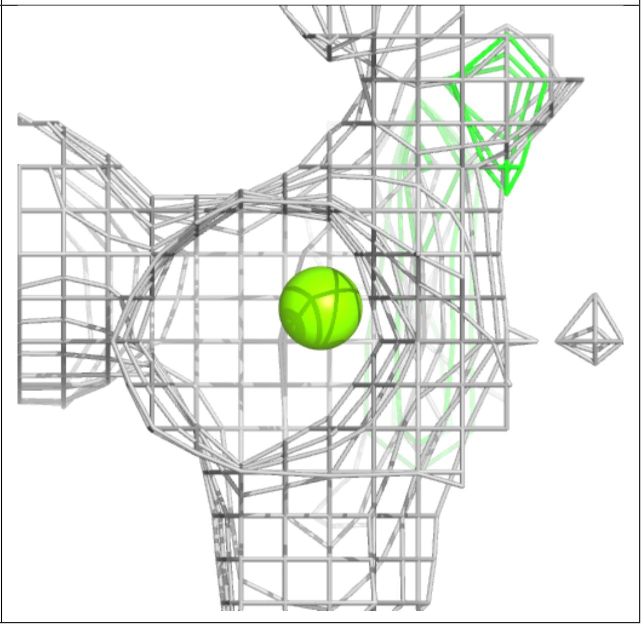
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MG B 902:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

