wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 06:55 PM EDT

PDB ID	:	7KKG
Title	:	Dihydrodipicolinate synthase (DHDPS) from C.jejuni, N84D mutant with pyruvate bound in the active site and L-lysine bound at the allosteric site
Authors	:	Saran, S.; Majdi Yazdi, M.; Sanders, D.A.R.
Deposited on	:	2020-10-27
Resolution	:	1.64 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:

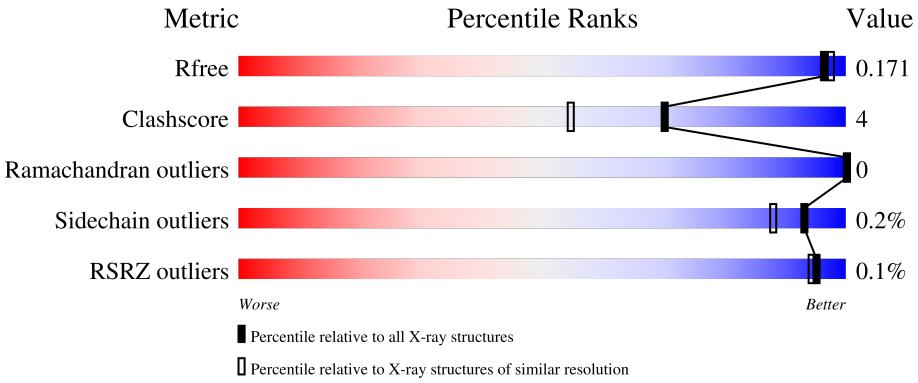
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	310	91% 5% ·
1	B	310	93% 6% ·
1	C	310	89% 6% 5%
1	D	310	95% · ··
1	E	310	92% · 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	310	89% 6% 5%

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
4	PG4	D	304	-	-	X	-
5	PEG	E	304	-	-	X	-
6	PGE	F	305	-	-	X	-
7	EDO	E	305	-	-	X	-
7	EDO	F	307	-	-	X	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 16387 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 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	4	0
			2300	1459	384	444	13			
1	B	306	Total	C	N	O	S	0	4	0
			2374	1502	402	456	14			
1	C	295	Total	C	N	O	S	0	4	0
			2285	1449	380	443	13			
1	D	306	Total	C	N	O	S	0	5	0
			2380	1504	405	457	14			
1	E	296	Total	C	N	O	S	0	4	0
			2292	1455	383	441	13			
1	F	296	Total	C	N	O	S	0	5	0
			2295	1455	383	444	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	84	ASP	ASN	engineered mutation	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	84	ASP	ASN	engineered mutation	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	84	ASP	ASN	engineered mutation	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	84	ASP	ASN	engineered mutation	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	84	ASP	ASN	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	84	ASP	ASN	engineered mutation	UNP Q9PPB4

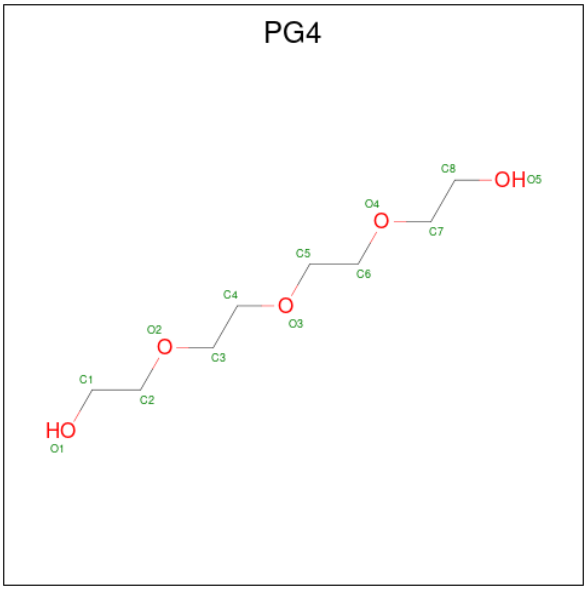
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	4	Total Mg 4 4	0	0
2	C	8	Total Mg 8 8	0	0
2	D	3	Total Mg 3 3	0	0
2	E	2	Total Mg 2 2	0	0
2	F	3	Total Mg 3 3	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

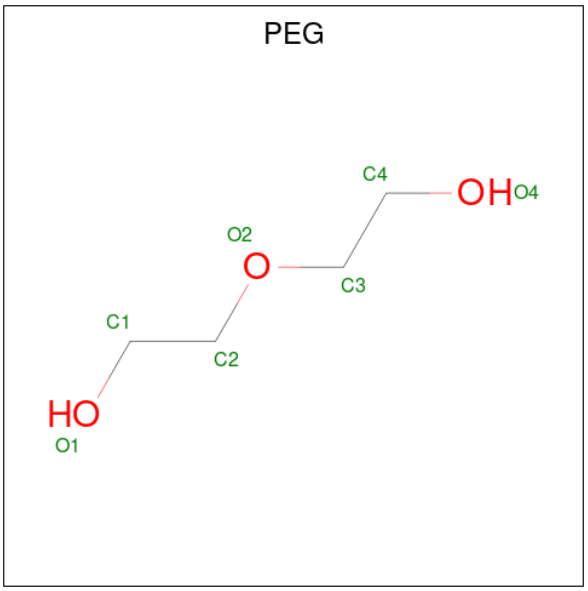
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	C	2	Total Na 2 2	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



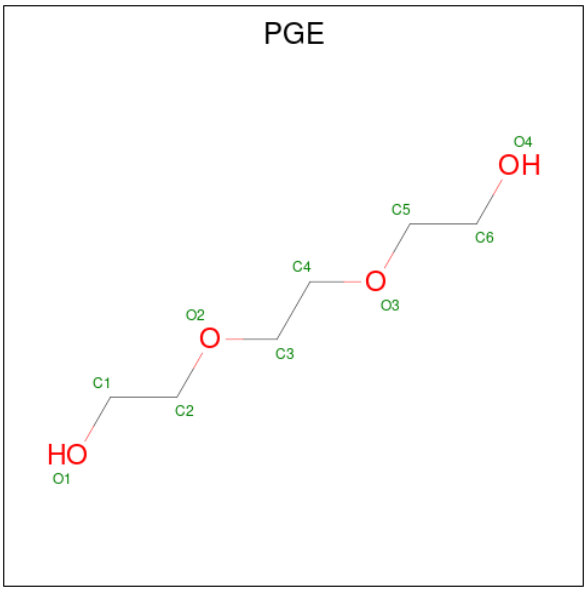
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	D	1	Total C O 13 8 5	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



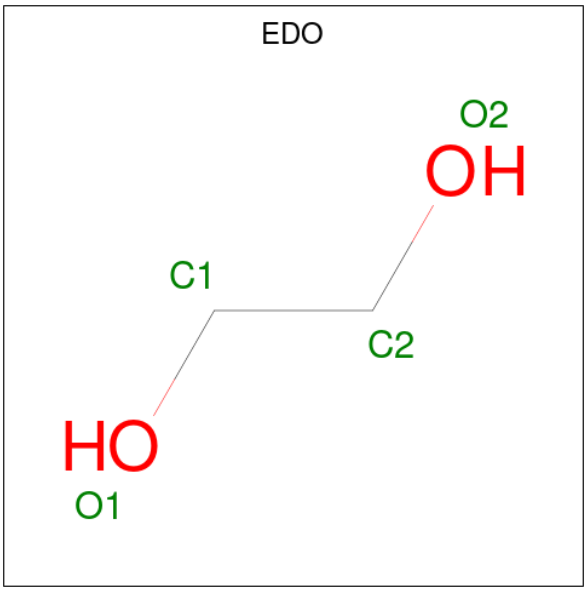
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	E	1	Total C O 7 4 3	0	0
5	E	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



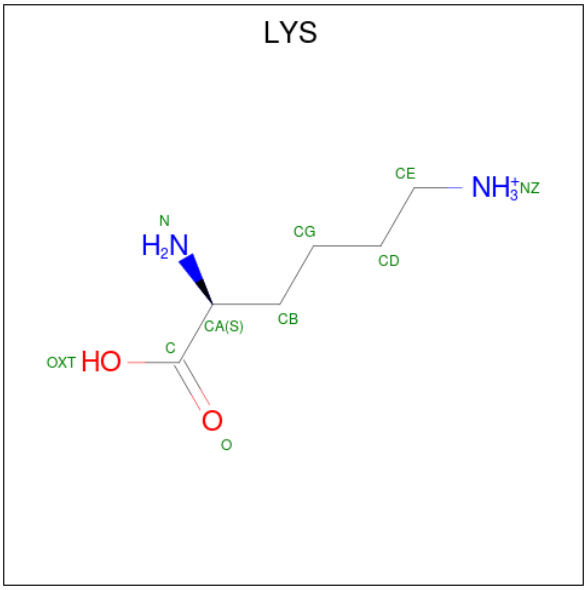
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	C	1	Total C O 10 6 4	0	0
6	C	1	Total C O 10 6 4	0	0
6	F	1	Total C O 10 6 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

- Molecule 8 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



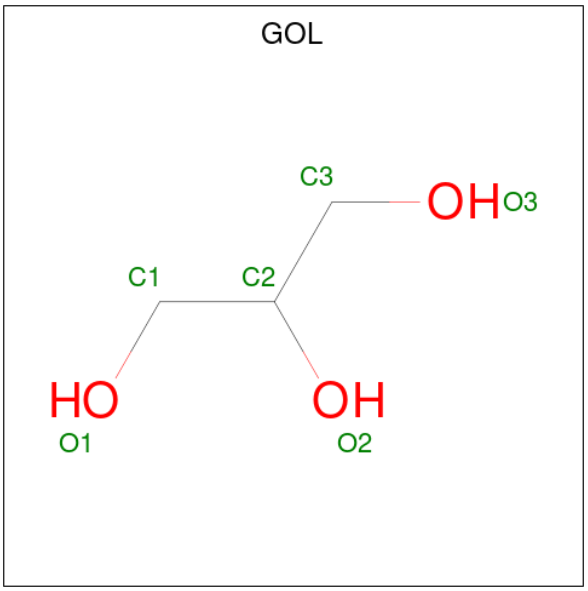
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 10 6 2 2	0	0
8	B	1	Total C N O 10 6 2 2	0	0

Continued on next page...

Continued from previous page...

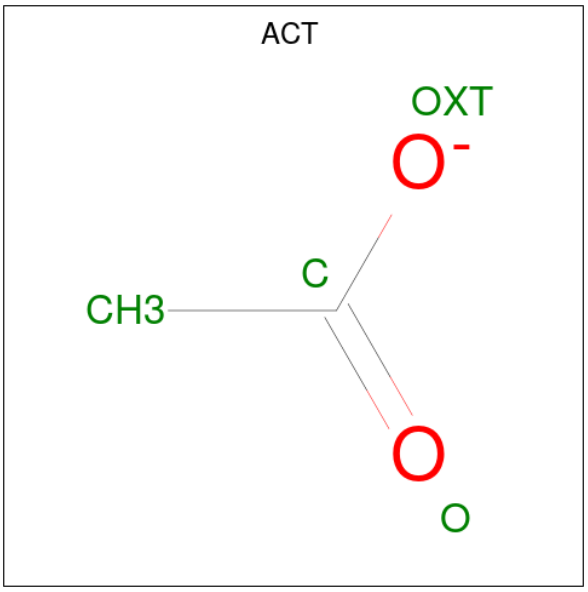
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C N O 10 6 2 2	0	0
8	D	1	Total C N O 10 6 2 2	0	0
8	E	1	Total C N O 10 6 2 2	0	0
8	F	1	Total C N O 10 6 2 2	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	1	Total C O 4 2 2	0	0
10	F	1	Total C O 4 2 2	0	0

- Molecule 11 is water.

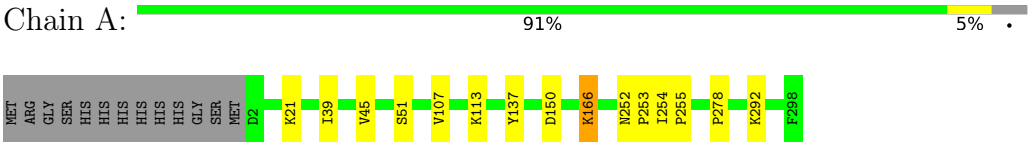
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	409	Total O 409 409	0	0
11	B	389	Total O 389 389	0	0
11	C	376	Total O 376 376	0	0
11	D	378	Total O 378 378	0	0
11	E	334	Total O 334 334	0	0
11	F	313	Total O 313 313	0	0

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.

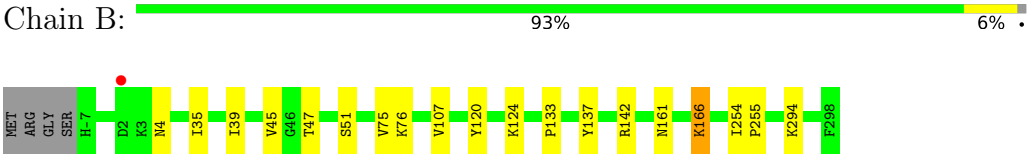
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A:



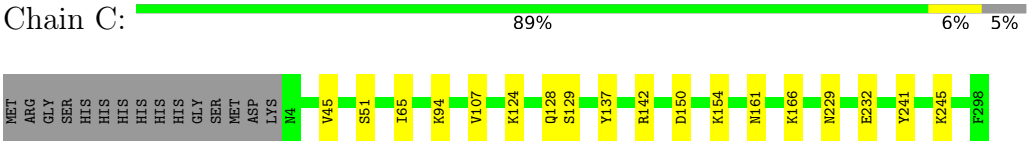
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B:



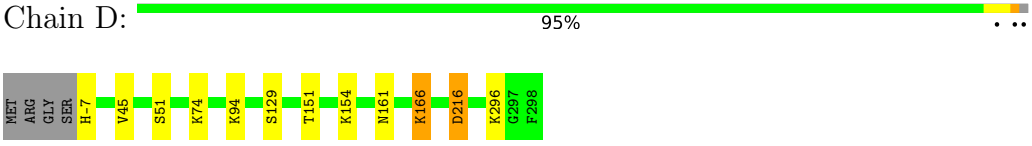
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C:



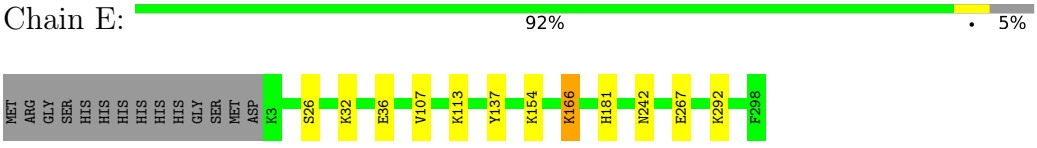
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D:



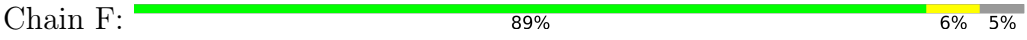
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

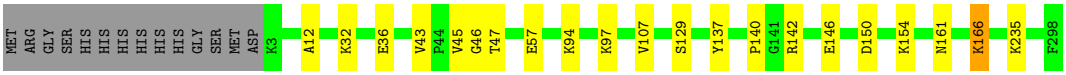
Chain E:



• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain F:




MET
ARG
GLY
SER
HIS
HIS
HIS
HIS
HIS
GLY
SER
MET
ASP
K3
A12
K32
E36
V43
P44
V45
G46
T47
E57
K94
K97
V107
S129
Y137
P140
G141
R142
E146
D150
K154
N161
K166
K235
F298

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	85.67Å 225.73Å 200.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 1.64 49.27 – 1.64	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.88-1.64) 98.8 (49.27-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.34 (at 1.64Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.138 , 0.169 0.140 , 0.171	Depositor DCC
R_{free} test set	11683 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.2	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.3	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	0.97	EDS
Total number of atoms	16387	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: PG4, PEG, ACT, GOL, MG, EDO, KPI, NA, PGE

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	0.60	0/2344	0.71	0/3166
1	B	0.56	0/2425	0.71	0/3276
1	C	0.59	0/2330	0.70	0/3148
1	D	0.67	0/2435	0.76	2/3289 (0.1%)
1	E	0.55	0/2336	0.69	0/3155
1	F	0.59	0/2344	0.71	0/3166
All	All	0.59	0/14214	0.71	2/19200 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	216	ASP	CB-CG-OD1	11.52	128.67	118.30
1	D	216	ASP	CB-CG-OD2	-5.68	113.18	118.30

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	2300	0	2340	15	0
1	B	2374	0	2386	13	0
1	C	2285	0	2309	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2380	0	2393	16	0
1	E	2292	0	2336	18	0
1	F	2295	0	2331	27	0
2	A	1	0	0	0	0
2	B	4	0	0	0	0
2	C	8	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
4	A	13	0	18	3	0
4	B	13	0	18	0	0
4	D	13	0	18	10	0
5	A	7	0	10	0	0
5	B	7	0	10	0	0
5	C	7	0	10	0	0
5	D	7	0	10	0	0
5	E	14	0	20	4	0
5	F	7	0	10	0	0
6	A	10	0	14	1	0
6	C	20	0	28	2	0
6	F	10	0	14	7	0
7	A	8	0	12	2	0
7	C	8	0	12	4	0
7	E	12	0	18	9	0
7	F	8	0	10	12	0
8	A	10	0	12	0	0
8	B	10	0	12	0	0
8	C	10	0	12	0	0
8	D	10	0	12	0	0
8	E	10	0	12	0	0
8	F	10	0	12	0	0
9	B	6	0	8	1	0
10	F	8	0	6	0	0
11	A	409	0	0	3	0
11	B	389	0	0	2	0
11	C	376	0	0	3	0
11	D	378	0	0	3	0
11	E	334	0	0	3	0
11	F	313	0	0	3	0
All	All	16387	0	14413	104	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 4.

The worst 5 of 104 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:GLY:H	7:F:307:EDO:H12	1.13	1.10
1:F:12:ALA:HA	7:F:307:EDO:H22	1.42	0.98
1:D:154:LYS:HZ2	4:D:304:PG4:H41	1.31	0.94
1:F:46:GLY:H	7:F:307:EDO:C1	1.82	0.92
1:F:46:GLY:N	7:F:307:EDO:H12	1.88	0.87

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/310 (96%)	293 (98%)	5 (2%)	0	100	100
1	B	307/310 (99%)	301 (98%)	6 (2%)	0	100	100
1	C	296/310 (96%)	291 (98%)	5 (2%)	0	100	100
1	D	308/310 (99%)	300 (97%)	8 (3%)	0	100	100
1	E	297/310 (96%)	291 (98%)	6 (2%)	0	100	100
1	F	298/310 (96%)	292 (98%)	6 (2%)	0	100	100
All	All	1804/1860 (97%)	1768 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	253/260 (97%)	253 (100%)	0	100 100
1	B	261/260 (100%)	260 (100%)	1 (0%)	91 84
1	C	251/260 (96%)	251 (100%)	0	100 100
1	D	262/260 (101%)	262 (100%)	0	100 100
1	E	252/260 (97%)	252 (100%)	0	100 100
1	F	253/260 (97%)	251 (99%)	2 (1%)	81 68
All	All	1532/1560 (98%)	1529 (100%)	3 (0%)	93 88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	THR
1	F	47	THR
1	F	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	KPI	E	166	1	11,13,14	2.22	4 (36%)	10,15,17	3.14	4 (40%)
1	KPI	A	166	1	11,13,14	1.87	3 (27%)	10,15,17	3.01	4 (40%)
1	KPI	D	166	1	11,13,14	1.86	3 (27%)	10,15,17	3.08	5 (50%)
1	KPI	F	166	1	11,13,14	2.06	3 (27%)	10,15,17	2.85	3 (30%)
1	KPI	C	166	1	11,13,14	3.65	4 (36%)	10,15,17	3.23	3 (30%)
1	KPI	B	166	1	11,13,14	2.00	4 (36%)	10,15,17	2.75	5 (50%)

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	KPI	E	166	1	-	2/13/14/16	-
1	KPI	A	166	1	-	4/13/14/16	-
1	KPI	D	166	1	-	2/13/14/16	-
1	KPI	F	166	1	-	2/13/14/16	-
1	KPI	C	166	1	-	5/13/14/16	-
1	KPI	B	166	1	-	2/13/14/16	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	CX2-CX1	9.05	1.60	1.49
1	C	166	KPI	O2-CX2	5.59	1.37	1.22
1	C	166	KPI	C1-CX1	4.95	1.59	1.49
1	F	166	KPI	O2-CX2	4.75	1.35	1.22
1	E	166	KPI	CX2-CX1	4.40	1.55	1.49

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	166	KPI	C1-CX1-CX2	8.07	126.01	118.17
1	A	166	KPI	O2-CX2-CX1	-6.54	113.03	121.38
1	B	166	KPI	CE-NZ-CX1	5.94	137.88	121.70
1	F	166	KPI	CE-NZ-CX1	5.88	137.71	121.70
1	F	166	KPI	C1-CX1-CX2	-5.65	112.68	118.17

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	166	KPI	NZ-CX1-CX2-O1
1	A	166	KPI	C1-CX1-CX2-O1
1	B	166	KPI	NZ-CX1-CX2-O1
1	B	166	KPI	NZ-CX1-CX2-O2
1	C	166	KPI	NZ-CX1-CX2-O1

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	166	KPI	1	0
1	A	166	KPI	2	0
1	D	166	KPI	1	0
1	F	166	KPI	1	0
1	B	166	KPI	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 24 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
8	LYS	C	316	-	8,9,9	0.96	0	9,10,10	1.17	1 (11%)
7	EDO	E	307	-	3,3,3	0.26	0	2,2,2	0.59	0
6	PGE	C	312	-	9,9,9	0.30	0	8,8,8	0.23	0
4	PG4	A	303	-	12,12,12	0.54	0	11,11,11	0.37	0
5	PEG	D	305	-	6,6,6	0.46	0	5,5,5	0.43	0
8	LYS	B	307	-	8,9,9	1.10	1 (12%)	9,10,10	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	ACT	F	309	-	3,3,3	0.66	0	3,3,3	1.92	2 (66%)
8	LYS	F	308	-	8,9,9	0.96	0	9,10,10	0.97	0
10	ACT	F	310	-	3,3,3	0.77	0	3,3,3	1.19	0
5	PEG	E	304	-	6,6,6	0.48	0	5,5,5	0.48	0
7	EDO	A	306	-	3,3,3	0.60	0	2,2,2	0.63	0
5	PEG	A	304	-	6,6,6	0.48	0	5,5,5	0.62	0
5	PEG	C	311	-	6,6,6	0.46	0	5,5,5	0.29	0
6	PGE	F	305	-	9,9,9	0.30	0	8,8,8	0.55	0
7	EDO	C	315	-	3,3,3	0.53	0	2,2,2	0.24	0
9	GOL	B	308	-	5,5,5	0.33	0	5,5,5	0.34	0
4	PG4	B	305	-	12,12,12	0.49	0	11,11,11	0.31	0
6	PGE	A	305	-	9,9,9	0.33	0	8,8,8	0.36	0
7	EDO	E	305	-	3,3,3	0.37	0	2,2,2	0.13	0
7	EDO	E	306	-	3,3,3	0.47	0	2,2,2	0.33	0
5	PEG	E	303	-	6,6,6	0.48	0	5,5,5	0.35	0
6	PGE	C	313	-	9,9,9	0.35	0	8,8,8	0.51	0
7	EDO	F	307	-	3,3,3	1.41	0	2,2,2	1.40	0
5	PEG	B	306	-	6,6,6	0.48	0	5,5,5	0.32	0
7	EDO	F	306	-	3,3,3	0.39	0	2,2,2	0.45	0
4	PG4	D	304	-	12,12,12	0.49	0	11,11,11	0.79	0
8	LYS	E	308	-	8,9,9	0.90	0	9,10,10	1.12	0
8	LYS	A	308	-	8,9,9	0.92	0	9,10,10	0.91	0
5	PEG	F	304	-	6,6,6	0.48	0	5,5,5	0.34	0
7	EDO	A	307	-	3,3,3	0.31	0	2,2,2	0.55	0
8	LYS	D	306	-	8,9,9	0.80	0	9,10,10	0.91	0
7	EDO	C	314	-	3,3,3	0.36	0	2,2,2	0.73	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
8	LYS	C	316	-	-	0/9/9/9	-
7	EDO	E	307	-	-	1/1/1/1	-
6	PGE	C	312	-	-	2/7/7/7	-
4	PG4	A	303	-	-	2/10/10/10	-
5	PEG	D	305	-	-	1/4/4/4	-
8	LYS	B	307	-	-	0/9/9/9	-
8	LYS	F	308	-	-	0/9/9/9	-
5	PEG	E	304	-	-	3/4/4/4	-
7	EDO	A	306	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	304	-	-	1/4/4/4	-
5	PEG	C	311	-	-	3/4/4/4	-
6	PGE	F	305	-	-	4/7/7/7	-
7	EDO	C	315	-	-	1/1/1/1	-
9	GOL	B	308	-	-	4/4/4/4	-
4	PG4	B	305	-	-	2/10/10/10	-
6	PGE	A	305	-	-	5/7/7/7	-
7	EDO	E	305	-	-	1/1/1/1	-
7	EDO	E	306	-	-	1/1/1/1	-
5	PEG	E	303	-	-	1/4/4/4	-
6	PGE	C	313	-	-	2/7/7/7	-
7	EDO	F	307	-	-	1/1/1/1	-
5	PEG	B	306	-	-	1/4/4/4	-
7	EDO	F	306	-	-	1/1/1/1	-
4	PG4	D	304	-	-	7/10/10/10	-
8	LYS	E	308	-	-	0/9/9/9	-
8	LYS	A	308	-	-	0/9/9/9	-
5	PEG	F	304	-	-	2/4/4/4	-
7	EDO	A	307	-	-	0/1/1/1	-
8	LYS	D	306	-	-	0/9/9/9	-
7	EDO	C	314	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	307	LYS	OXT-C	-2.15	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	309	ACT	OXT-C-CH3	2.52	125.61	115.18
8	C	316	LYS	OXT-C-CA	2.39	121.52	113.38
10	F	309	ACT	OXT-C-O	-2.07	114.42	122.05

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	308	GOL	O1-C1-C2-C3
6	A	305	PGE	C3-C4-O3-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	305	PGE	O2-C3-C4-O3
6	C	313	PGE	O3-C5-C6-O4
7	E	306	EDO	O1-C1-C2-O2

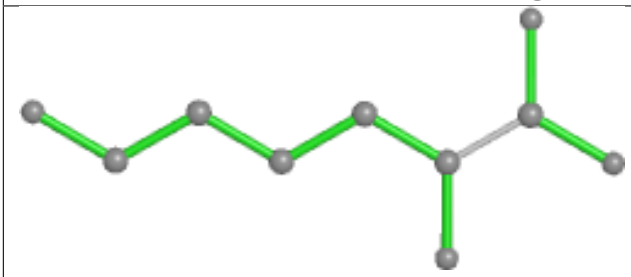
There are no ring outliers.

15 monomers are involved in 55 short contacts:

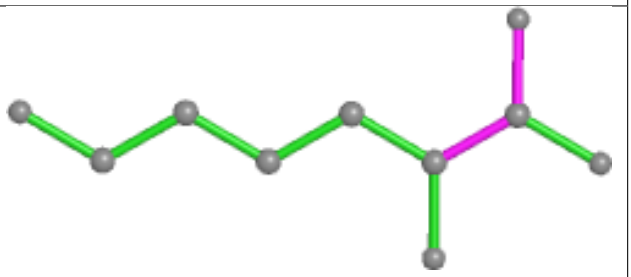
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	307	EDO	3	0
4	A	303	PG4	3	0
5	E	304	PEG	4	0
6	F	305	PGE	7	0
7	C	315	EDO	1	0
9	B	308	GOL	1	0
6	A	305	PGE	1	0
7	E	305	EDO	5	0
7	E	306	EDO	1	0
6	C	313	PGE	2	0
7	F	307	EDO	11	0
7	F	306	EDO	1	0
4	D	304	PG4	10	0
7	A	307	EDO	2	0
7	C	314	EDO	3	0

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.

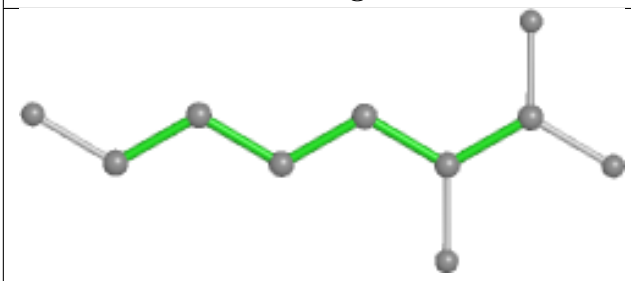
Ligand LYS C 316



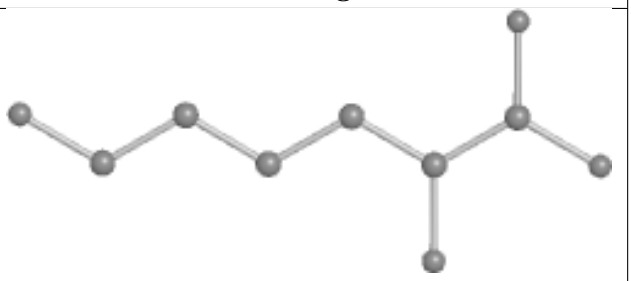
Bond lengths



Bond angles

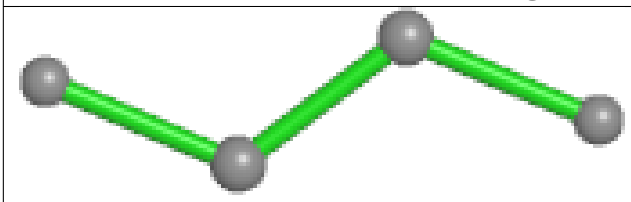


Torsions

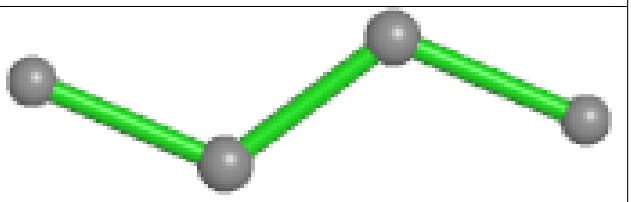


Rings

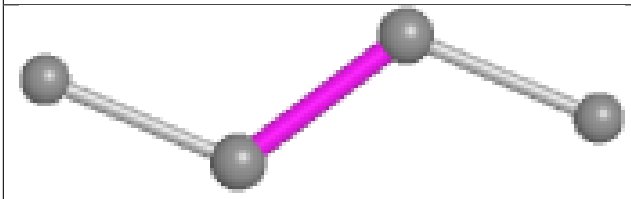
Ligand EDO E 307



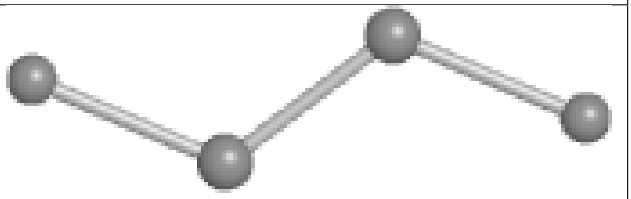
Bond lengths



Bond angles

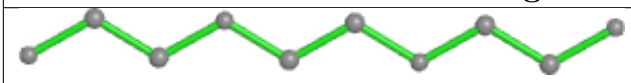


Torsions

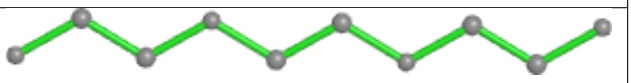


Rings

Ligand PGE C 312

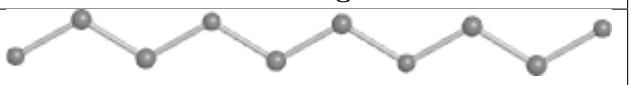


Bond lengths



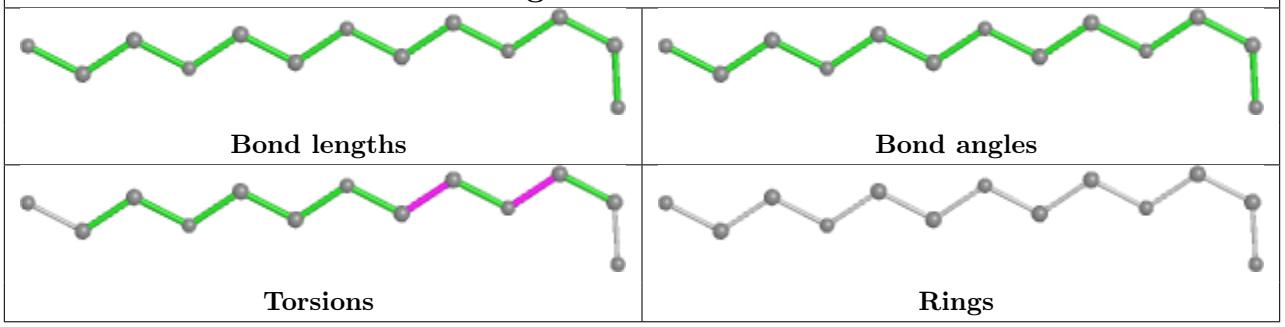
Bond angles

Torsions

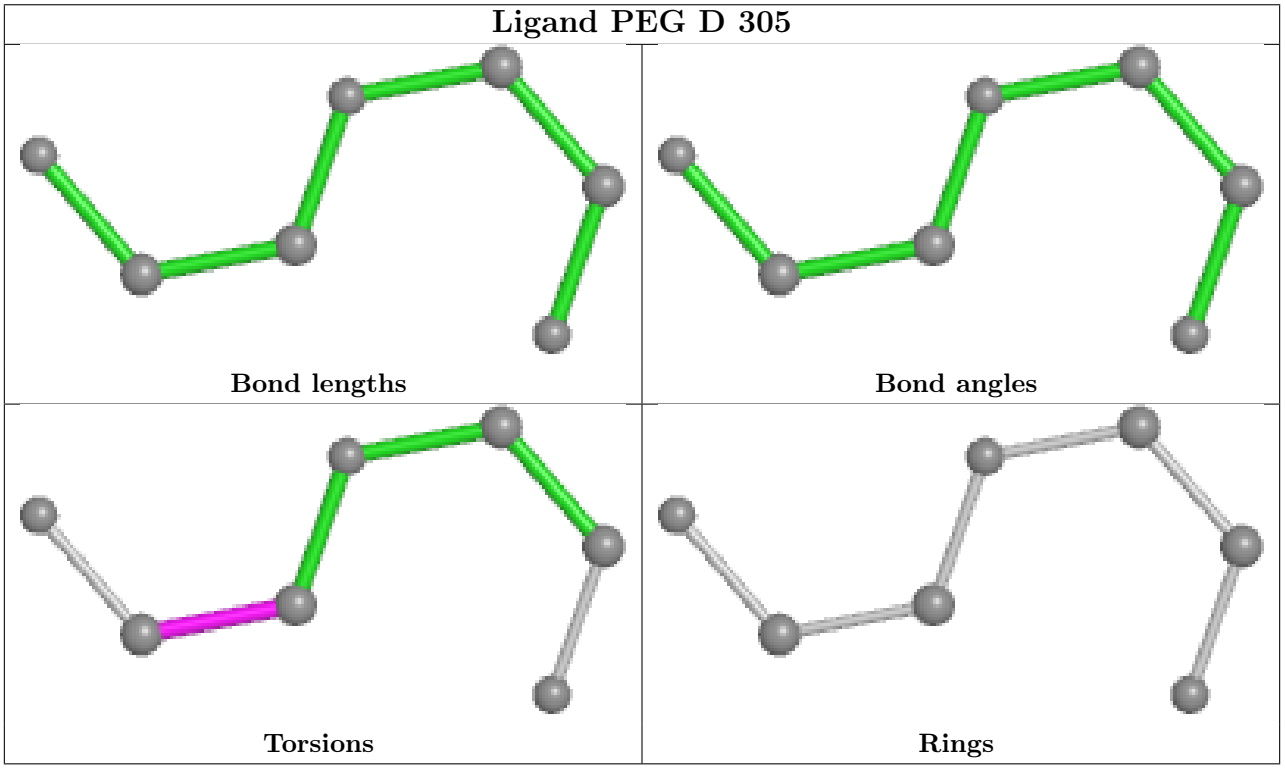


Rings

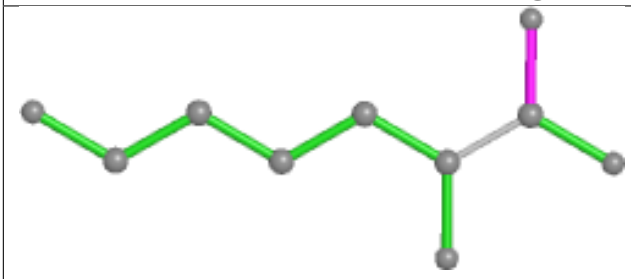
Ligand PG4 A 303



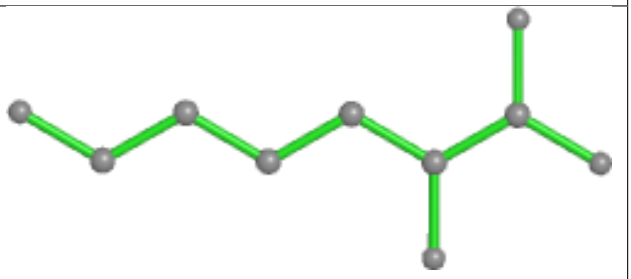
Ligand PEG D 305



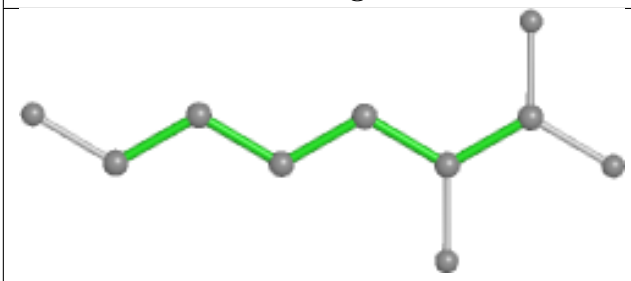
Ligand LYS B 307



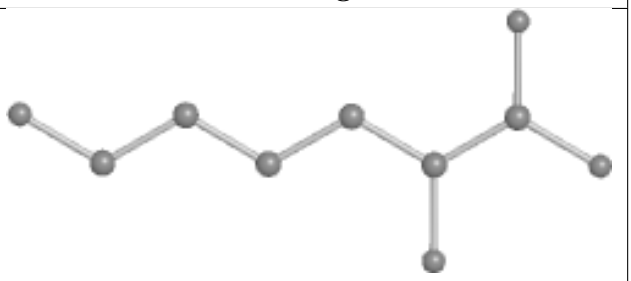
Bond lengths



Bond angles

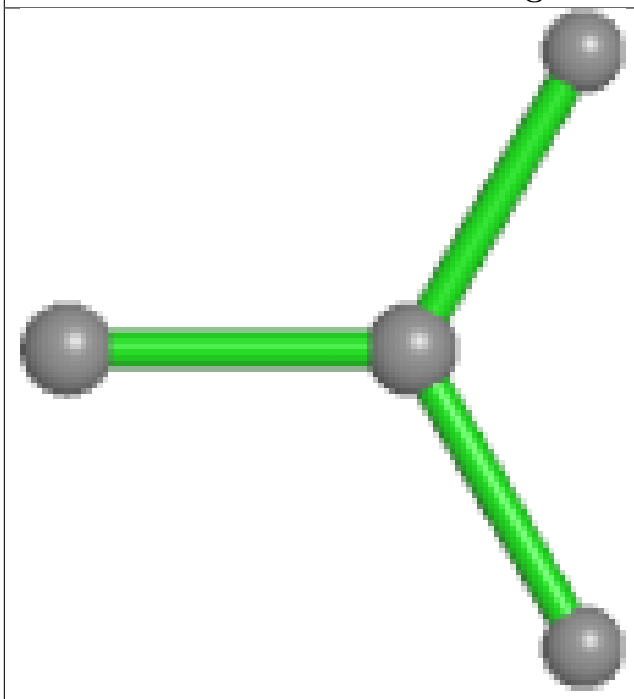


Torsions

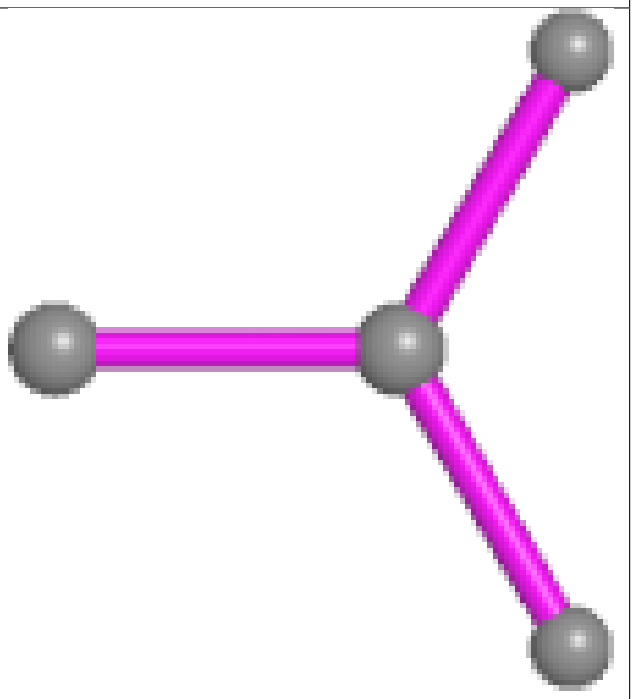


Rings

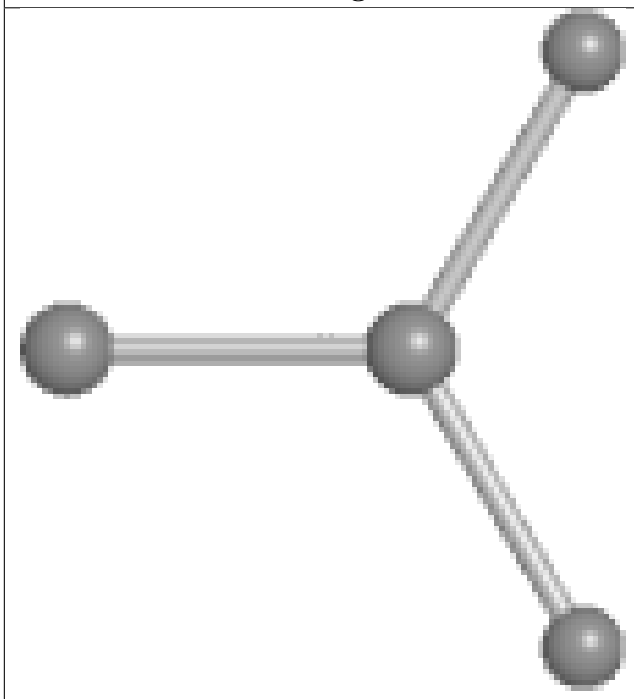
Ligand ACT F 309



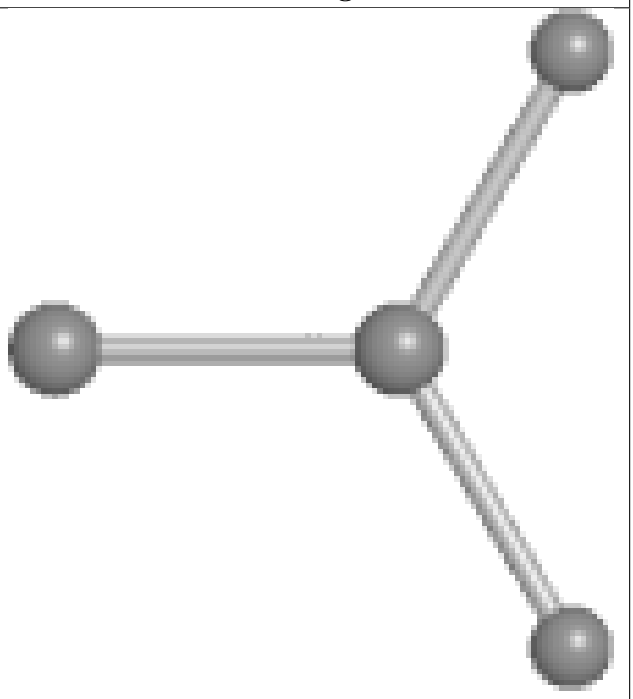
Bond lengths



Bond angles

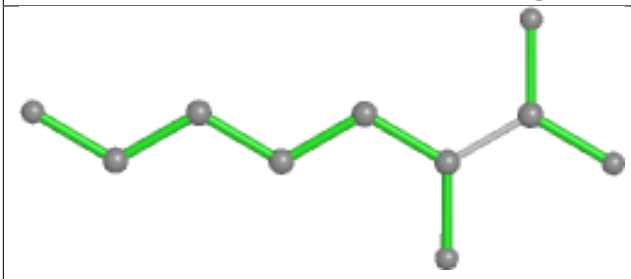


Torsions

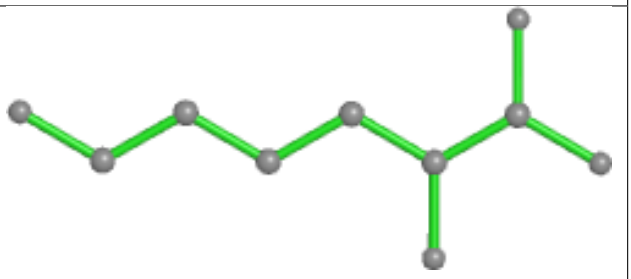


Rings

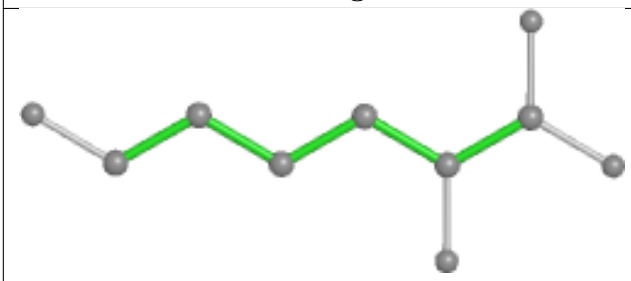
Ligand LYS F 308



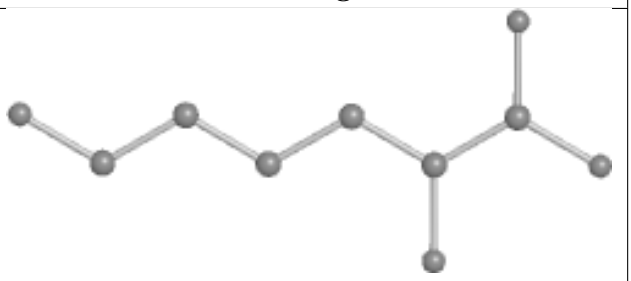
Bond lengths



Bond angles

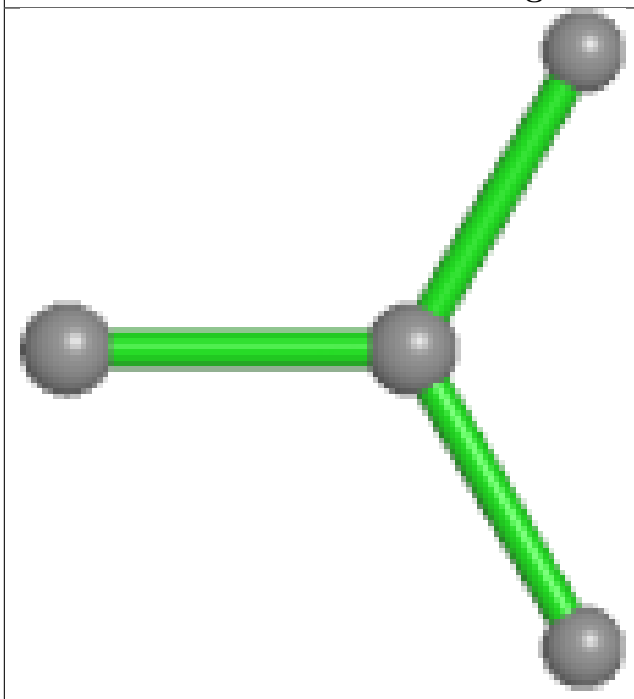


Torsions

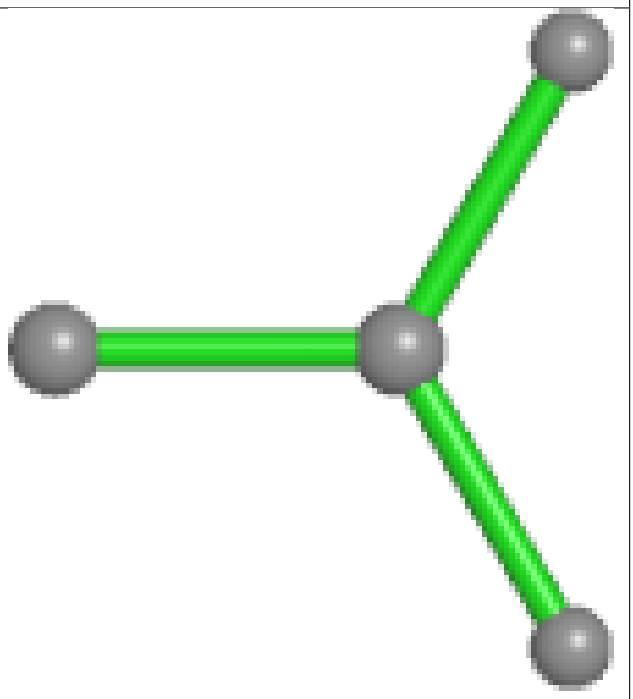


Rings

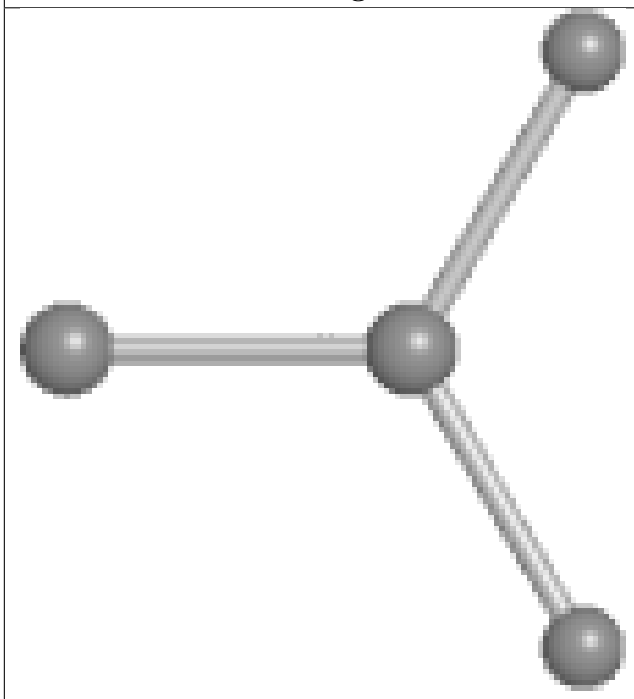
Ligand ACT F 310



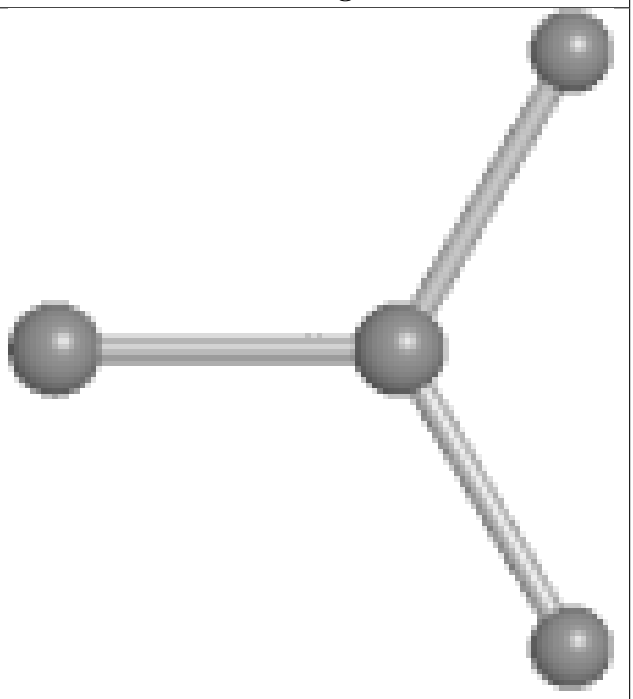
Bond lengths



Bond angles

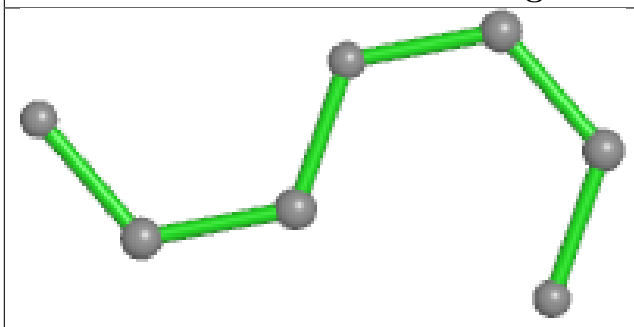


Torsions

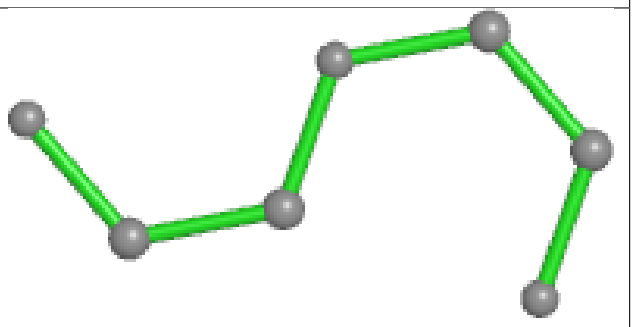


Rings

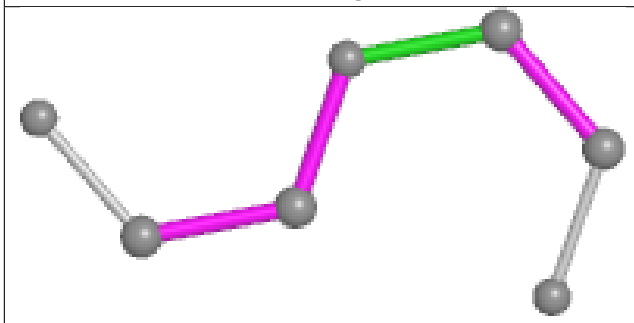