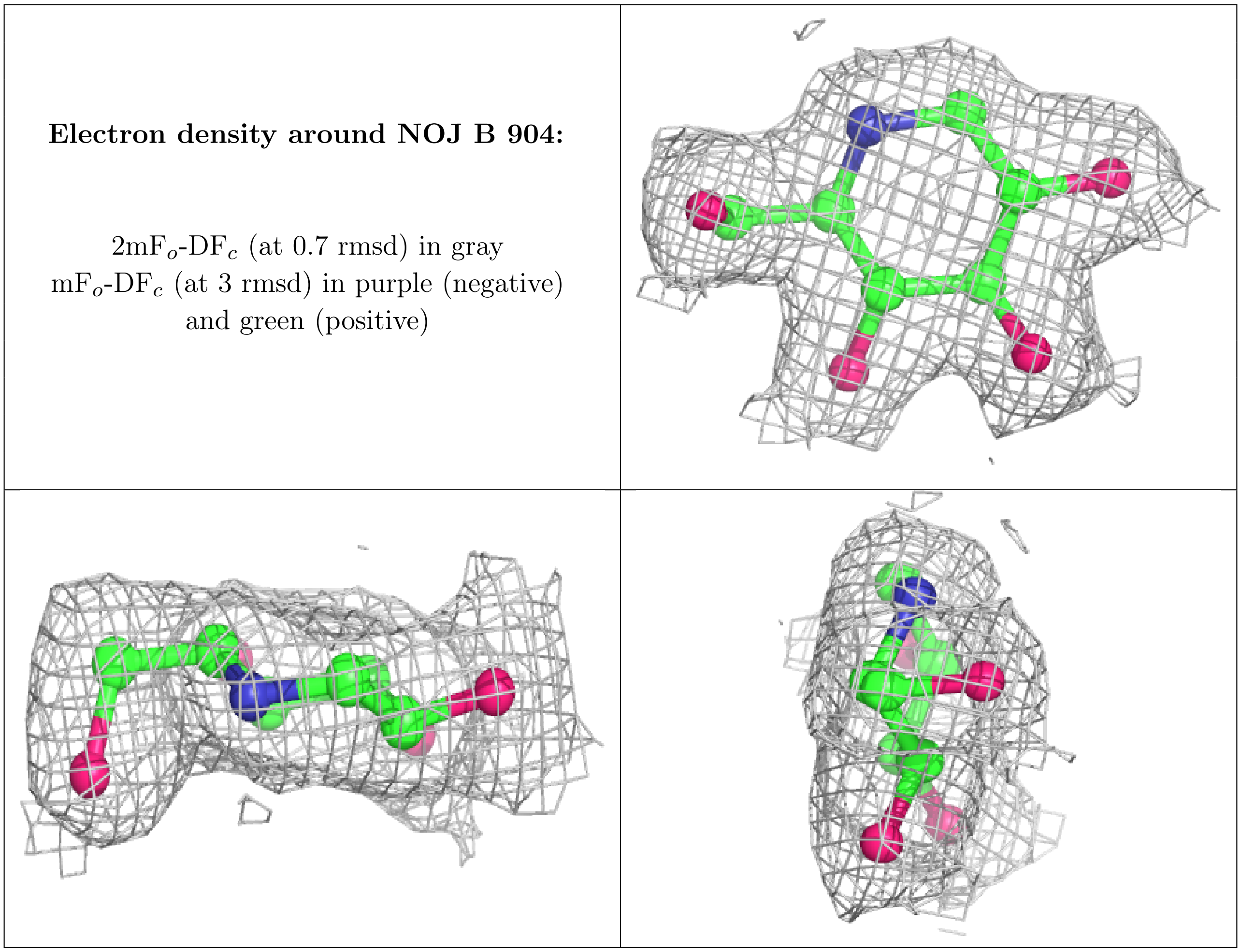






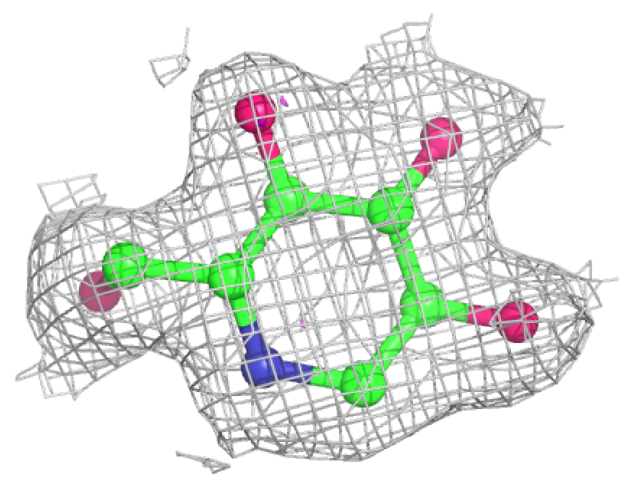
Electron density around NOJ B 904:

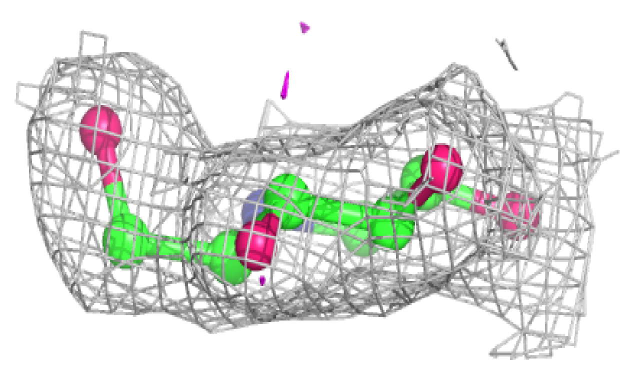
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

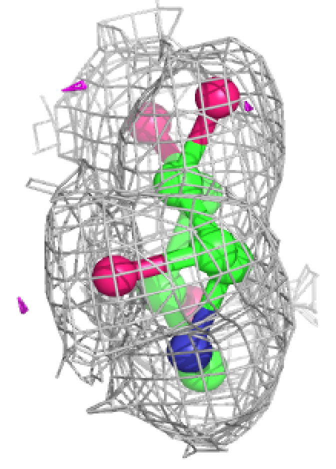


Electron density around NOJ C 904:

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

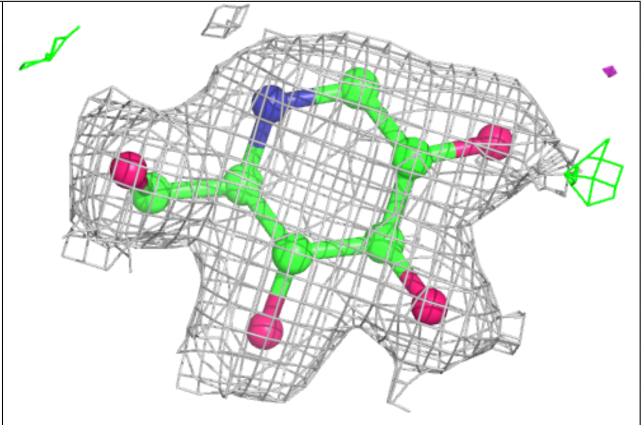


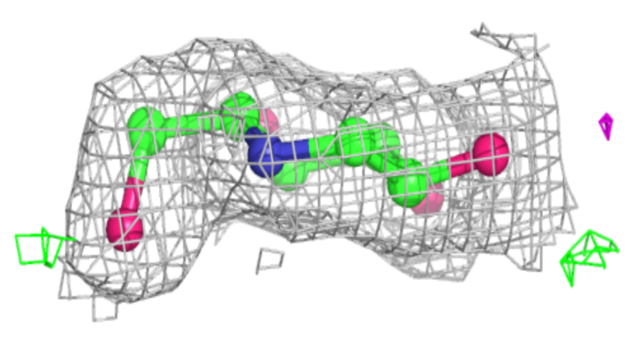


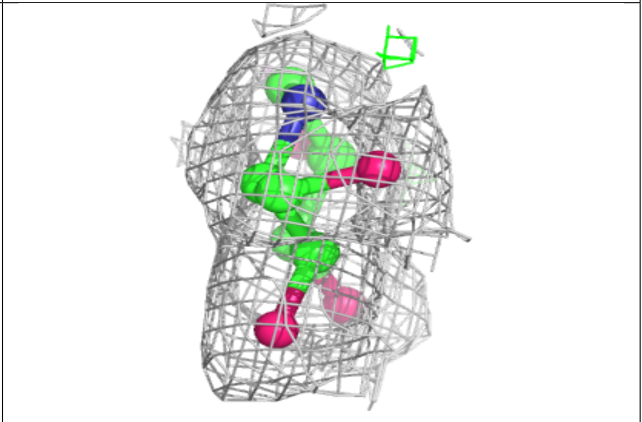


Electron density around NOJ A 904:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