Ligand PEG E 304



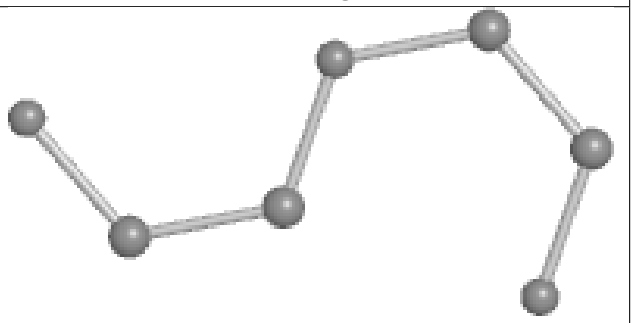
Bond lengths



Bond angles

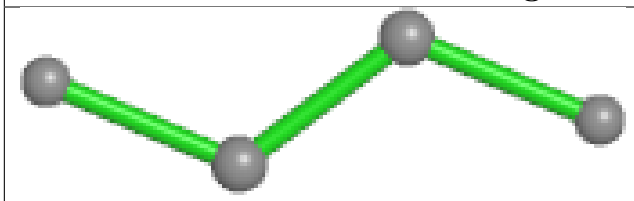


Torsions

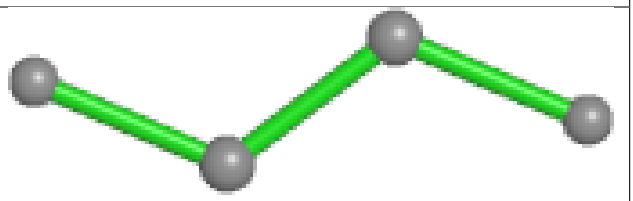


Rings

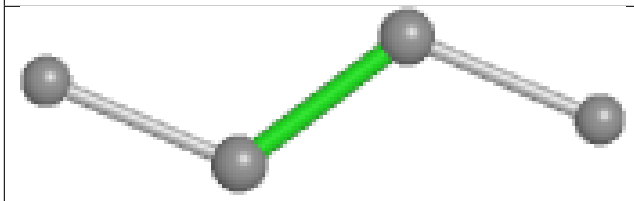
Ligand EDO A 306



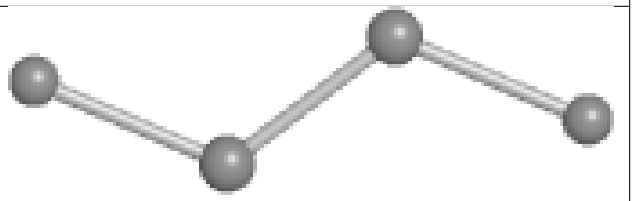
Bond lengths



Bond angles

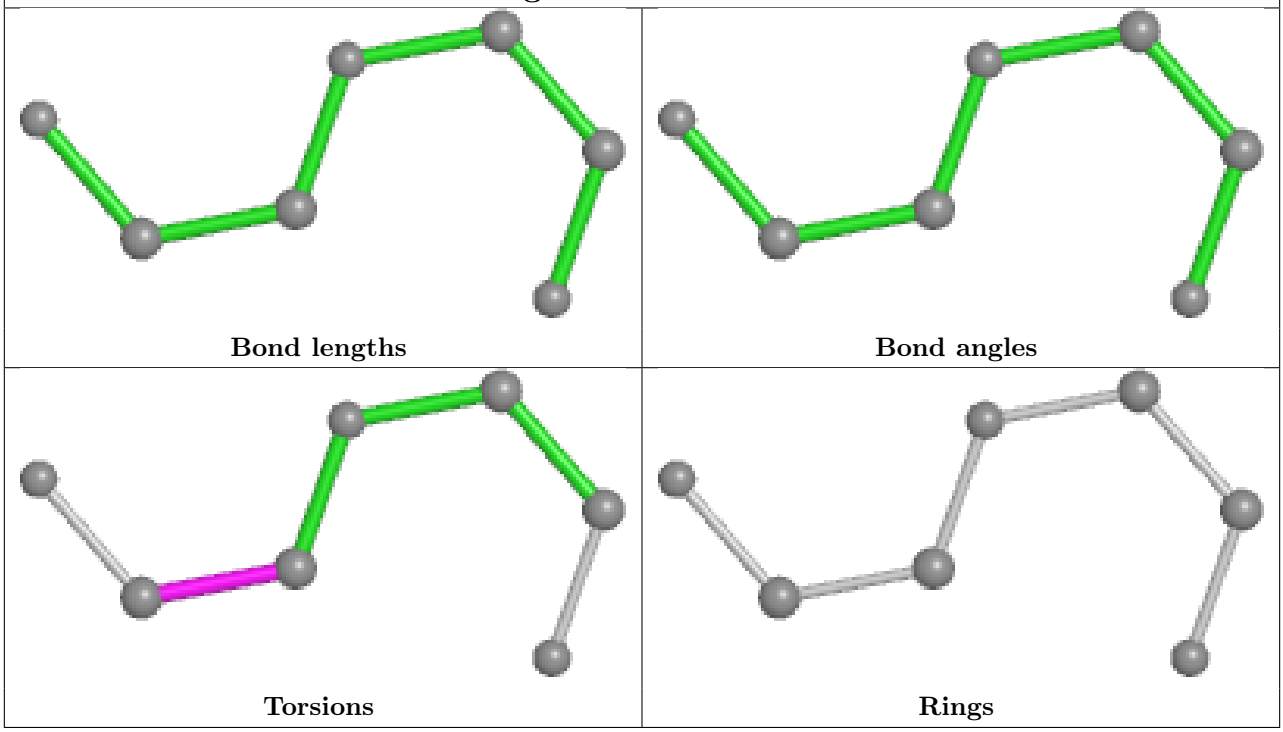


Torsions

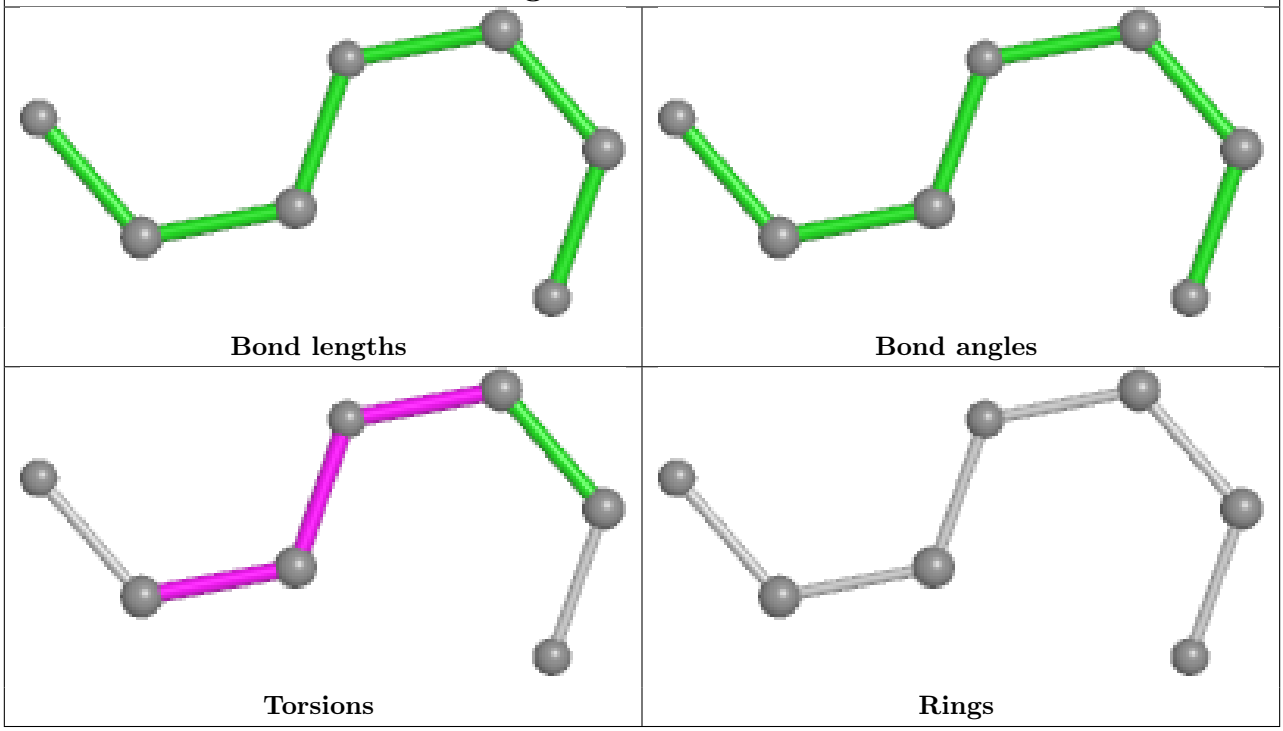


Rings

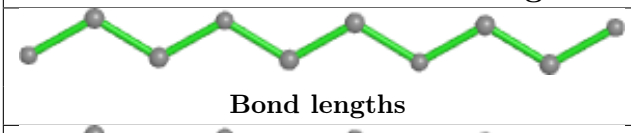
Ligand PEG A 304

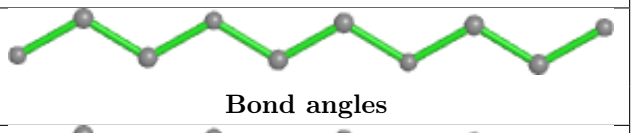


Ligand PEG C 311

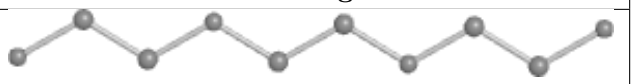


Ligand PGE F 305

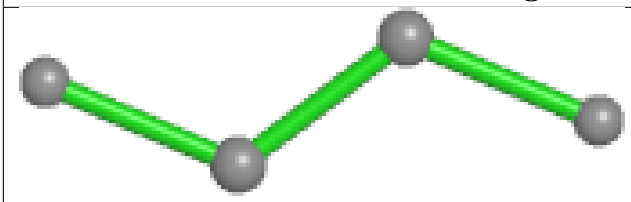

Bond lengths

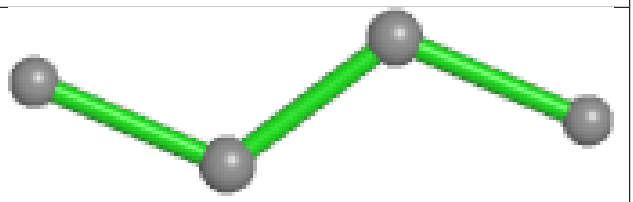

Bond angles

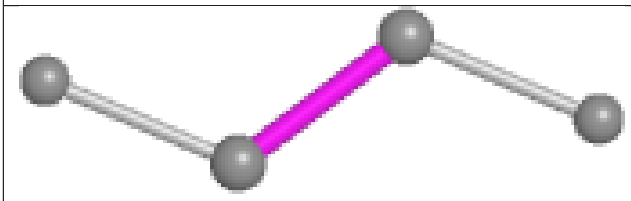

Torsions

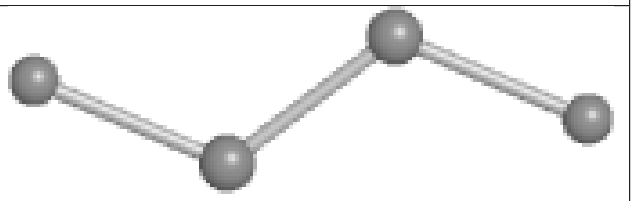

Rings

Ligand EDO C 315

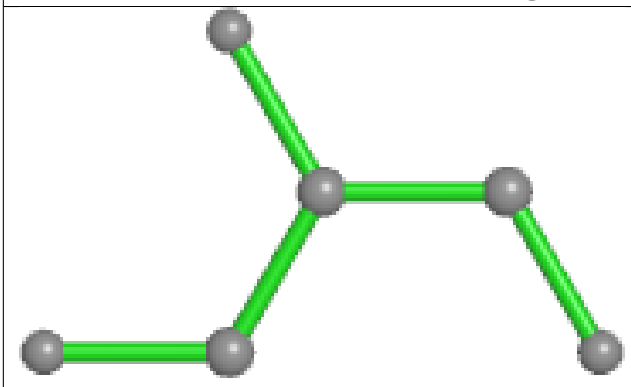

Bond lengths

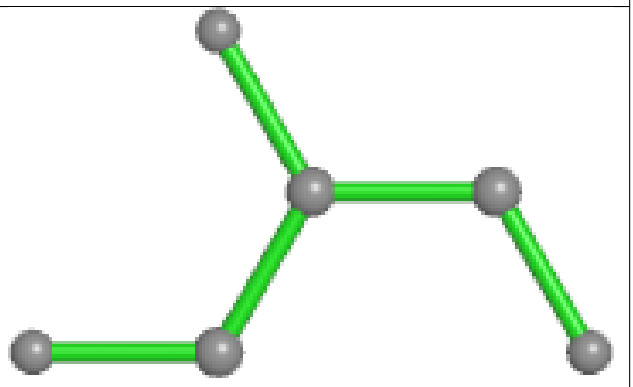

Bond angles

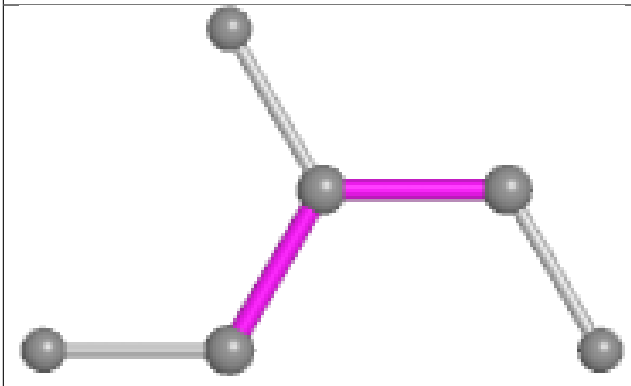

Torsions

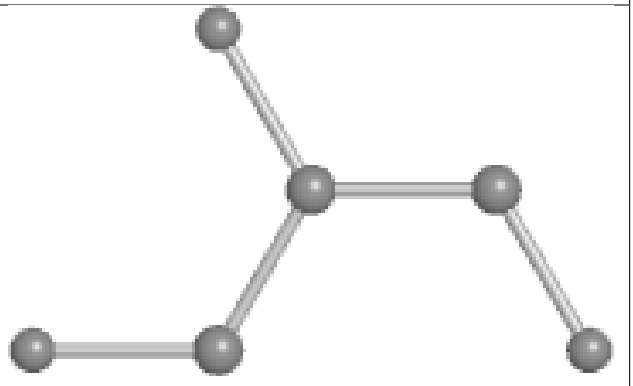

Rings

Ligand GOL B 308

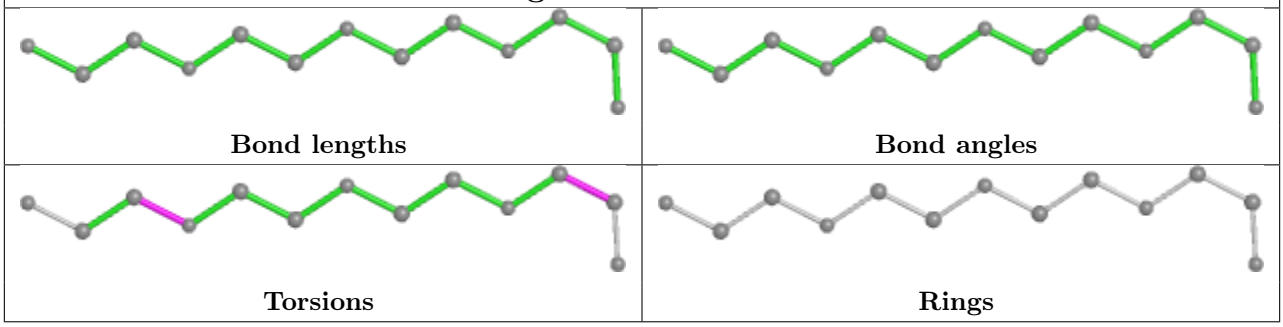

Bond lengths


Bond angles

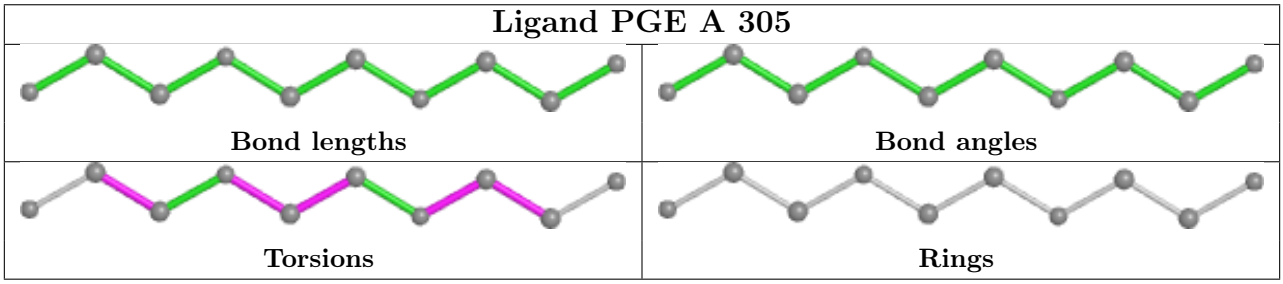

Torsions


Rings

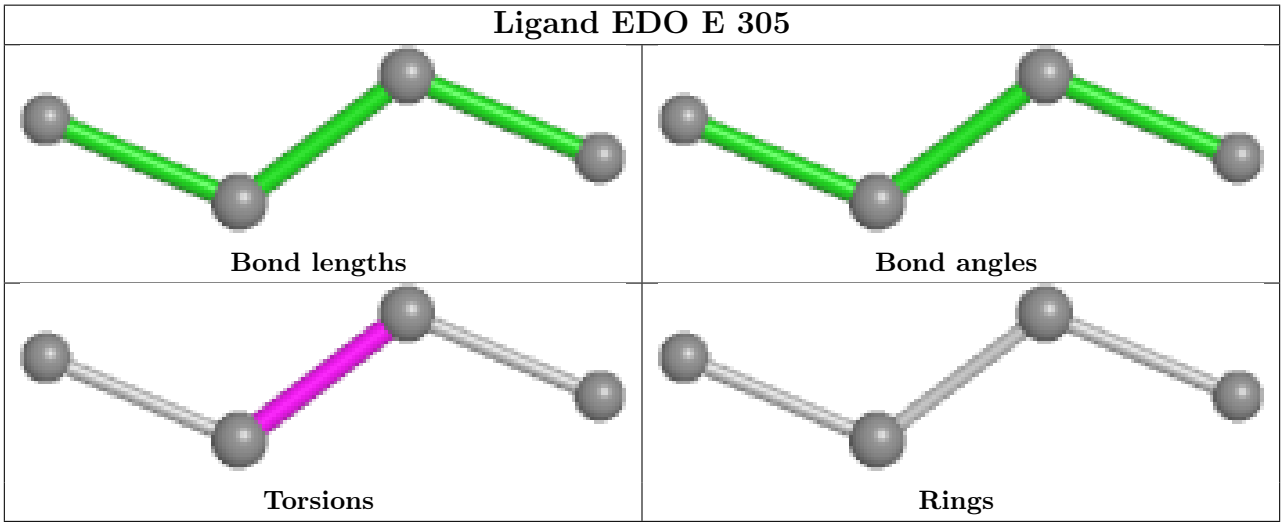
Ligand PG4 B 305



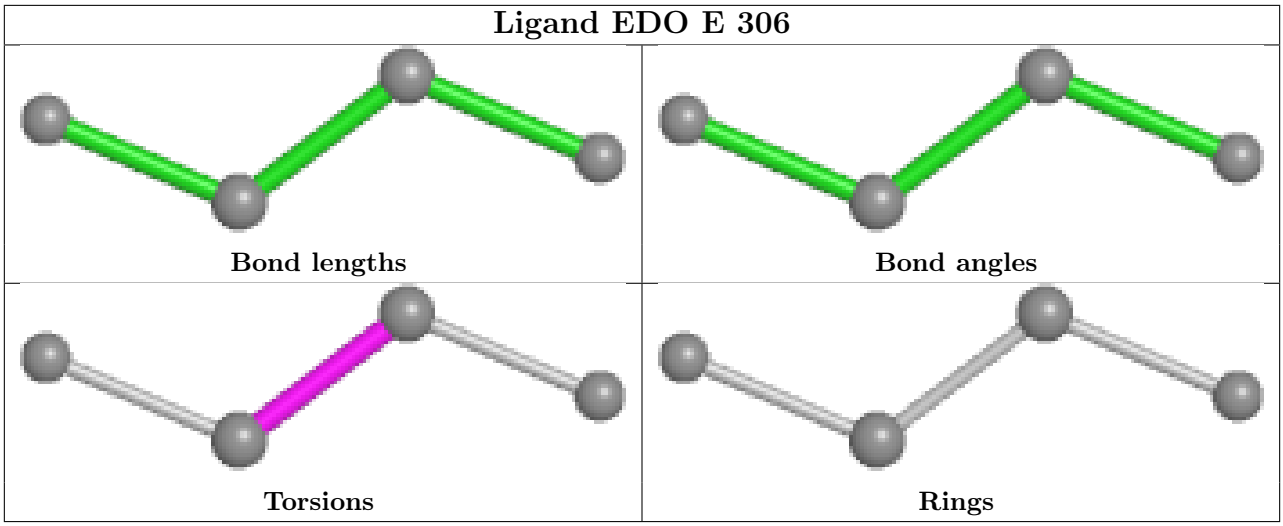
Ligand PGE A 305



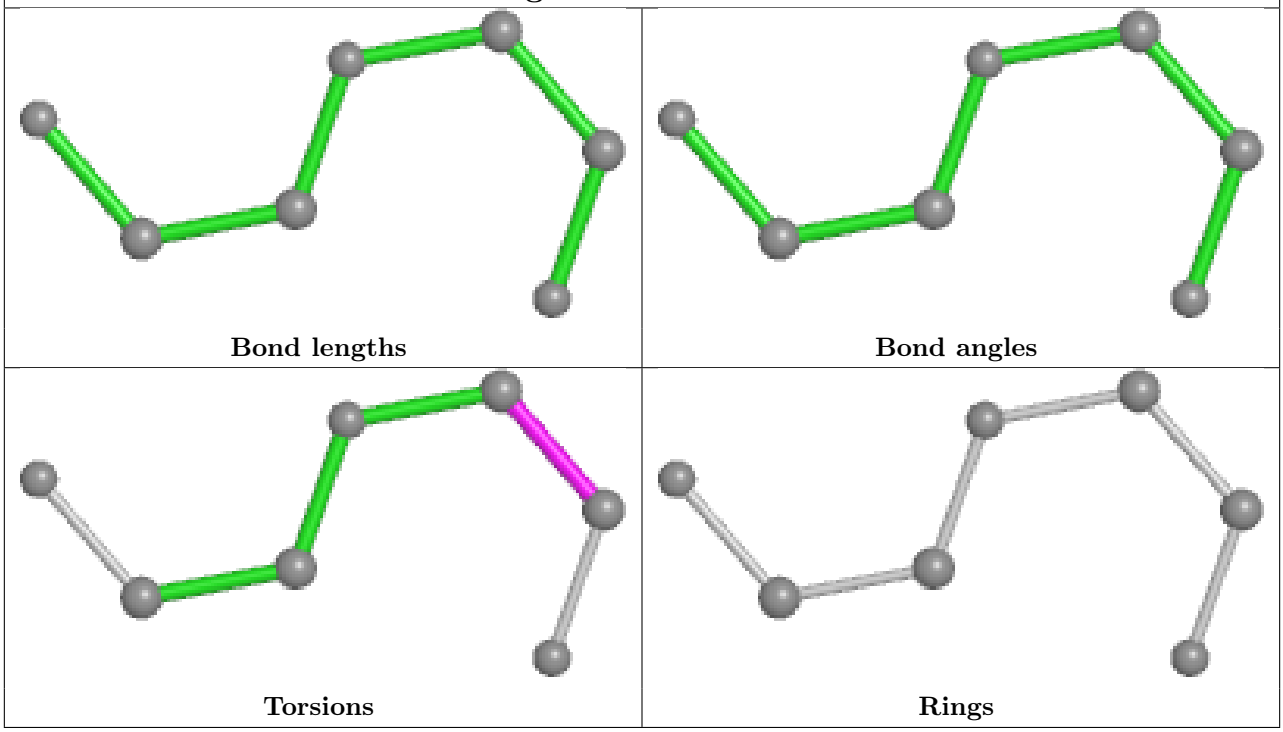
Ligand EDO E 305



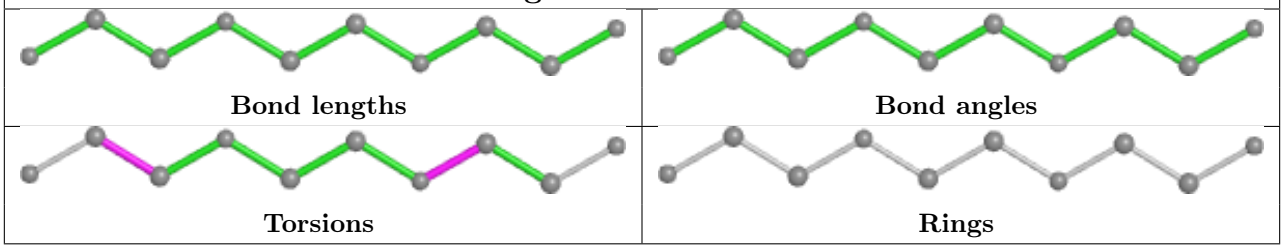
Ligand EDO E 306



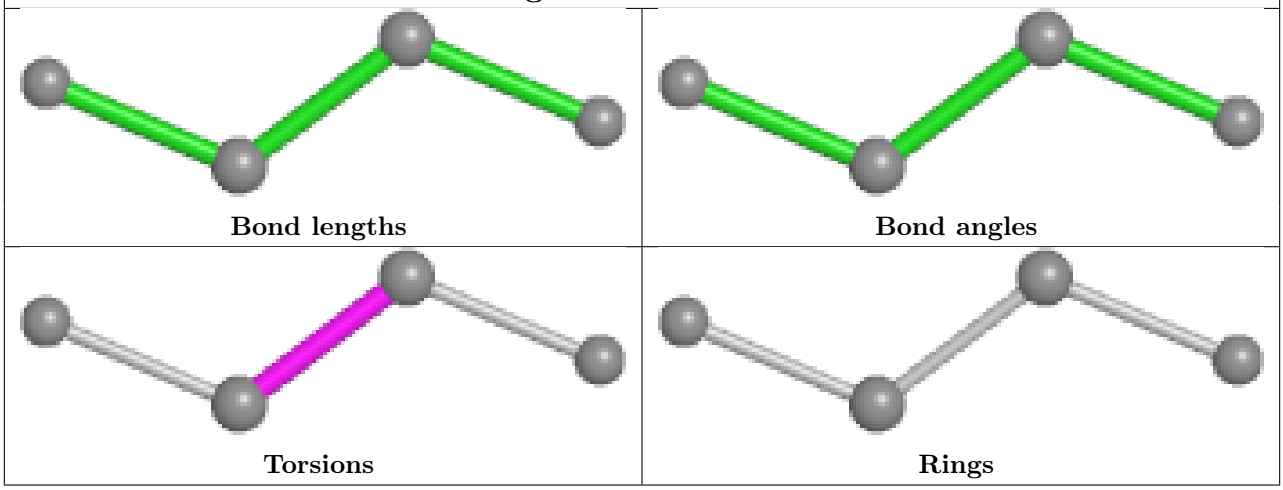
Ligand PEG E 303



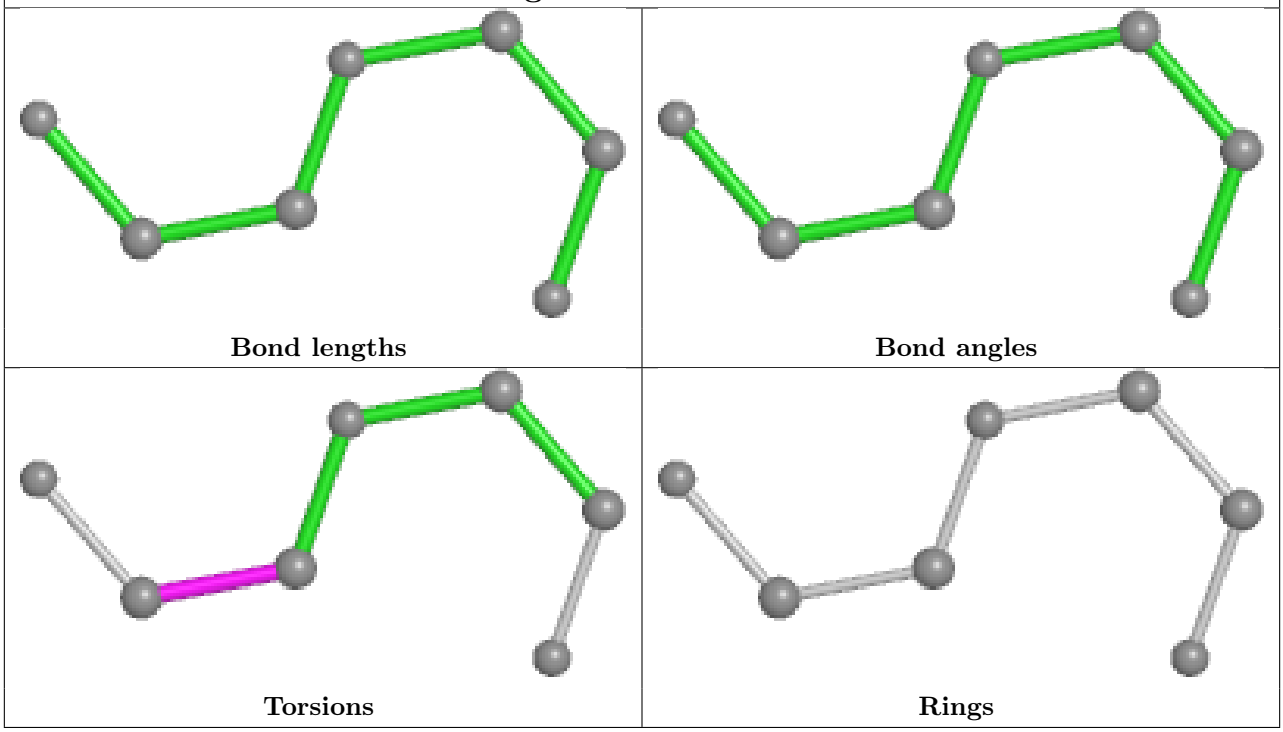
Ligand PGE C 313



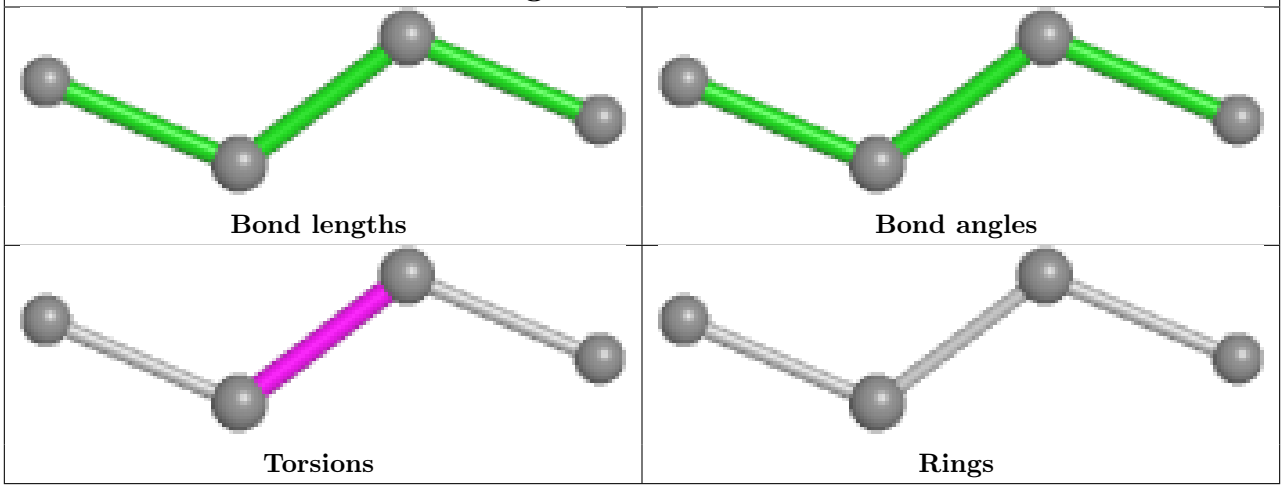
Ligand EDO F 307



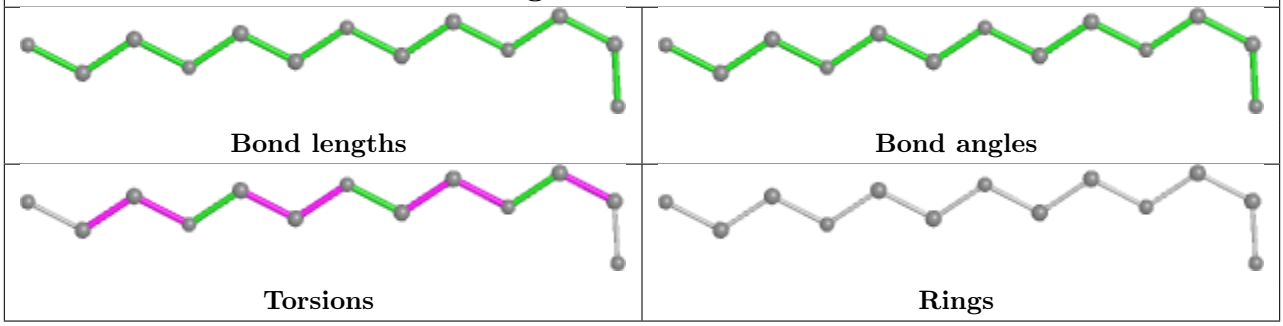
Ligand PEG B 306



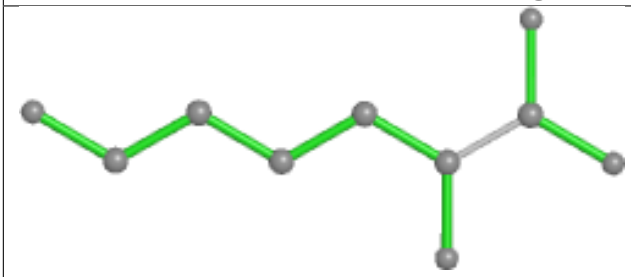
Ligand EDO F 306



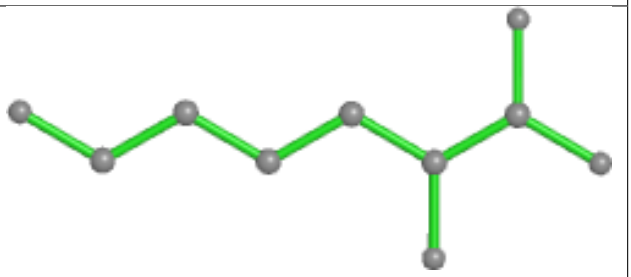
Ligand PG4 D 304



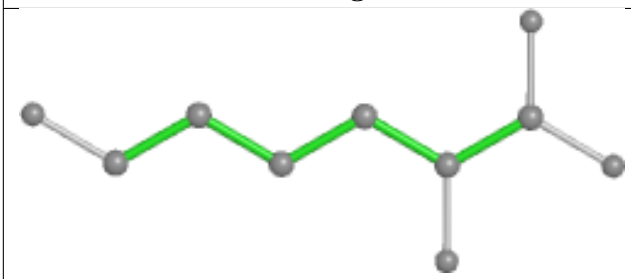
Ligand LYS E 308



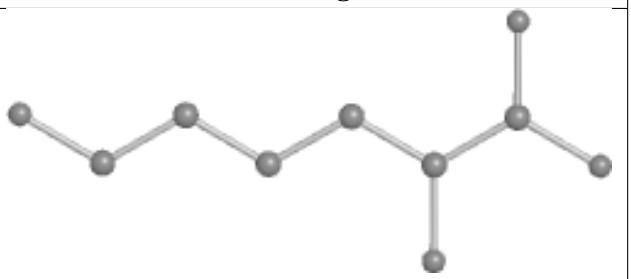
Bond lengths



Bond angles

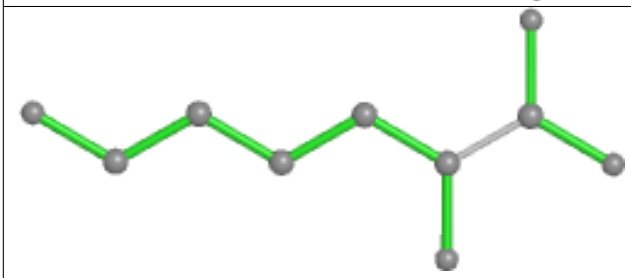


Torsions

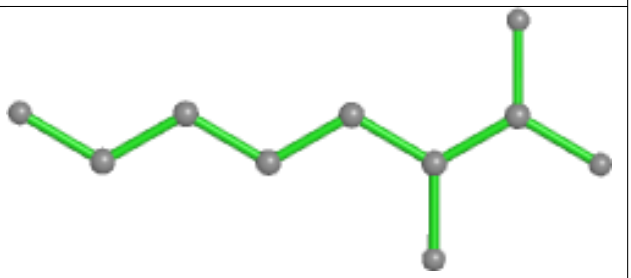


Rings

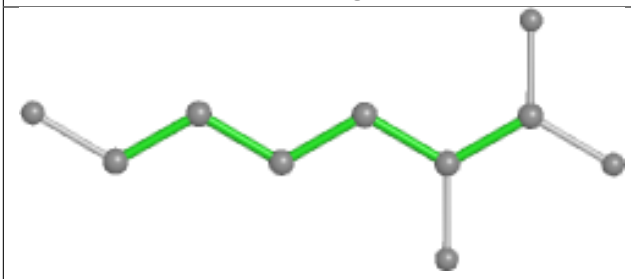
Ligand LYS A 308



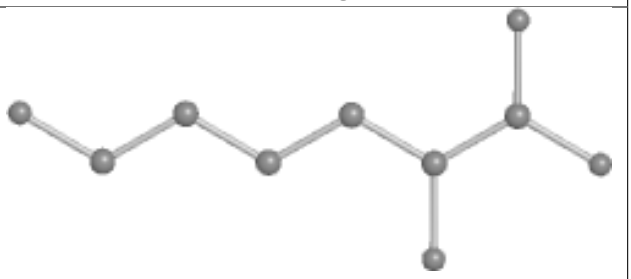
Bond lengths



Bond angles

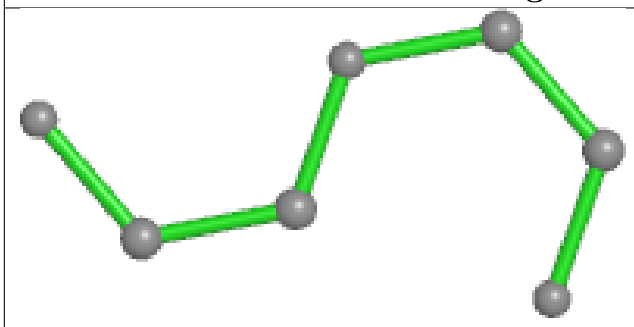


Torsions

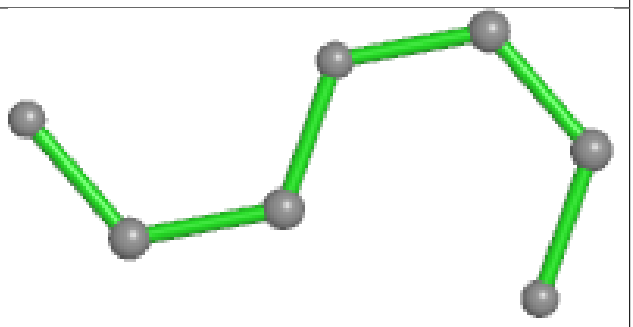


Rings

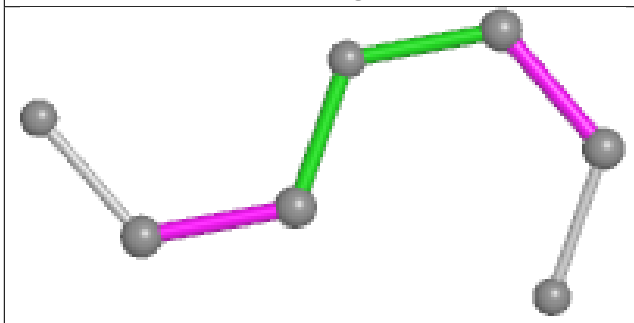
Ligand PEG F 304



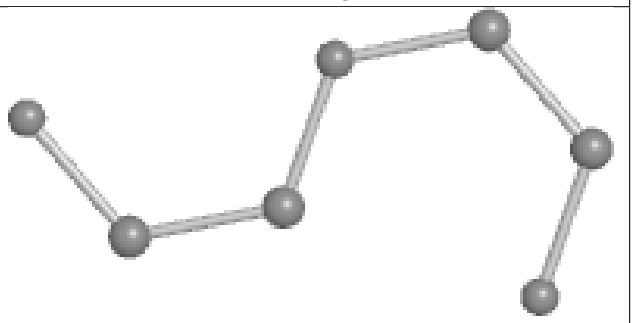
Bond lengths



Bond angles

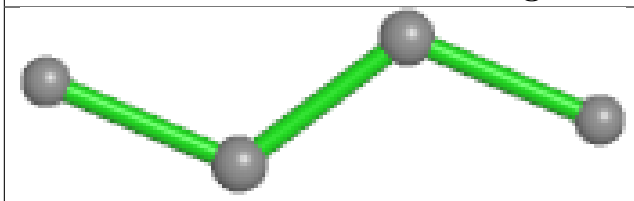


Torsions

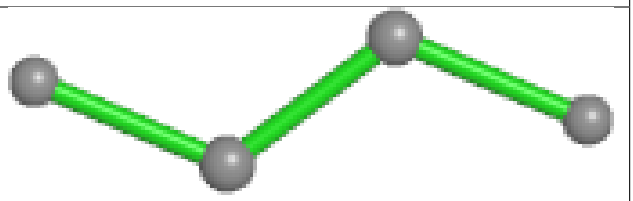


Rings

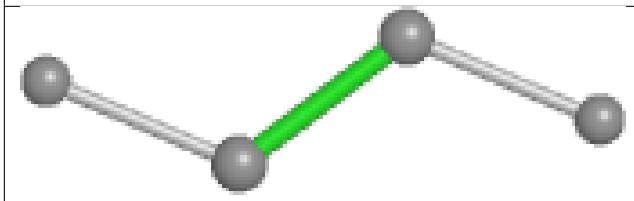
Ligand EDO A 307



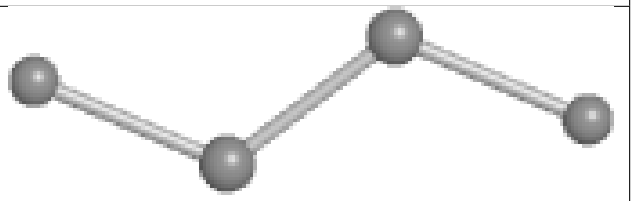
Bond lengths



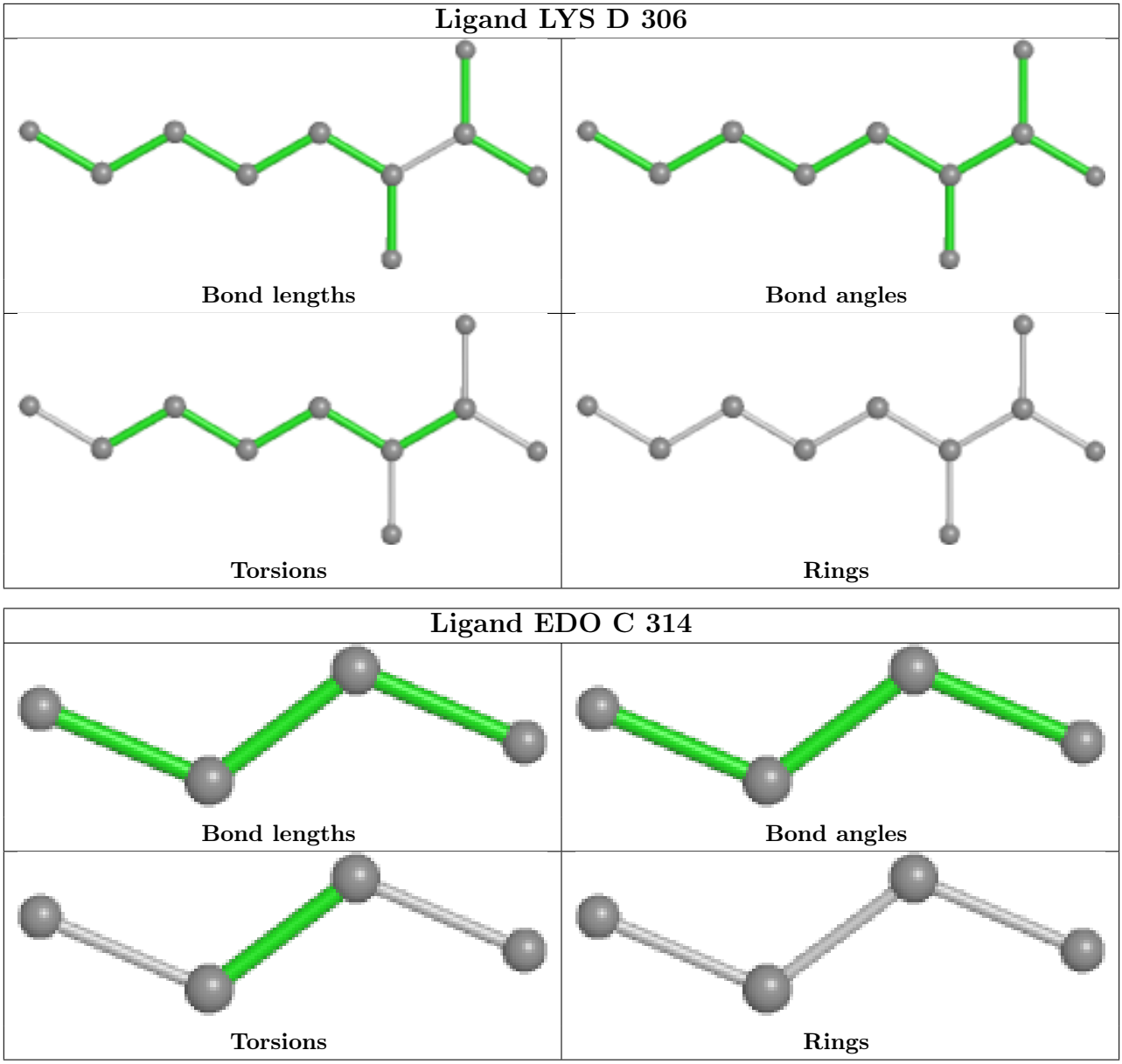
Bond angles



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, 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	296/310 (95%)	-0.71	0 100 100	7, 10, 21, 41	0
1	B	305/310 (98%)	-0.68	1 (0%) 94 94	7, 11, 24, 58	0
1	C	294/310 (94%)	-0.65	0 100 100	7, 11, 21, 35	0
1	D	305/310 (98%)	-0.66	0 100 100	8, 11, 25, 39	0
1	E	295/310 (95%)	-0.61	0 100 100	8, 12, 25, 37	0
1	F	295/310 (95%)	-0.57	0 100 100	8, 12, 26, 40	0
All	All	1790/1860 (96%)	-0.65	1 (0%) 95 94	7, 11, 24, 58	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ASP	2.6

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	KPI	B	166	14/15	0.61	0.26	20,20,20,20	0
1	KPI	D	166	14/15	0.63	0.25	20,20,20,20	0
1	KPI	C	166	14/15	0.64	0.28	20,20,20,20	0
1	KPI	F	166	14/15	0.65	0.25	20,20,20,20	0
1	KPI	E	166	14/15	0.67	0.25	20,20,20,20	0
1	KPI	A	166	14/15	0.68	0.25	20,20,20,20	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
6	PGE	A	305	10/10	0.77	0.20	35,45,49,53	0
7	EDO	F	307	4/4	0.78	0.59	20,20,20,20	0
5	PEG	E	303	7/7	0.82	0.18	26,36,49,50	0
5	PEG	B	306	7/7	0.83	0.16	27,38,45,47	0
2	MG	C	307	1/1	0.84	0.11	40,40,40,40	0
5	PEG	A	304	7/7	0.84	0.12	26,41,44,46	0
6	PGE	C	313	10/10	0.84	0.17	31,34,47,59	0
2	MG	B	303	1/1	0.84	0.14	41,41,41,41	0
2	MG	C	304	1/1	0.85	0.12	39,39,39,39	0
7	EDO	C	314	4/4	0.86	0.18	26,27,30,48	0
7	EDO	E	306	4/4	0.86	0.23	32,34,36,46	0
5	PEG	F	304	7/7	0.86	0.13	29,38,52,54	0
7	EDO	A	307	4/4	0.88	0.35	36,42,42,47	0
2	MG	C	306	1/1	0.88	0.19	35,35,35,35	0
7	EDO	C	315	4/4	0.89	0.21	28,29,37,44	0
2	MG	C	303	1/1	0.89	0.18	43,43,43,43	0
5	PEG	C	311	7/7	0.89	0.11	28,37,44,46	0
7	EDO	E	307	4/4	0.90	0.36	33,36,37,41	0
2	MG	D	303	1/1	0.90	0.16	35,35,35,35	0
7	EDO	F	306	4/4	0.91	0.25	43,44,45,49	0
7	EDO	E	305	4/4	0.91	0.36	19,36,38,40	0