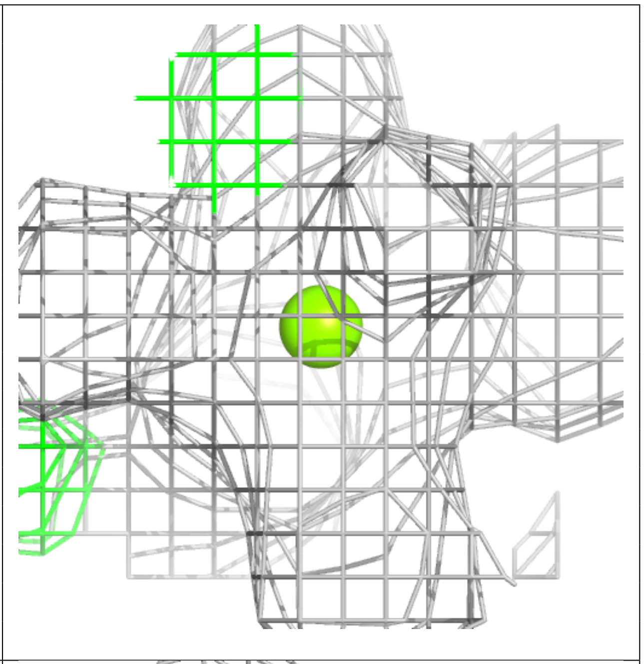


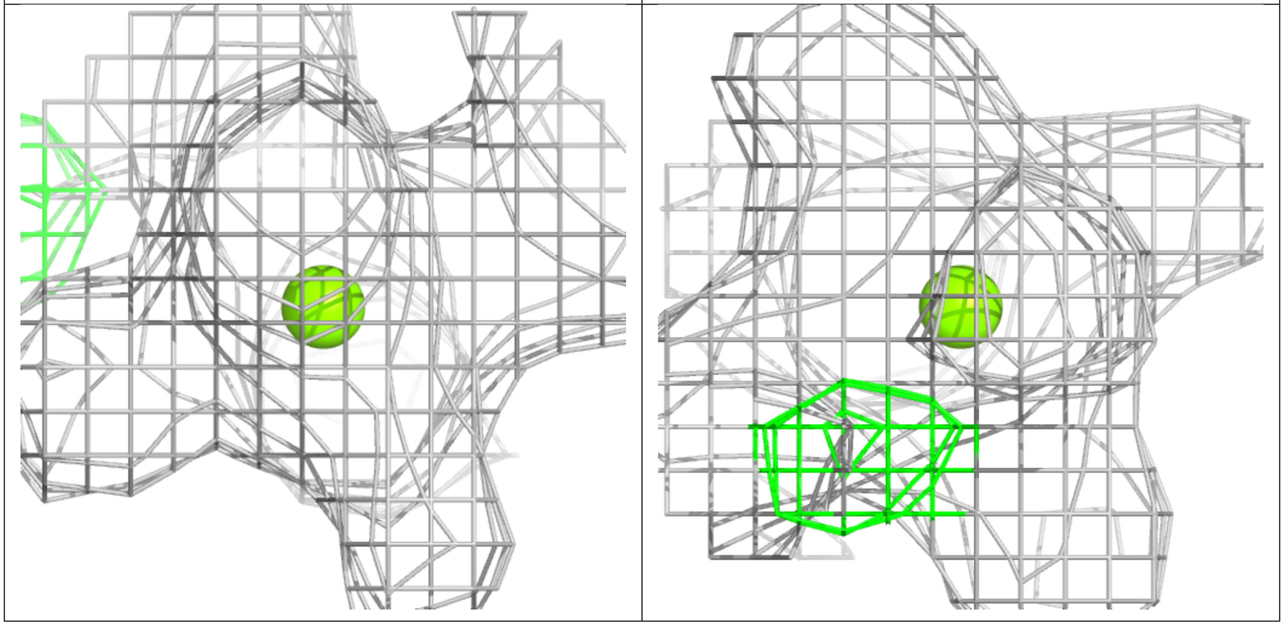




Electron density around MG D 901:

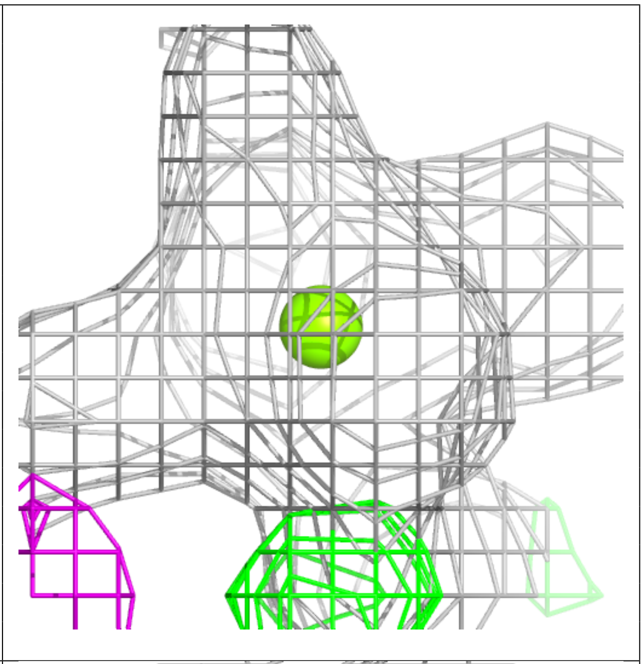
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

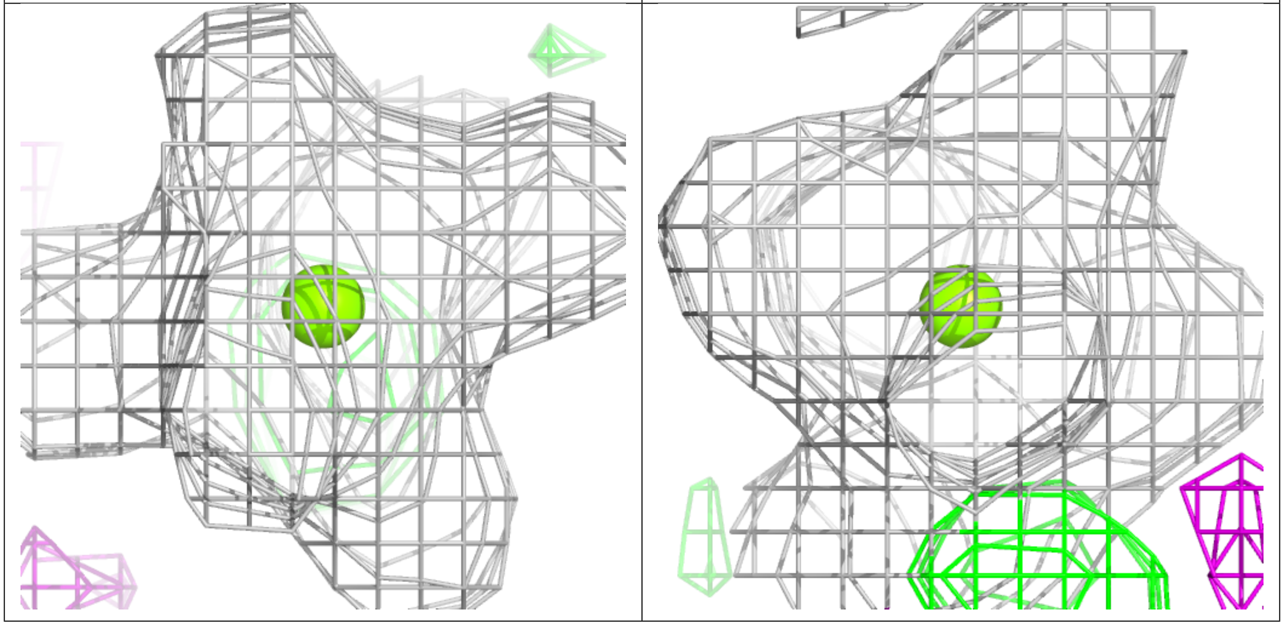




Electron density around MG D 903:

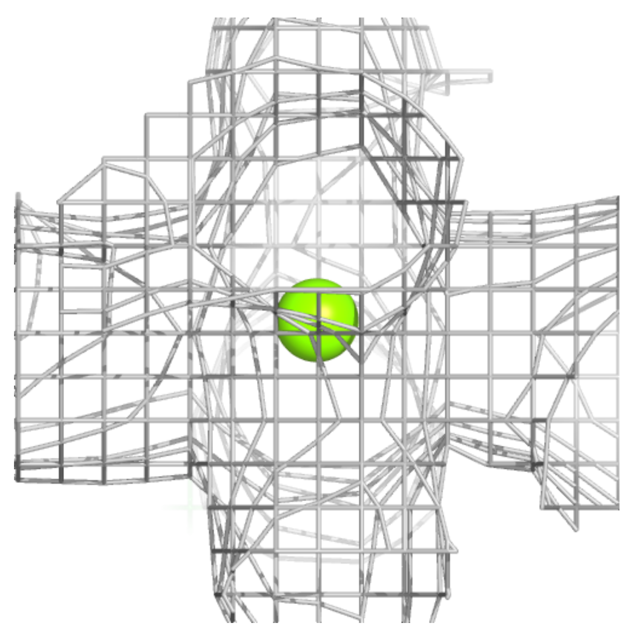
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

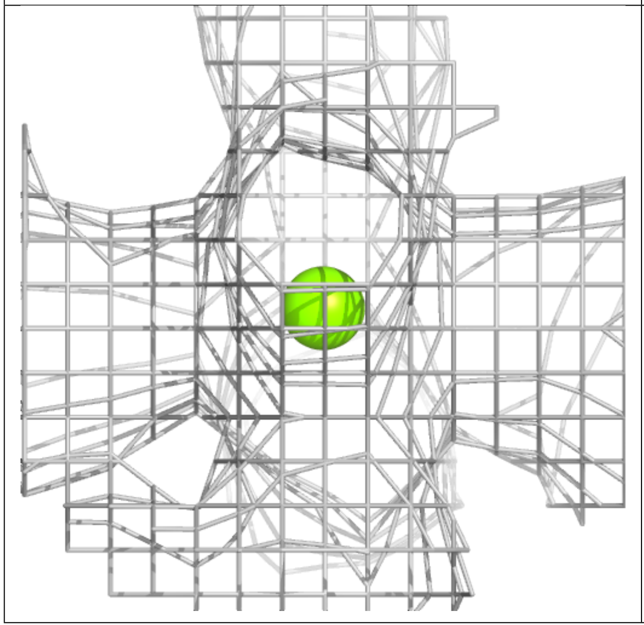




Electron density around MG A 902:

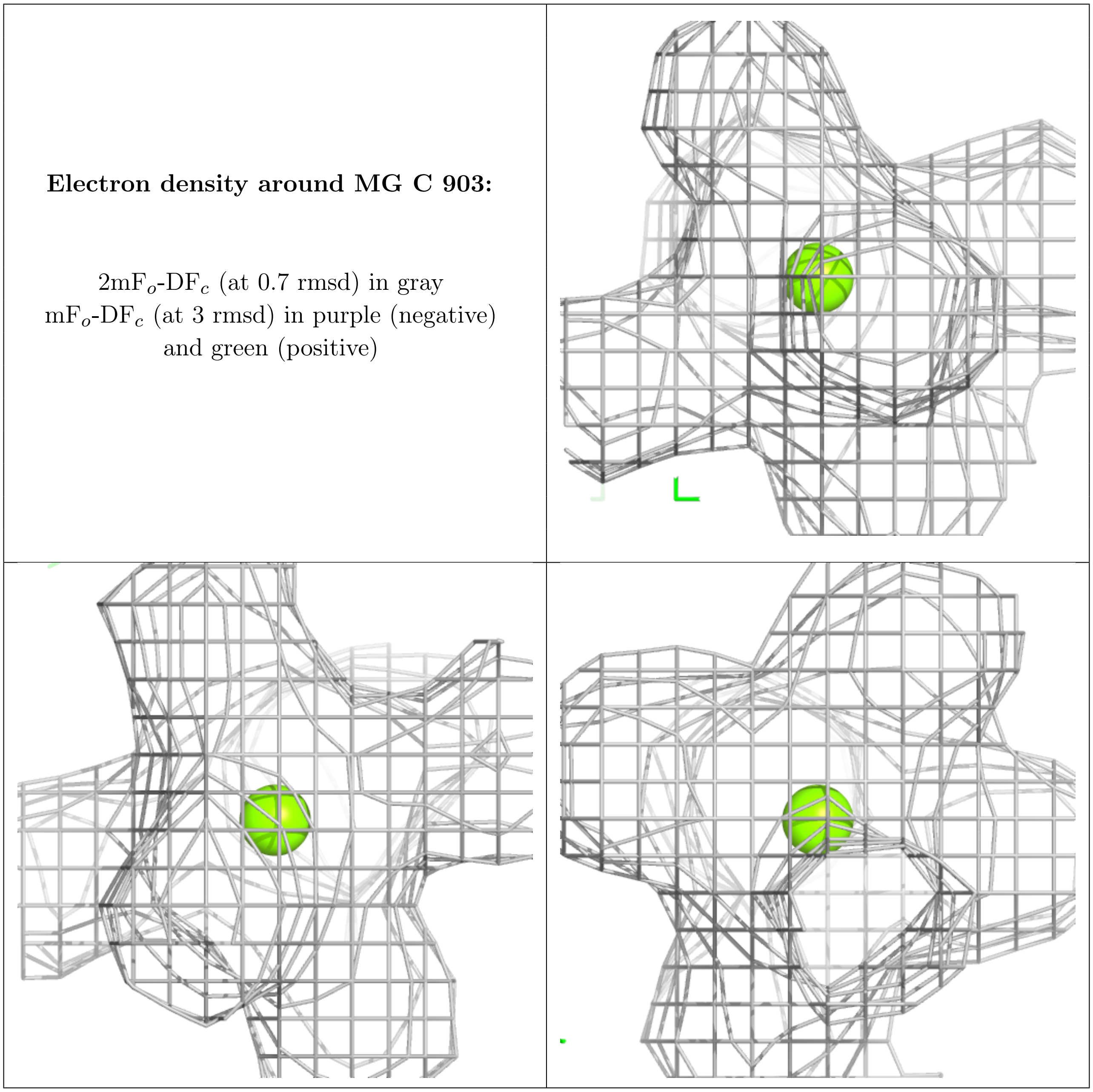
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





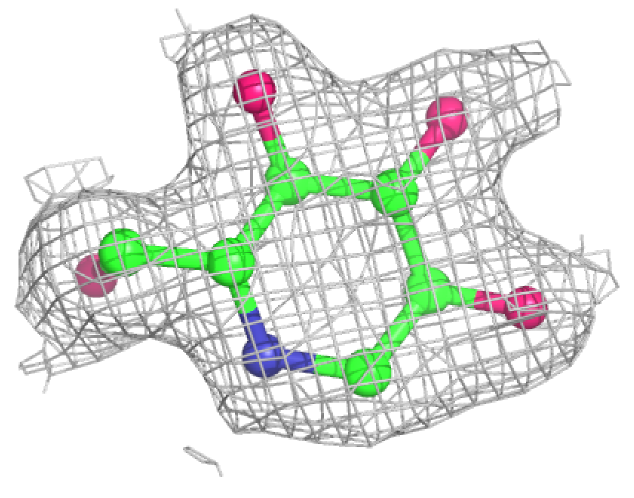
Electron density around MG C 903:

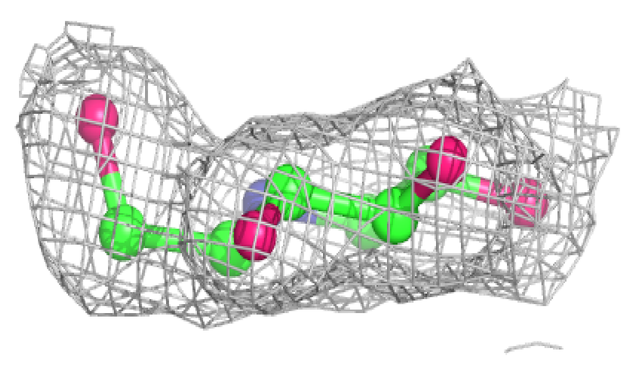
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

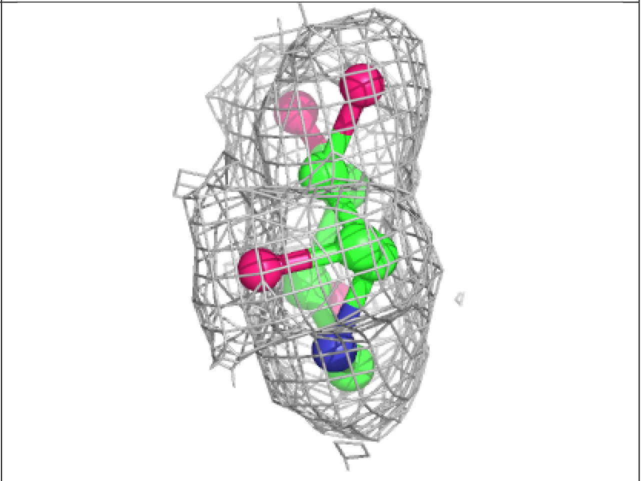


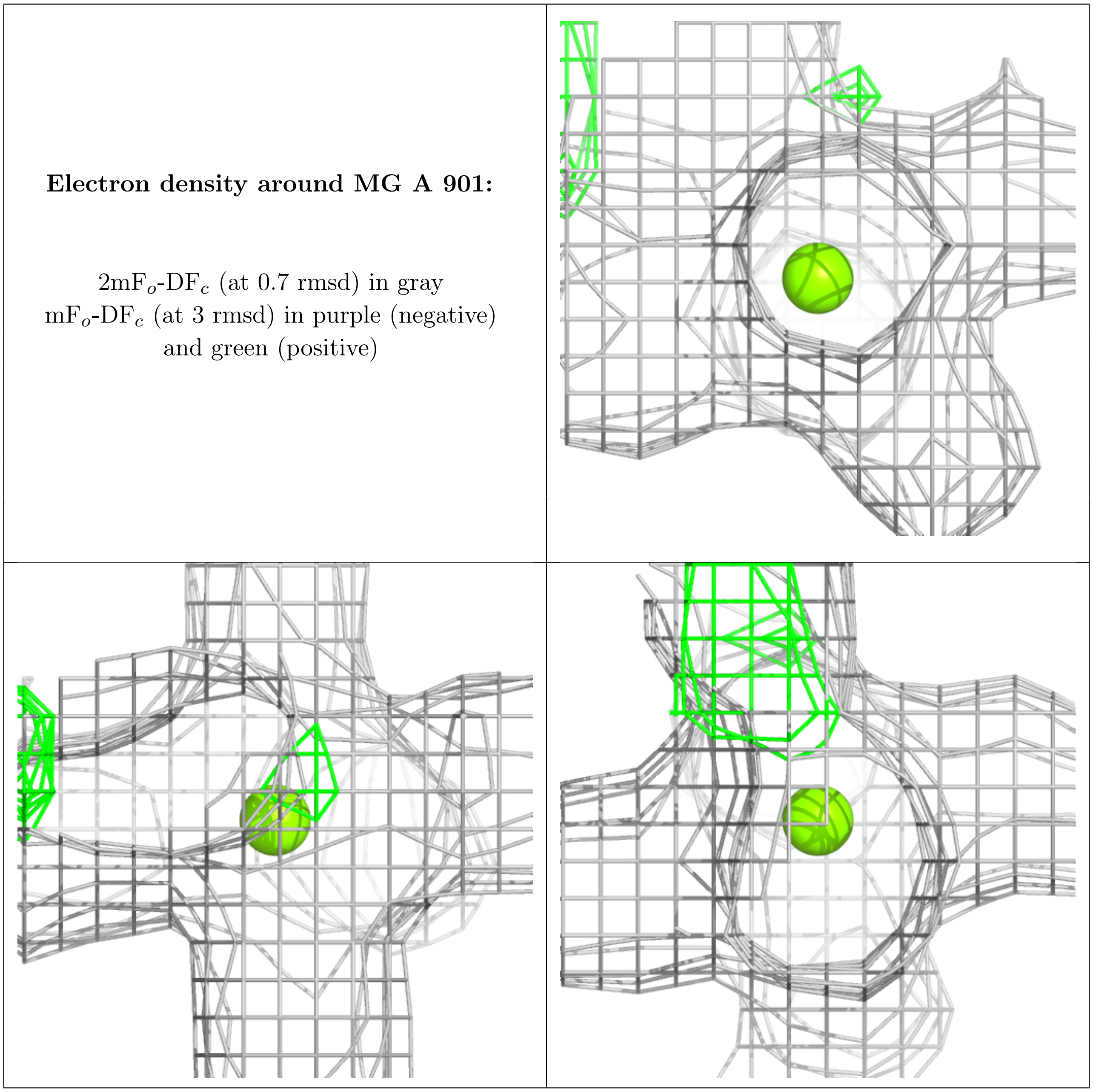
Electron density around NOJ D 904:

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



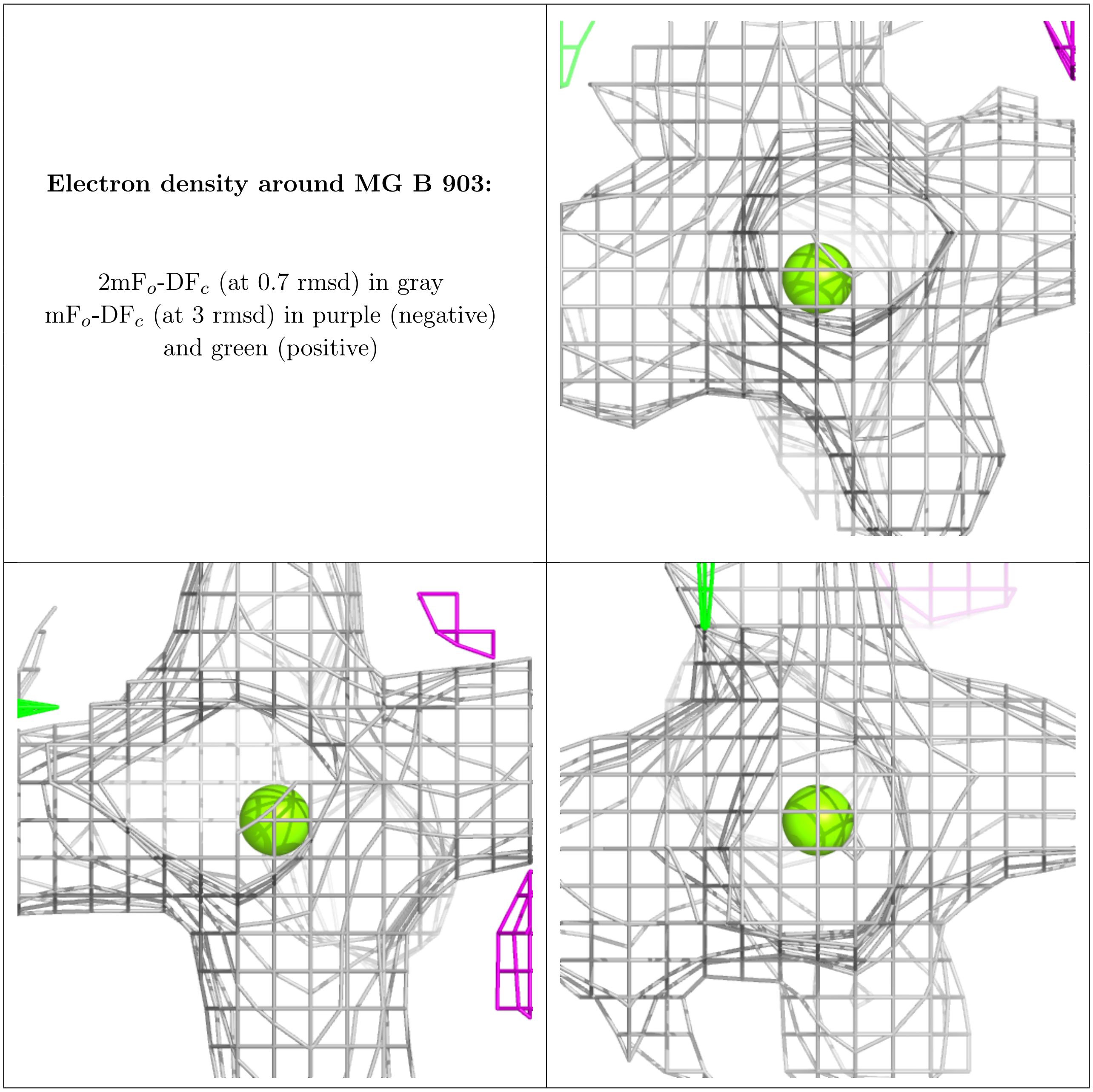






Electron density around MG A 901:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

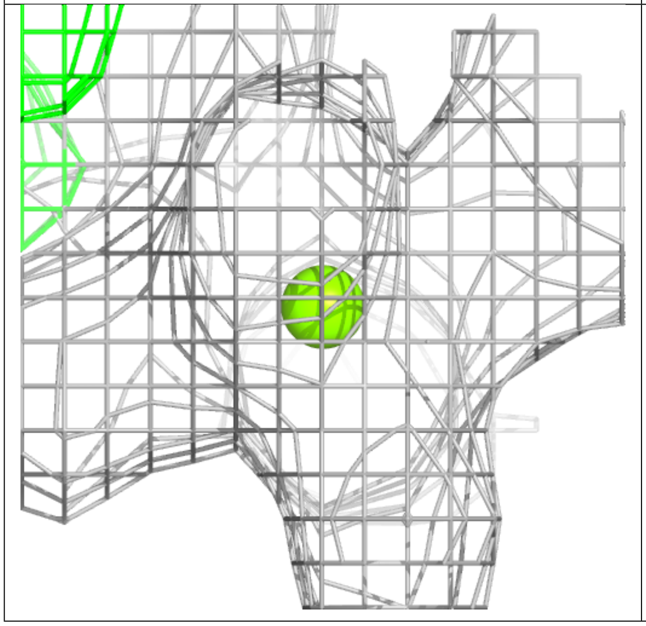


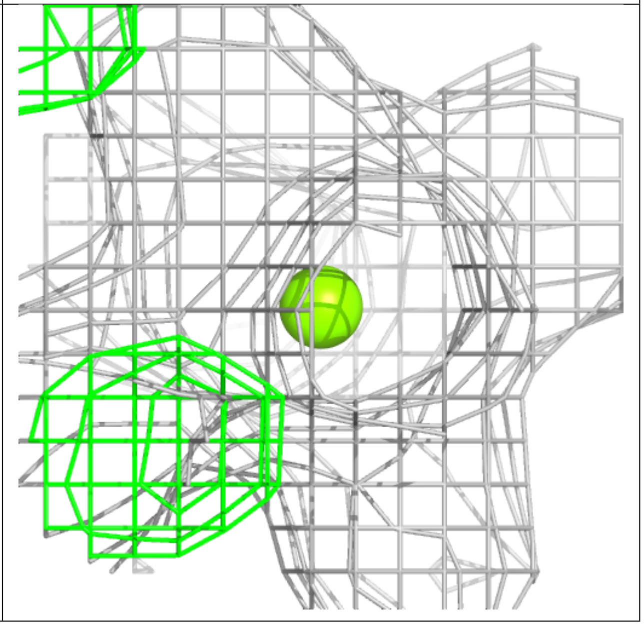
Electron density around MG B 903:

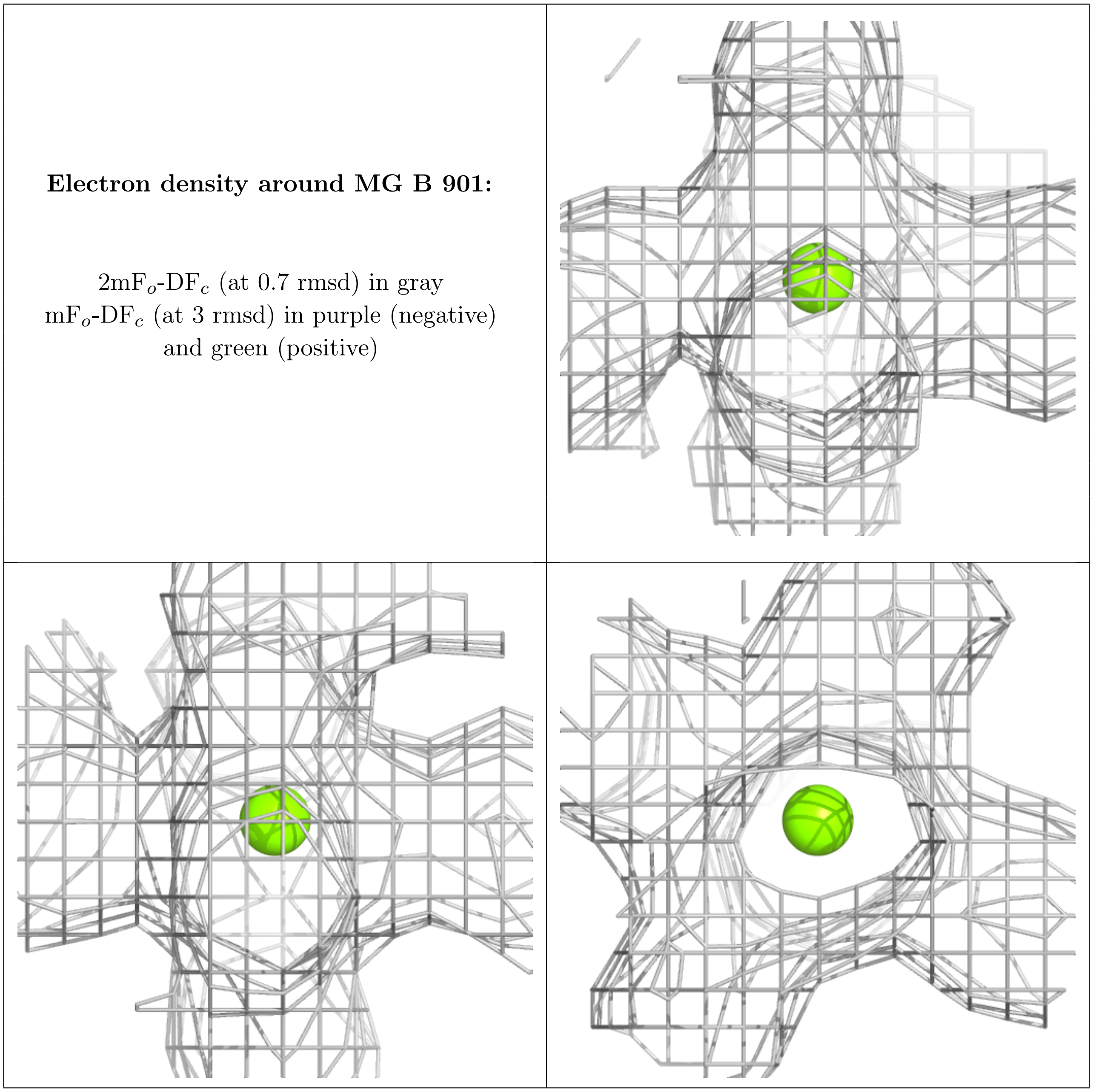
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MG C 901:

$2mF_o$-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 901:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.