9	GOL	B	308	6/6	0.91	0.18	39,40,47,50	0
6	PGE	F	305	10/10	0.92	0.15	23,32,44,52	0
2	MG	C	302	1/1	0.92	0.13	36,36,36,36	0
10	ACT	F	310	4/4	0.92	0.15	21,25,31,36	0
5	PEG	D	305	7/7	0.93	0.12	25,41,54,64	0
5	PEG	E	304	7/7	0.93	0.09	25,33,36,44	0
4	PG4	D	304	13/13	0.94	0.09	15,29,42,42	0
7	EDO	A	306	4/4	0.94	0.09	14,14,14,15	0
6	PGE	C	312	10/10	0.94	0.13	22,27,36,43	0
10	ACT	F	309	4/4	0.94	0.21	25,26,33,56	0
4	PG4	A	303	13/13	0.94	0.12	21,28,47,51	0

Continued on next page...

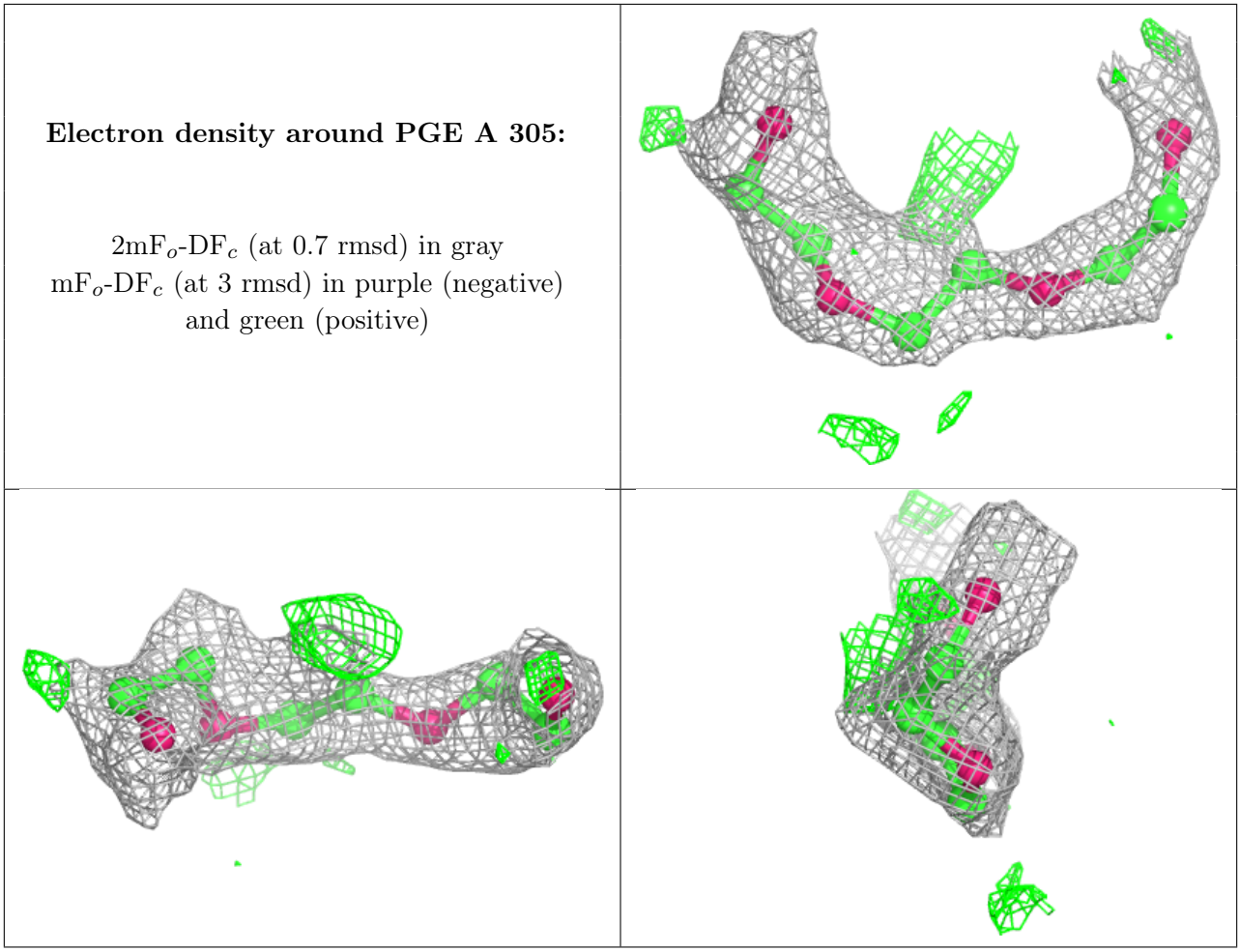
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	E	302	1/1	0.95	0.21	41,41,41,41	0
4	PG4	B	305	13/13	0.95	0.12	22,25,40,43	0
8	LYS	B	307	10/10	0.96	0.07	6,9,11,12	0
2	MG	C	308	1/1	0.96	0.25	38,38,38,38	0
8	LYS	C	316	10/10	0.97	0.08	8,9,10,10	0
3	NA	A	302	1/1	0.97	0.10	29,29,29,29	0
8	LYS	A	308	10/10	0.97	0.07	7,9,9,10	0
3	NA	C	309	1/1	0.97	0.05	25,25,25,25	0
8	LYS	E	308	10/10	0.98	0.07	7,9,11,12	0
8	LYS	F	308	10/10	0.98	0.08	7,9,10,10	0
2	MG	B	302	1/1	0.98	0.07	10,10,10,10	0
3	NA	C	310	1/1	0.98	0.08	26,26,26,26	0
8	LYS	D	306	10/10	0.98	0.06	7,8,10,13	0
2	MG	C	301	1/1	0.99	0.09	11,11,11,11	0
2	MG	D	301	1/1	0.99	0.08	17,17,17,17	0
2	MG	D	302	1/1	0.99	0.10	9,9,9,9	0
2	MG	B	301	1/1	0.99	0.12	9,9,9,9	0
2	MG	B	304	1/1	0.99	0.27	22,22,22,22	0
2	MG	F	302	1/1	0.99	0.19	17,17,17,17	0
2	MG	F	303	1/1	0.99	0.03	22,22,22,22	0
2	MG	E	301	1/1	1.00	0.15	9,9,9,9	0
2	MG	A	301	1/1	1.00	0.14	8,8,8,8	0
2	MG	F	301	1/1	1.00	0.16	10,10,10,10	0
2	MG	C	305	1/1	1.00	0.11	9,9,9,9	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.

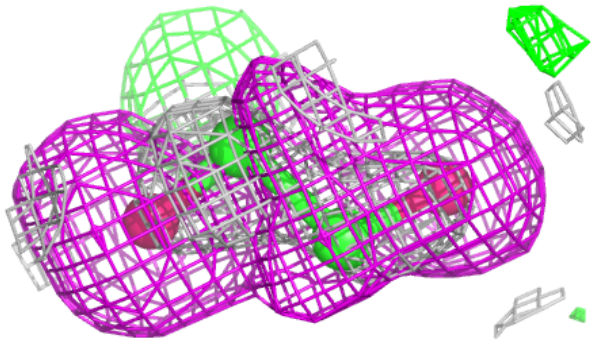
Electron density around PGE A 305:

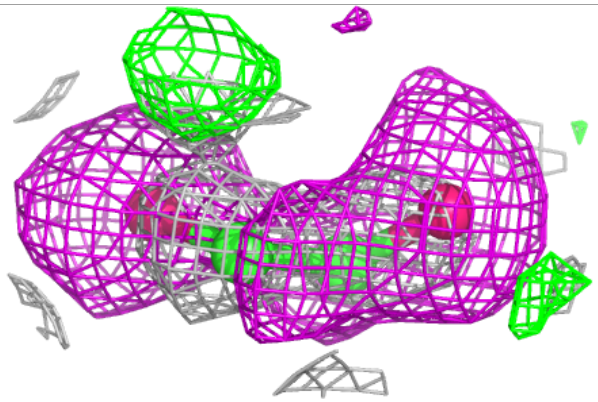
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

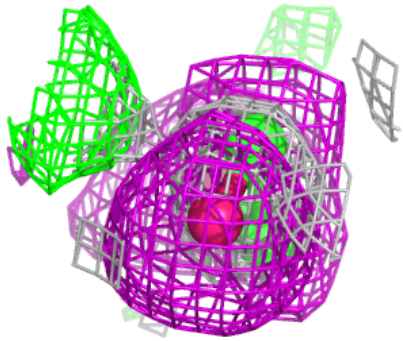


Electron density around EDO F 307:

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

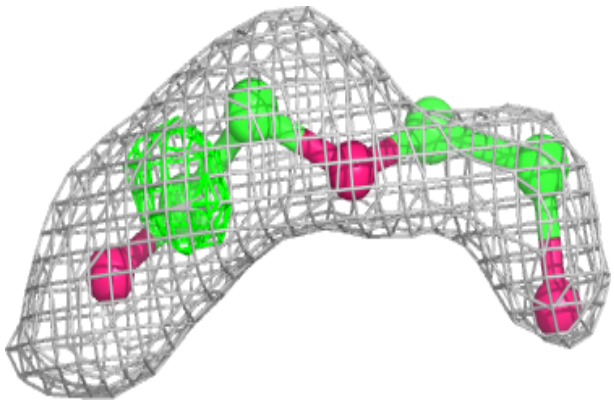


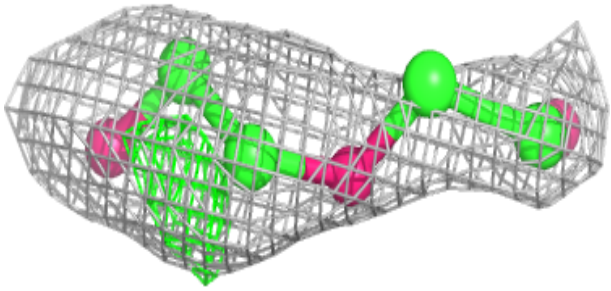


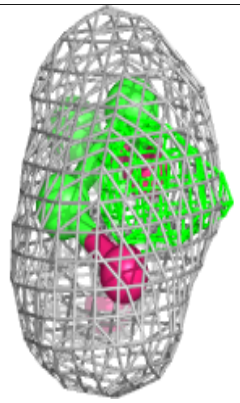


Electron density around PEG E 303:

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

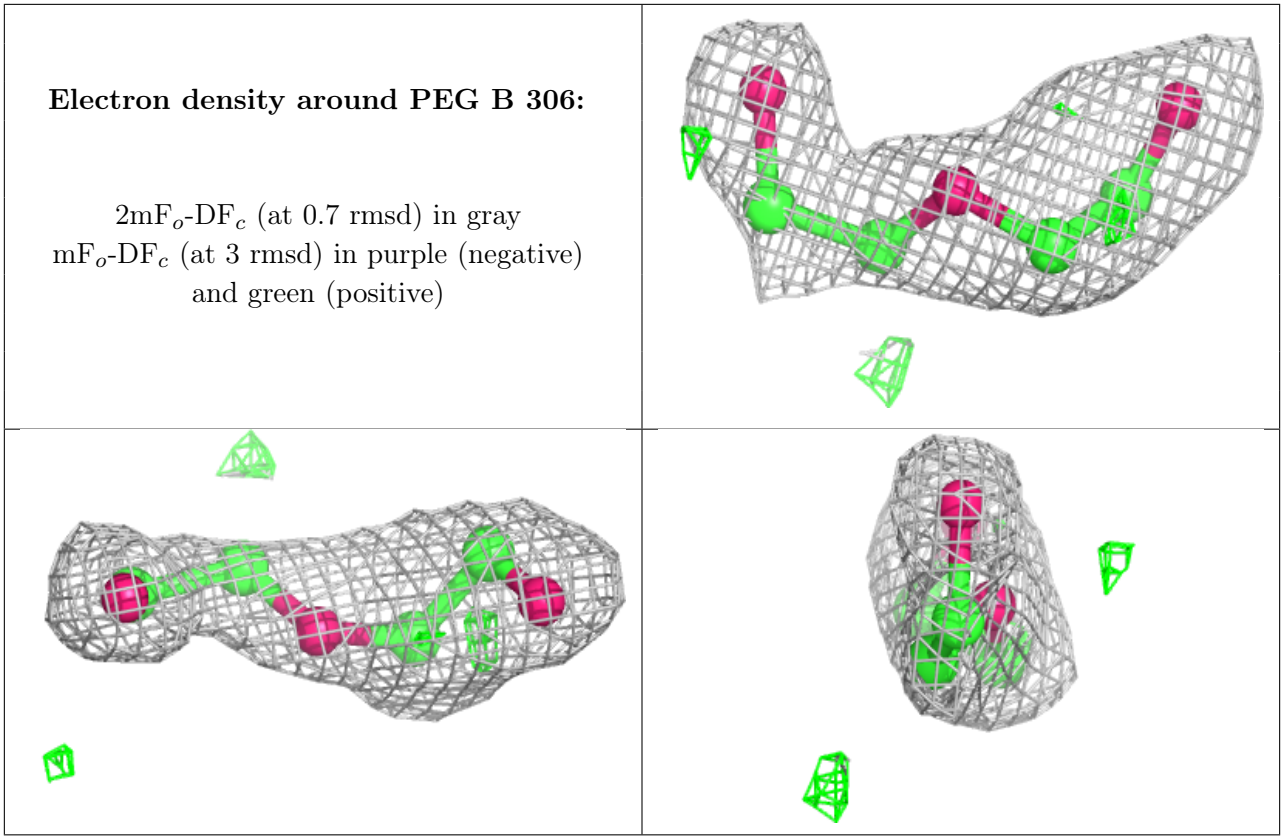






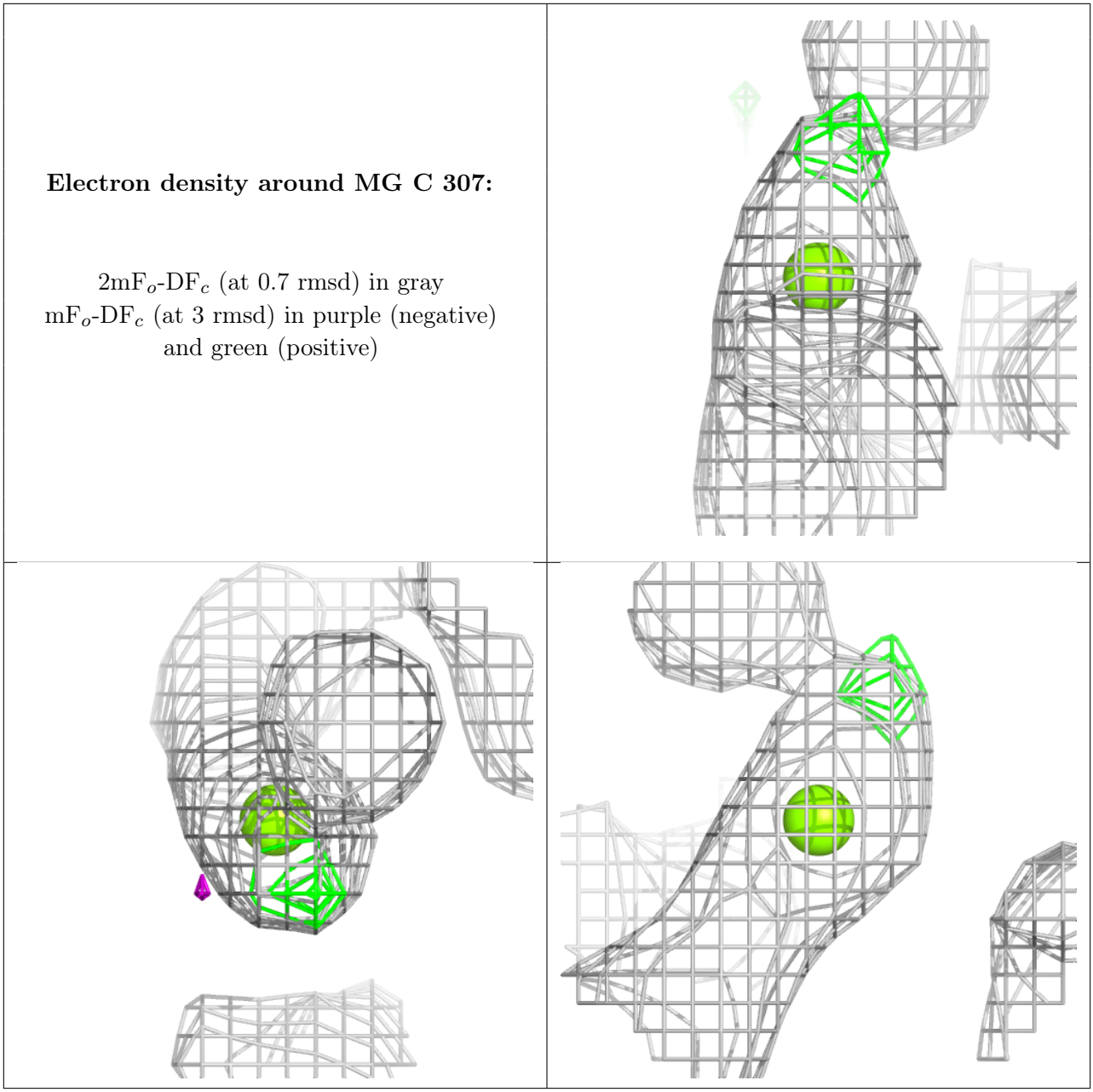
Electron density around PEG B 306:

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



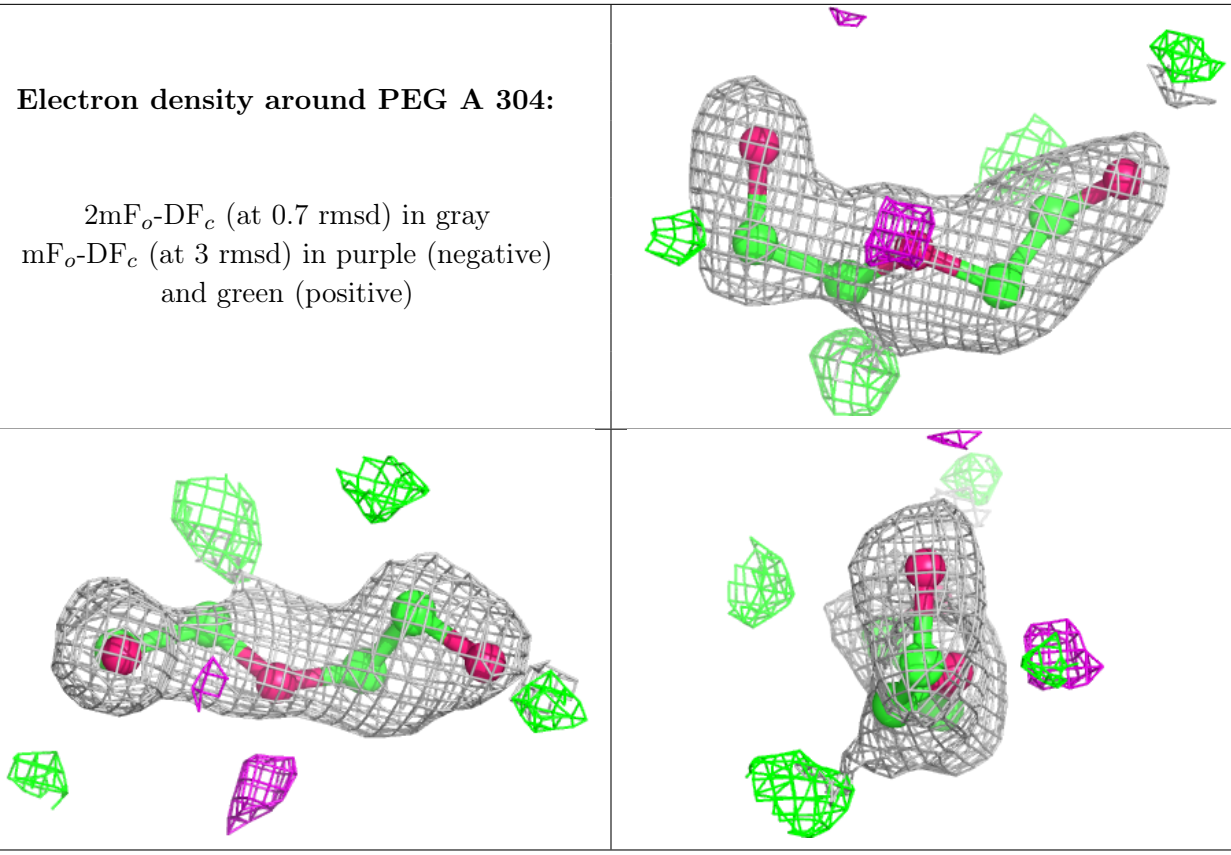
Electron density around MG C 307:

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



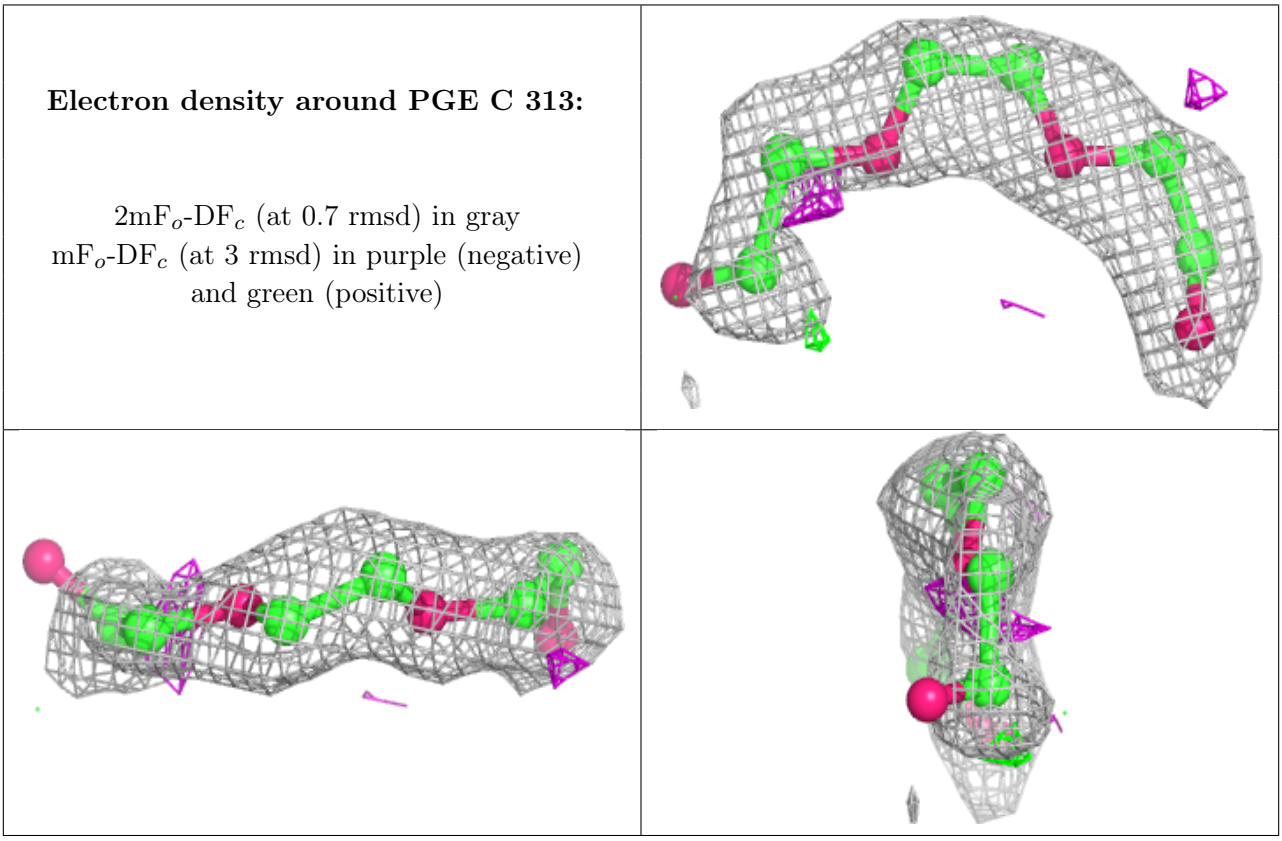
Electron density around PEG A 304:

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



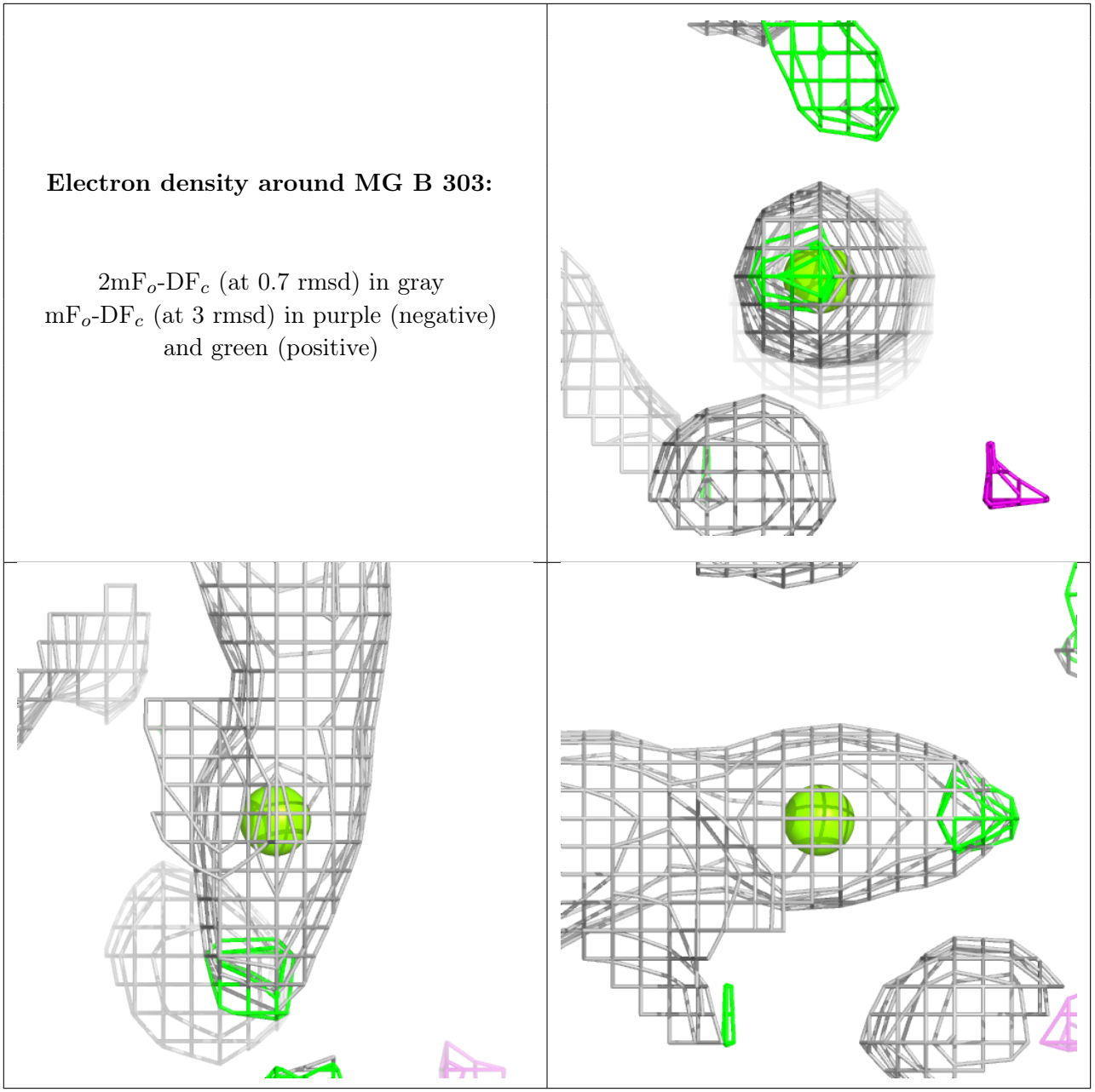
Electron density around PGE C 313:

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



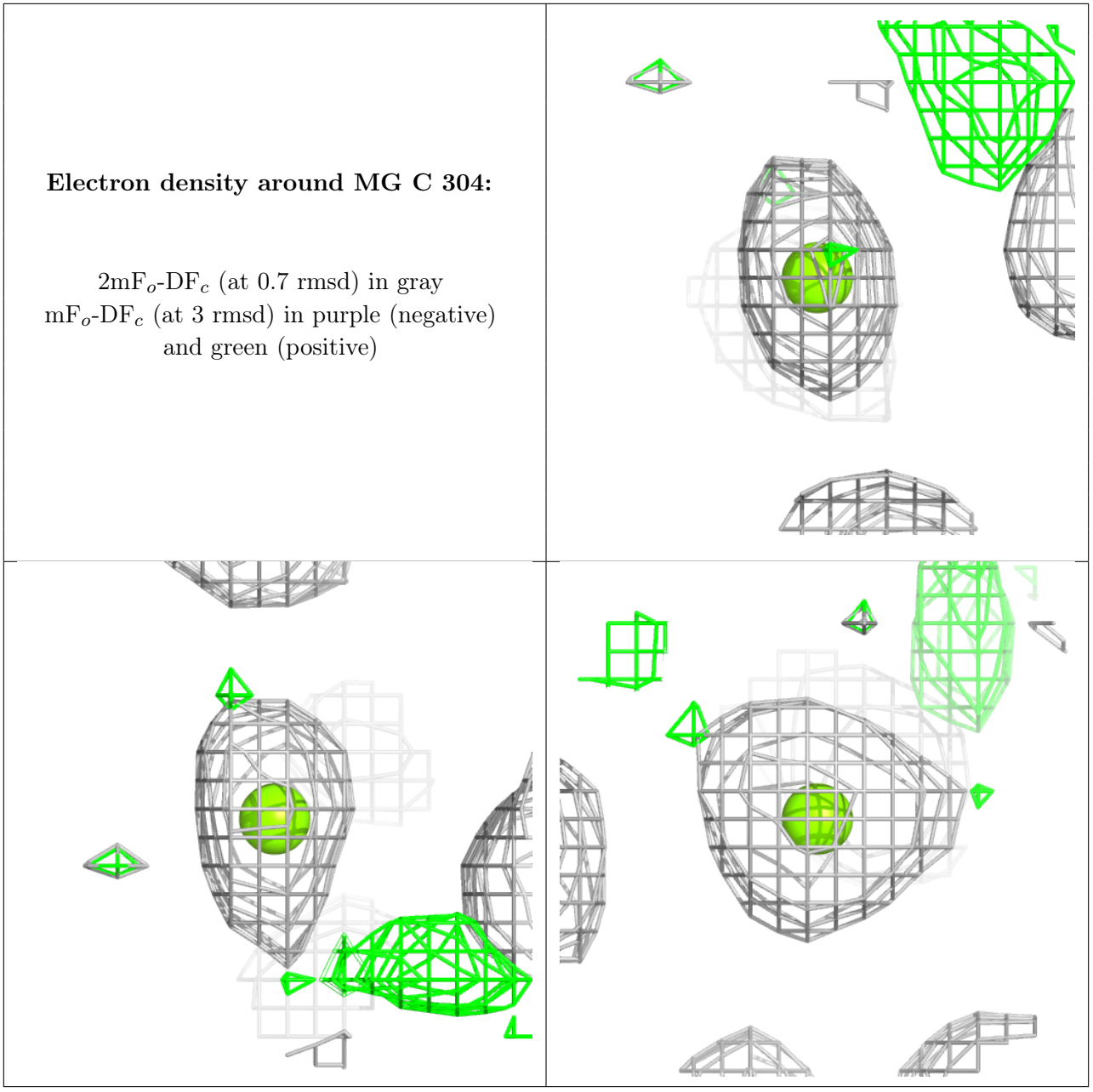
Electron density around MG B 303:

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



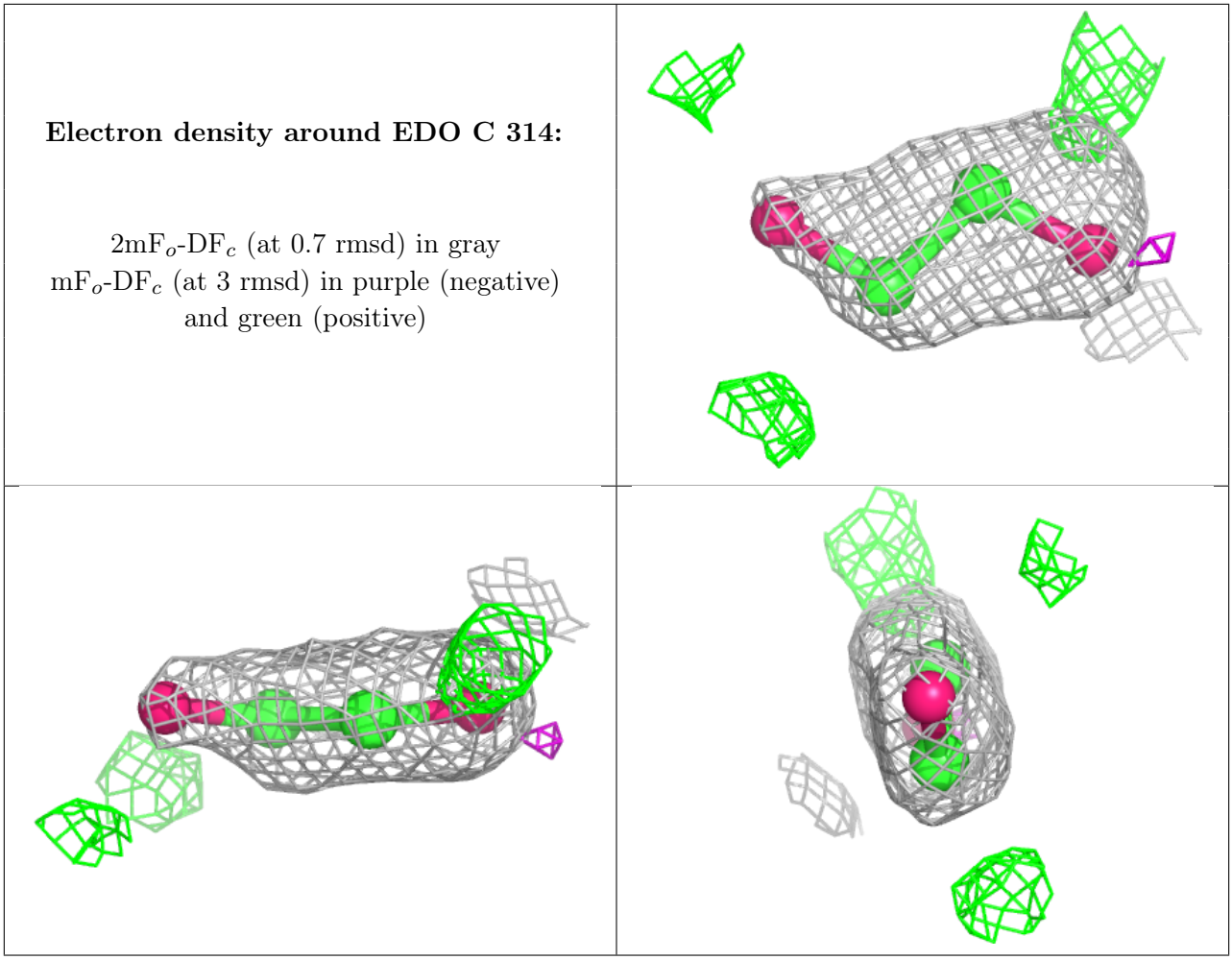
Electron density around MG C 304:

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



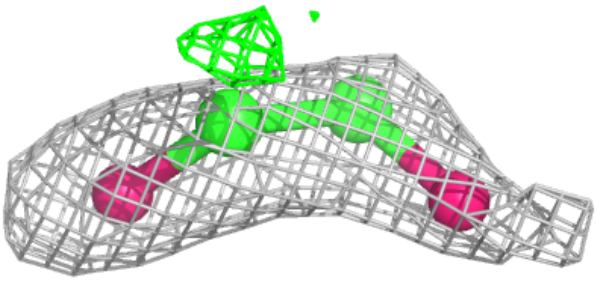
Electron density around EDO C 314:

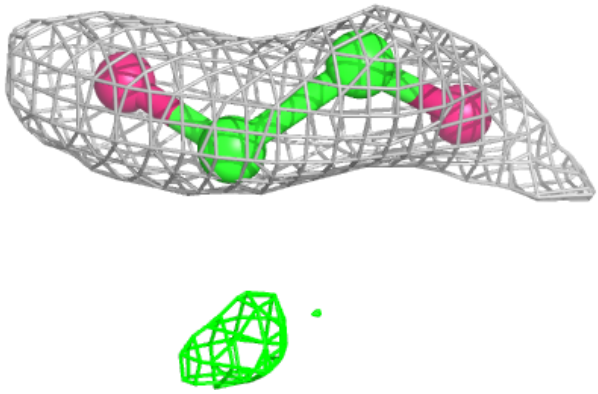
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

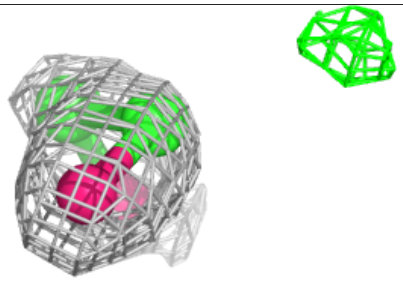


Electron density around EDO E 306:

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

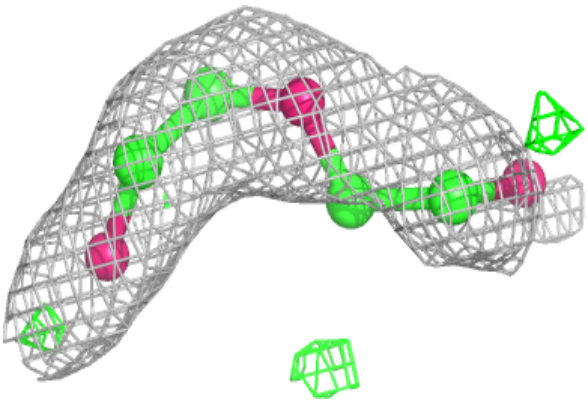


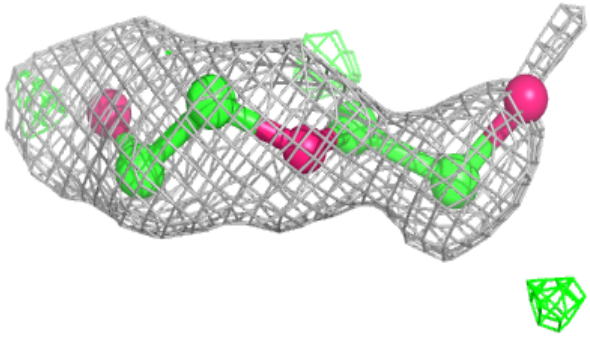


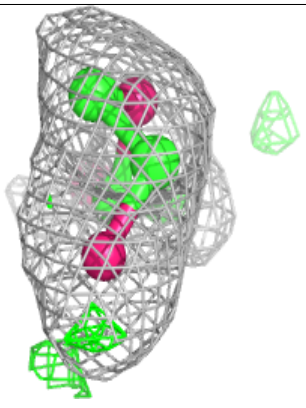


Electron density around PEG F 304:

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

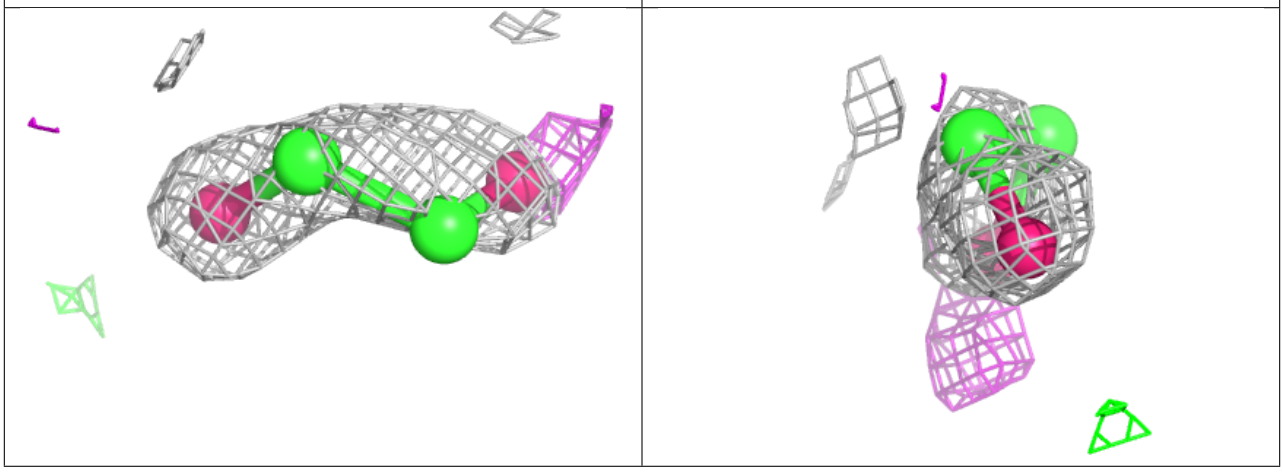






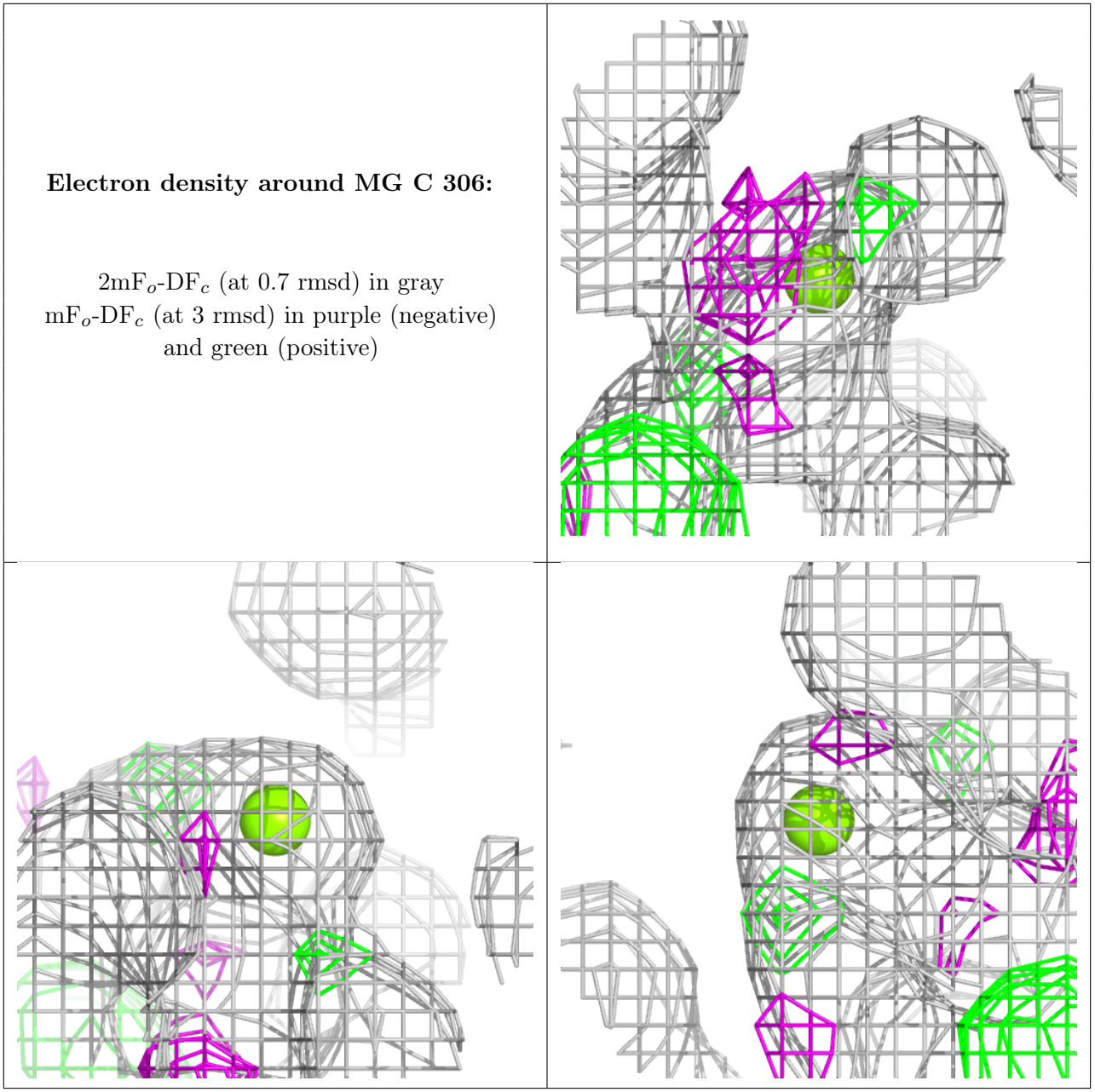
Electron density around EDO A 307:

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



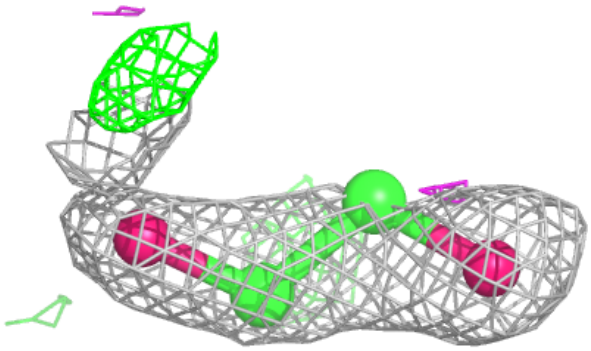
Electron density around MG C 306:

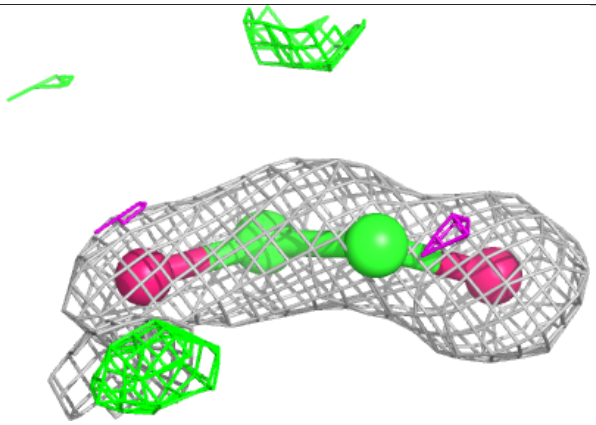
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

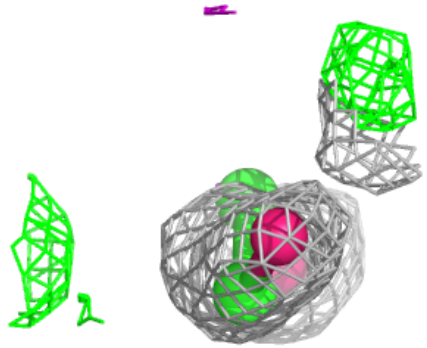


Electron density around EDO C 315:

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

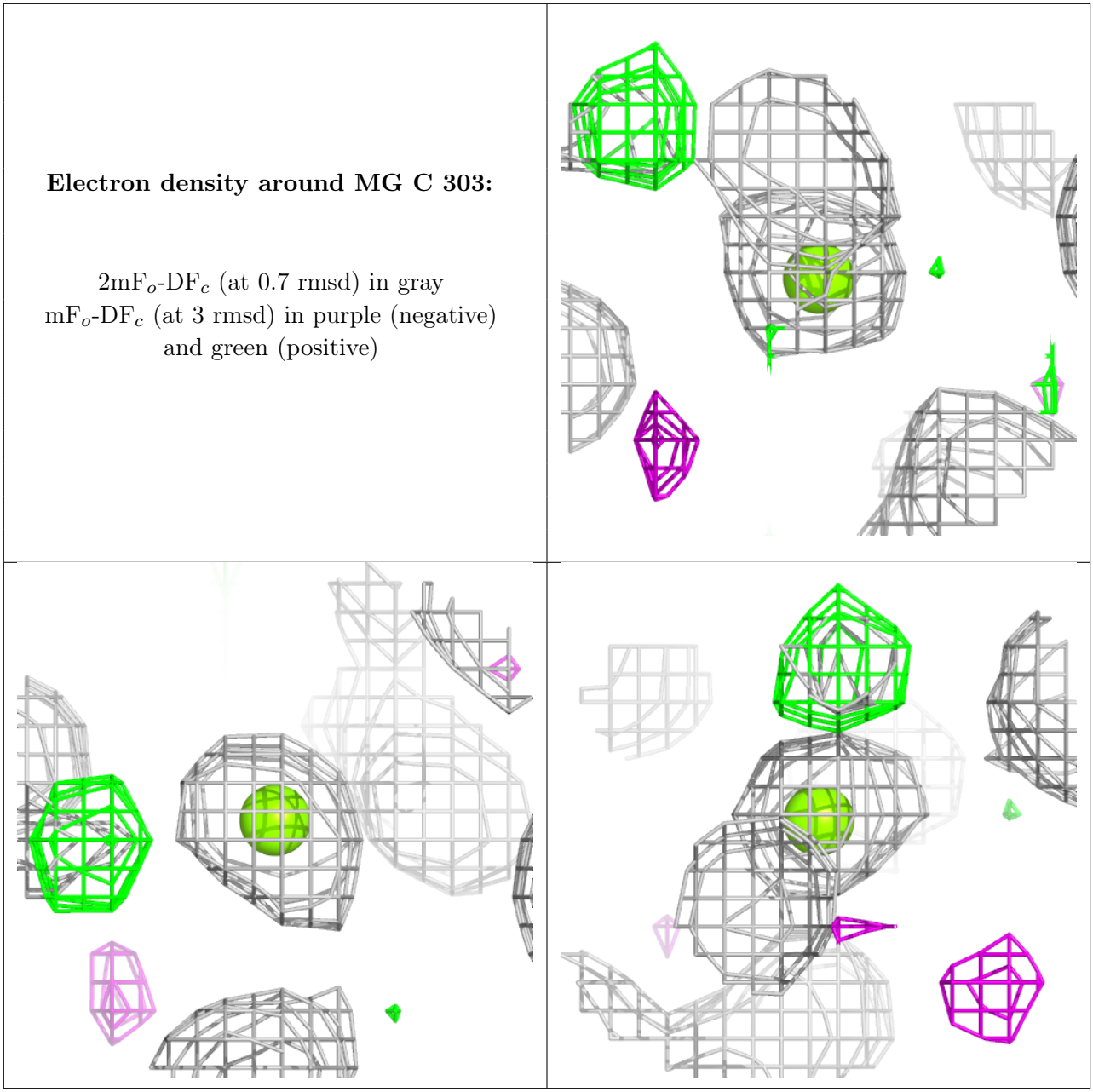






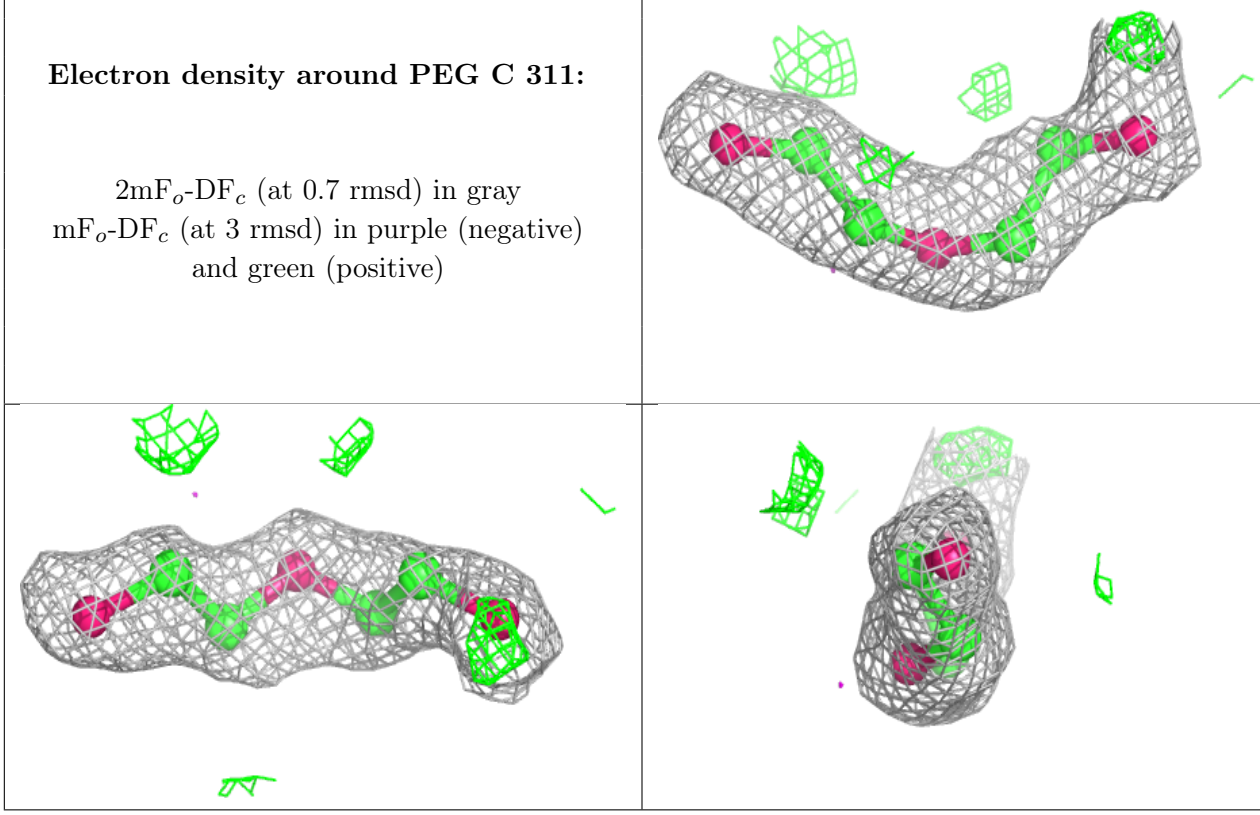
Electron density around MG C 303:

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



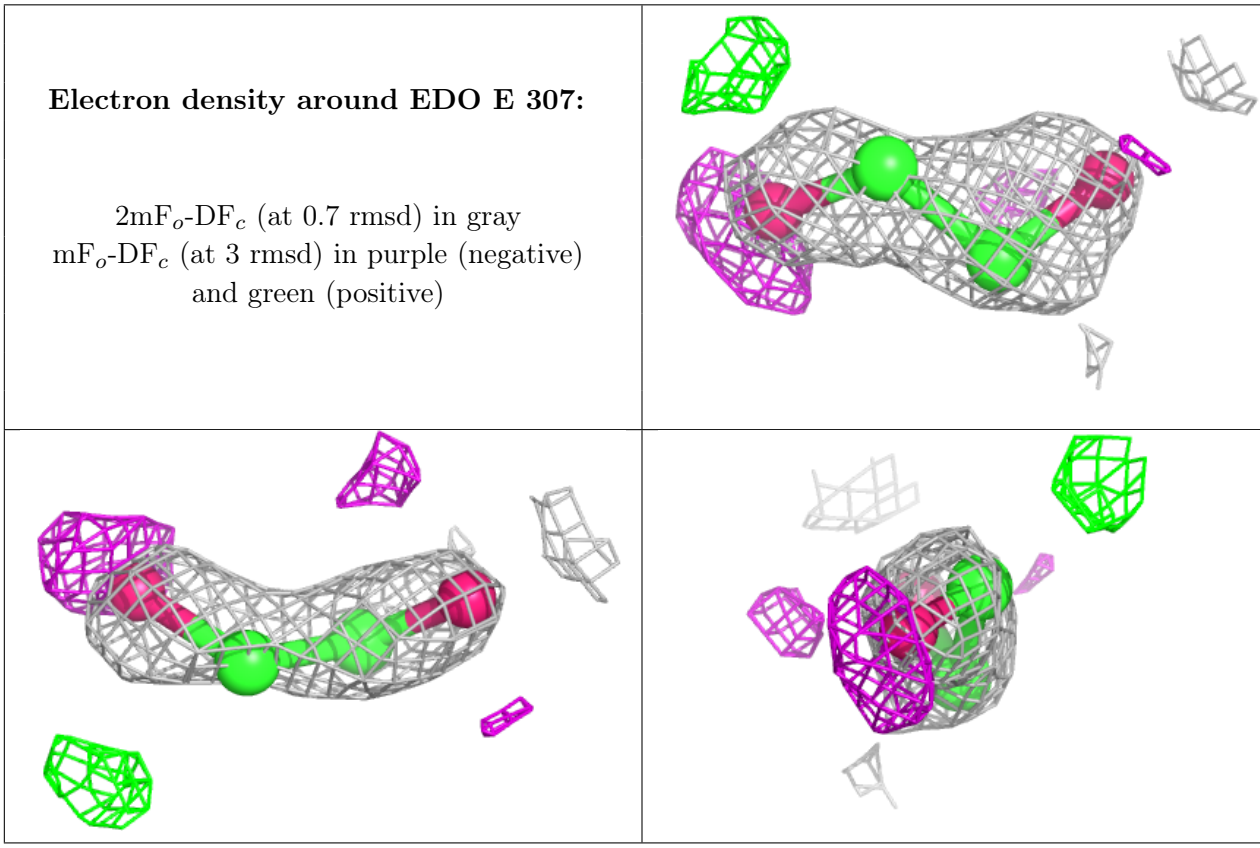
Electron density around PEG C 311:

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



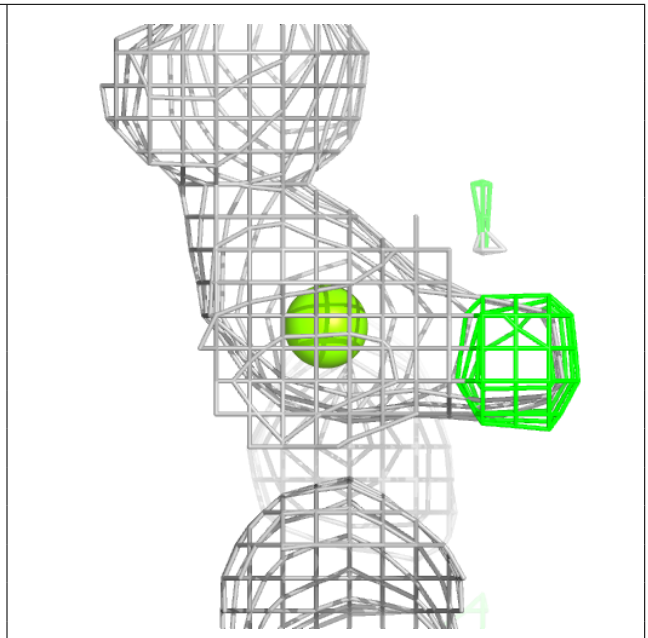
Electron density around EDO E 307:

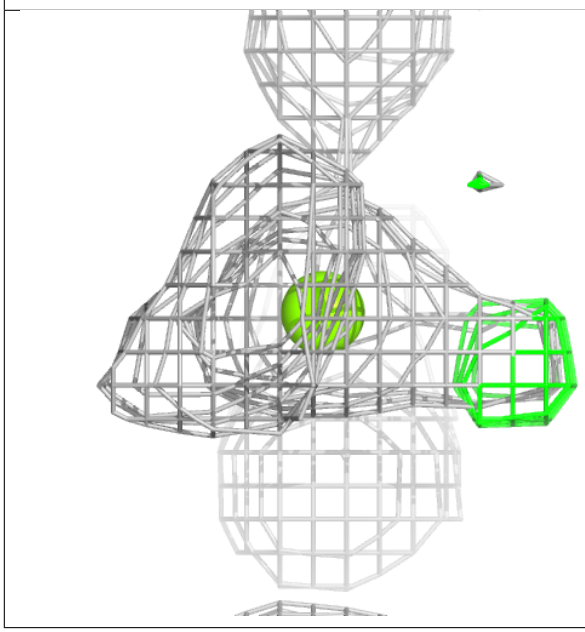
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

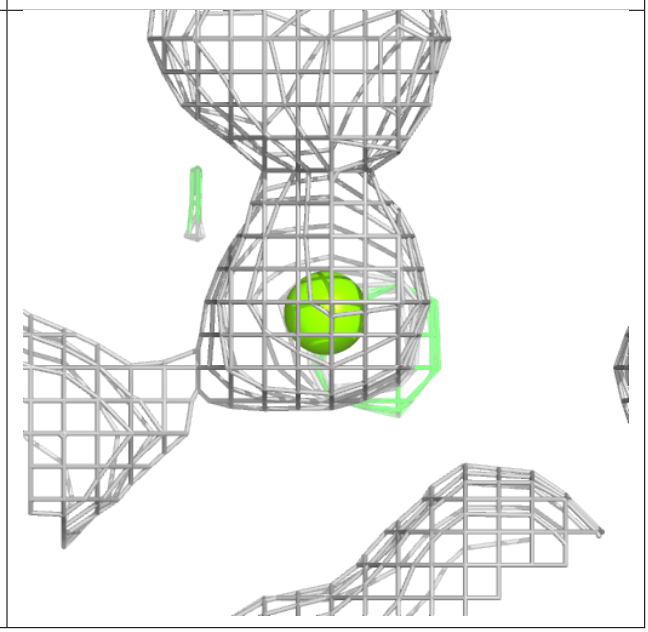


Electron density around MG D 303:

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

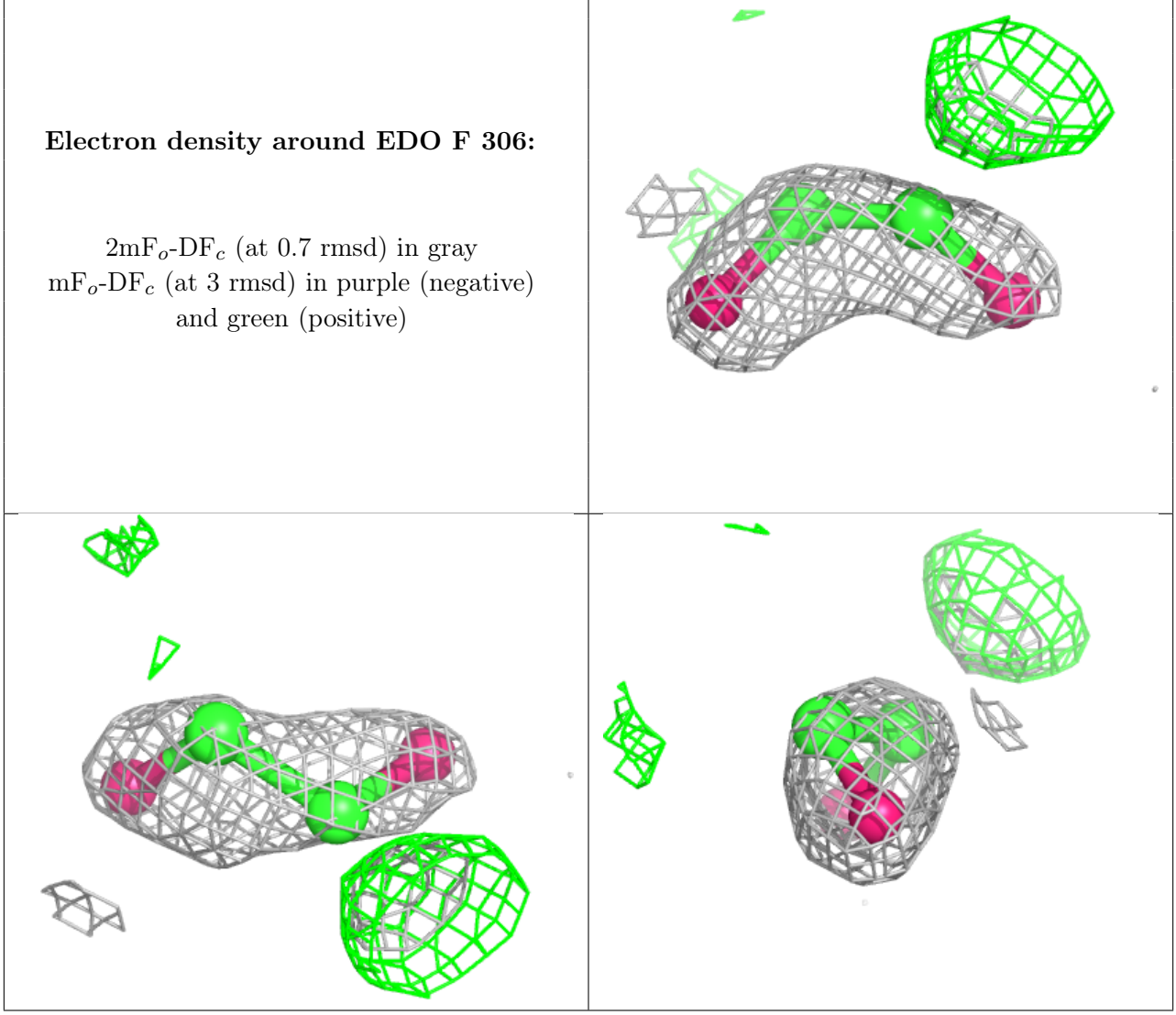






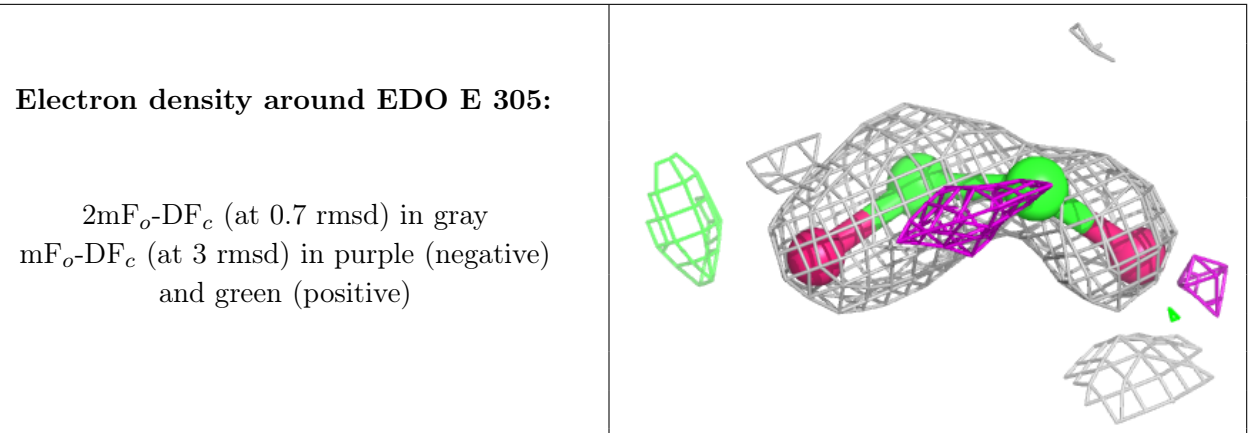
Electron density around EDO F 306:

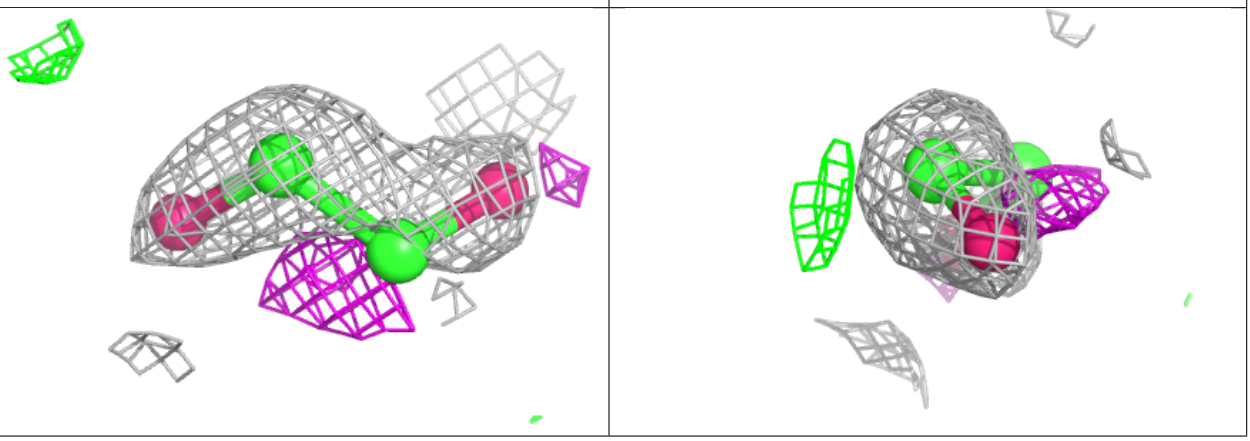
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around EDO E 305:

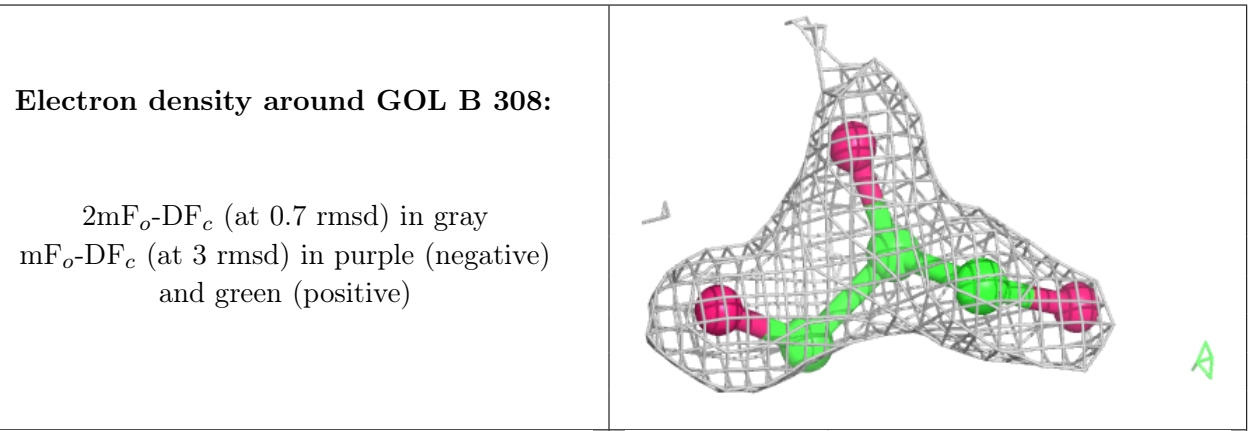
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

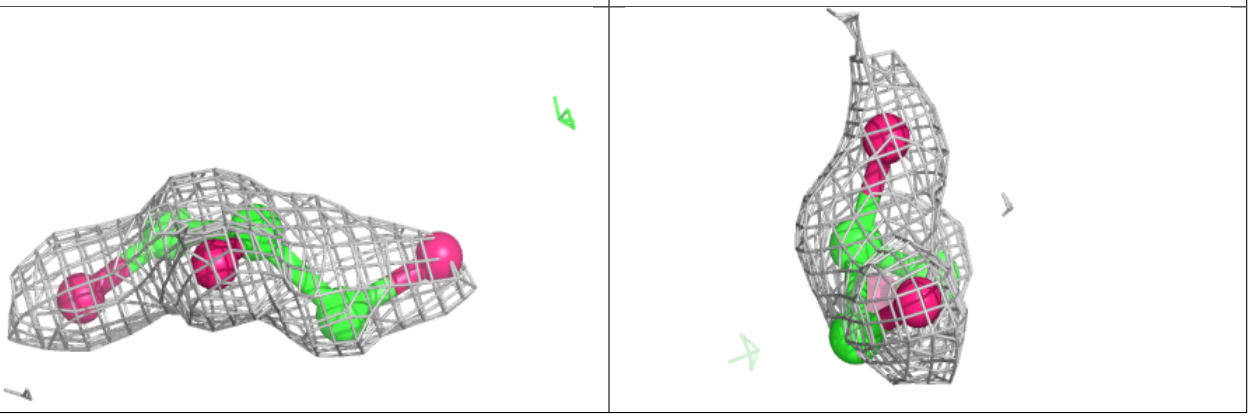




Electron density around GOL B 308:

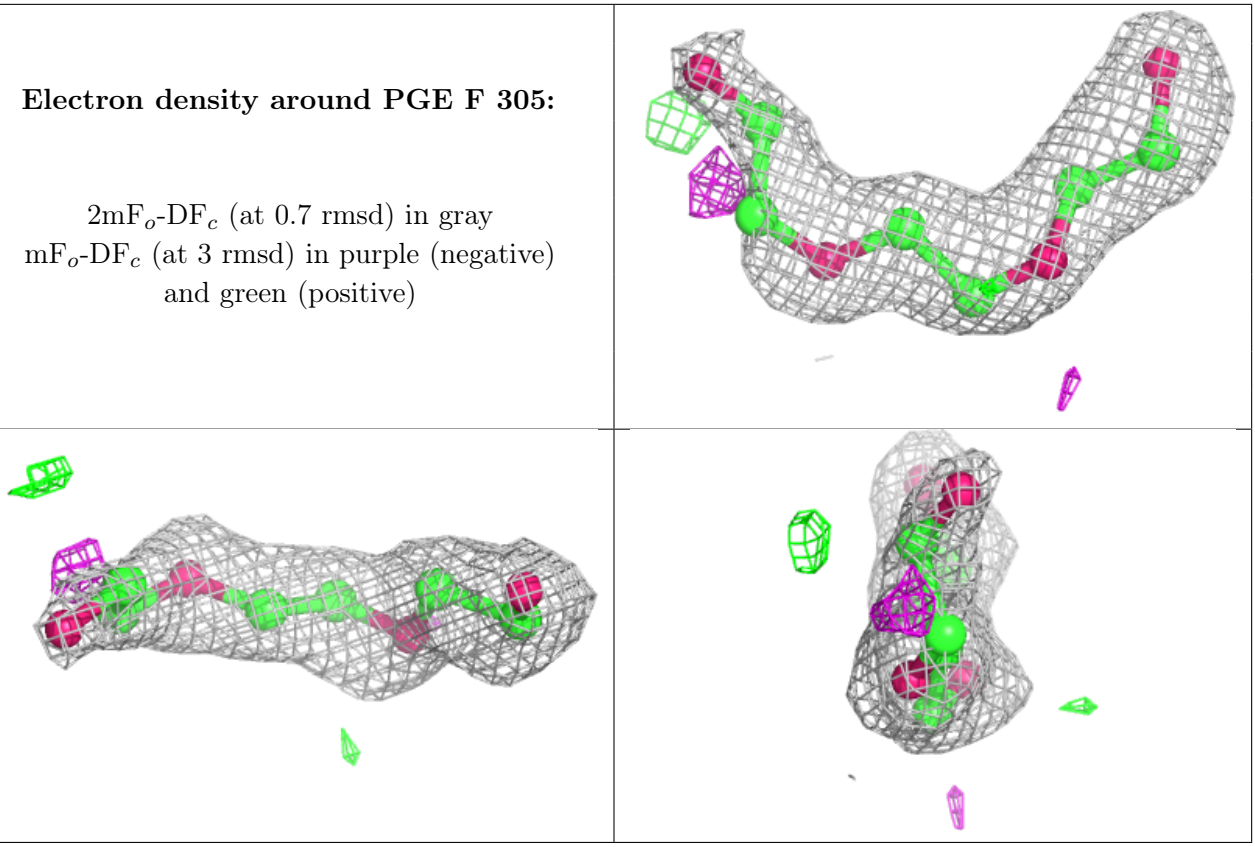
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





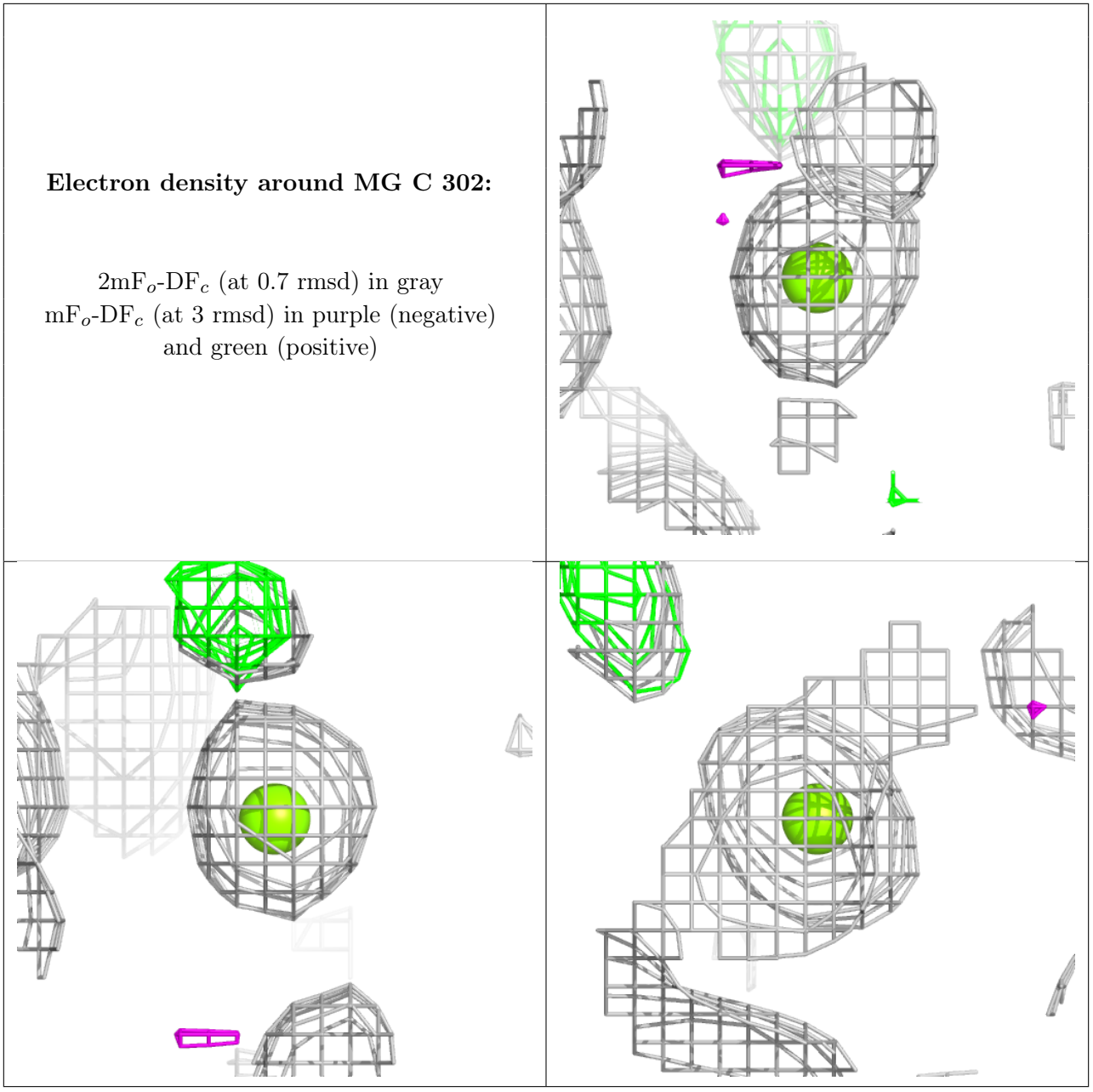
Electron density around PGE F 305:

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



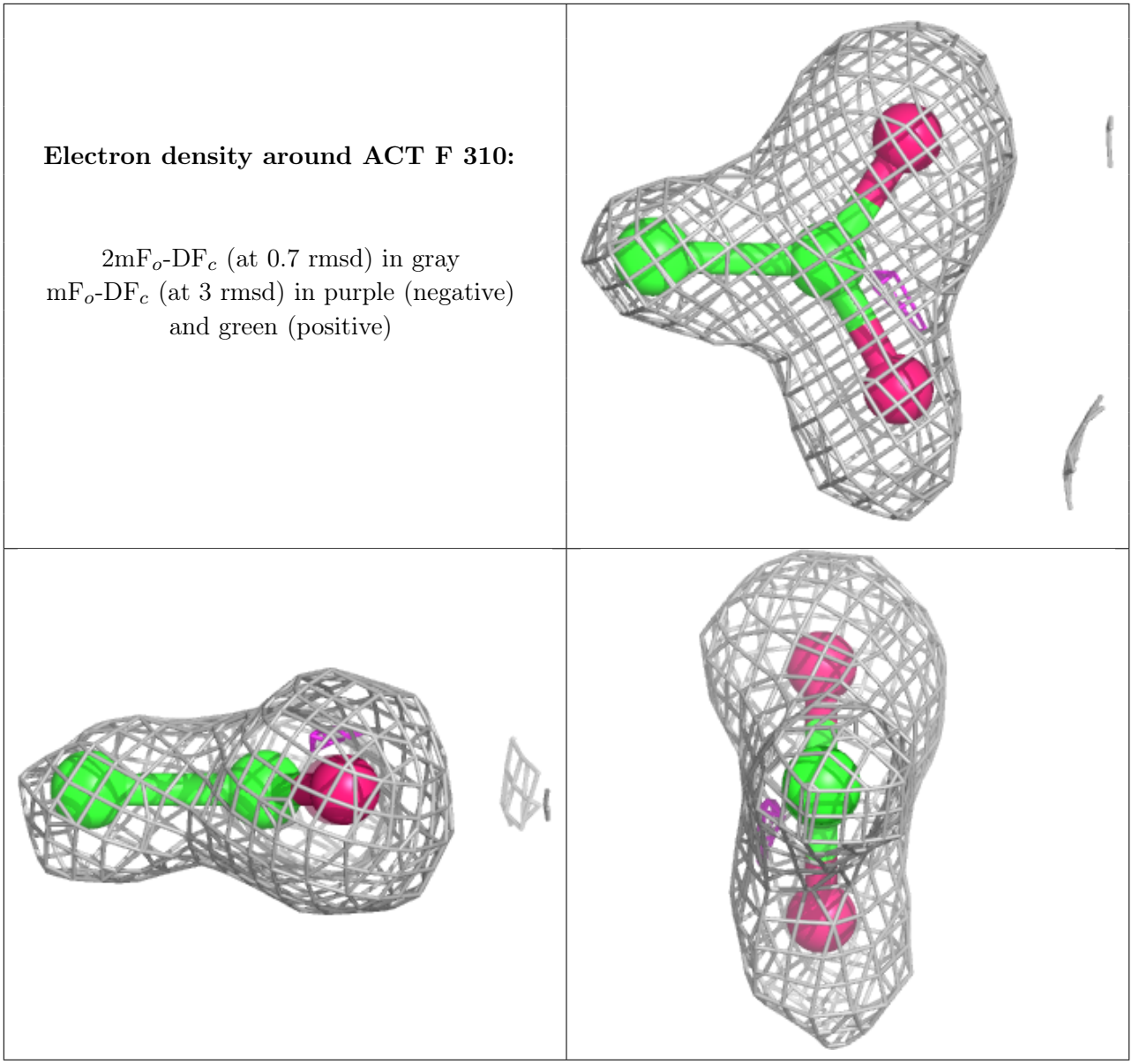
Electron density around MG C 302:

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



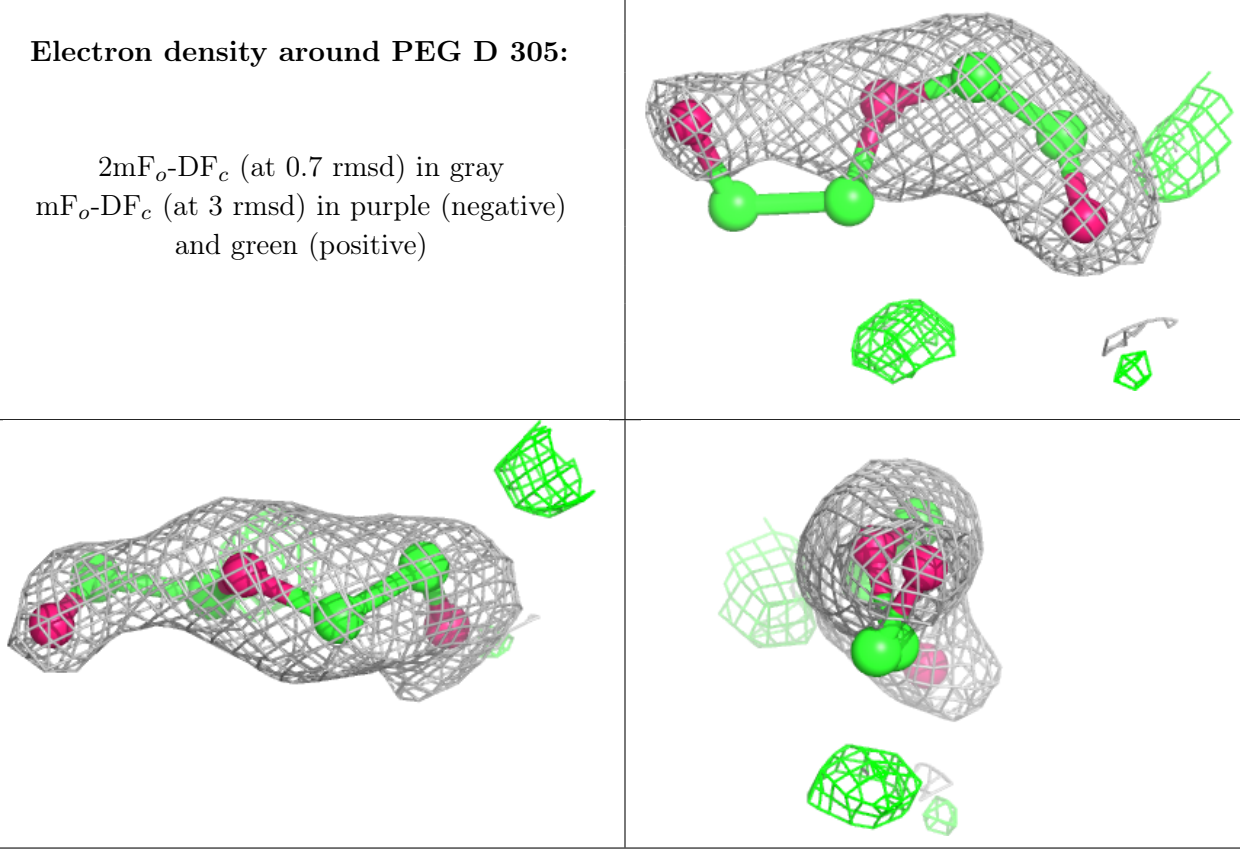
Electron density around ACT F 310:

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



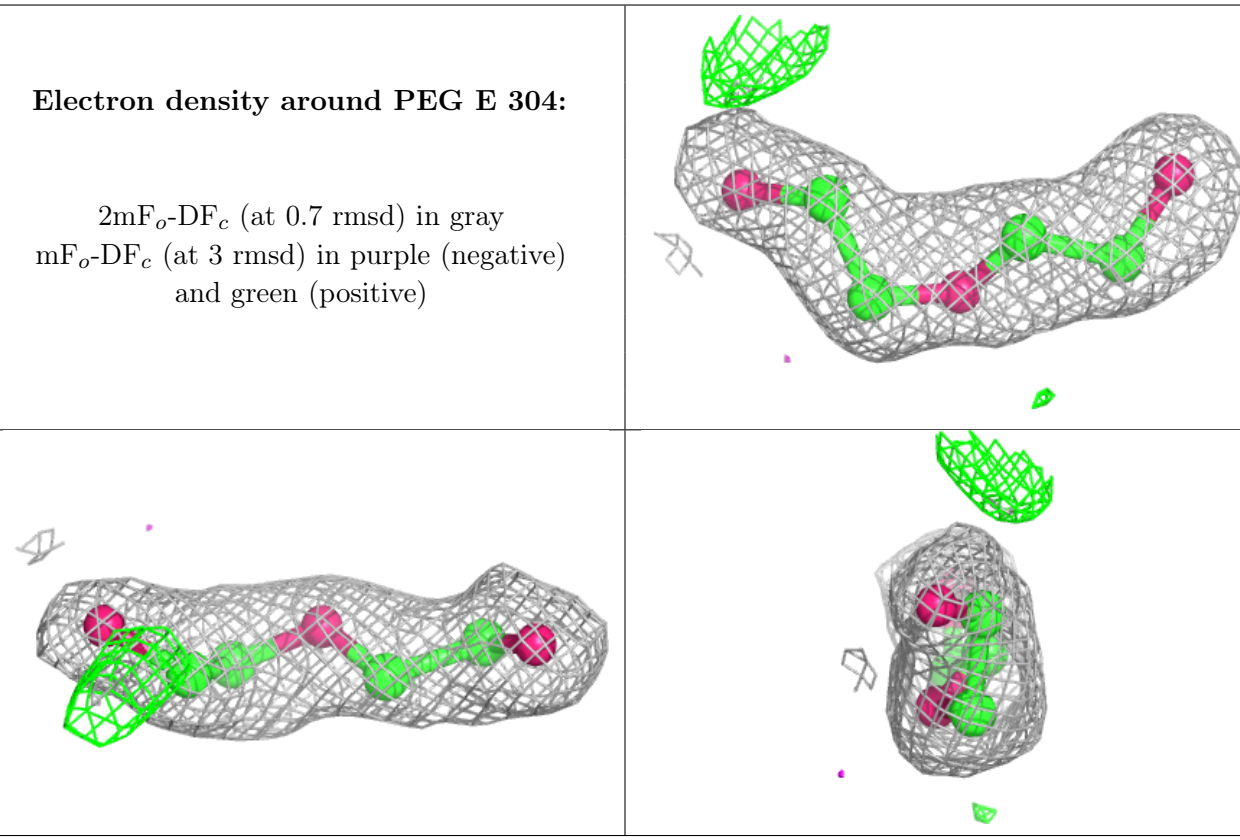
Electron density around PEG D 305:

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



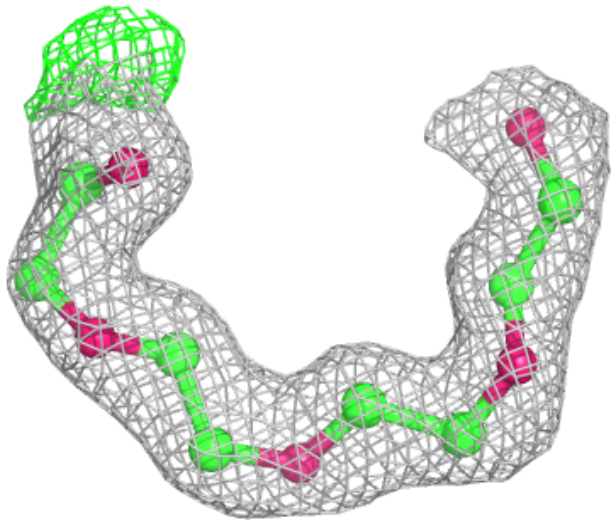
Electron density around PEG E 304:

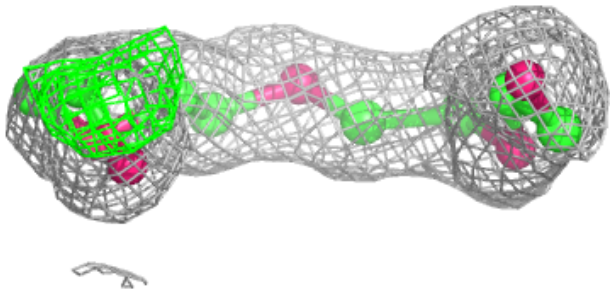
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

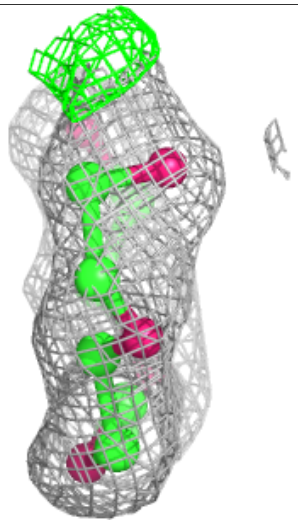


Electron density around PG4 D 304:

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

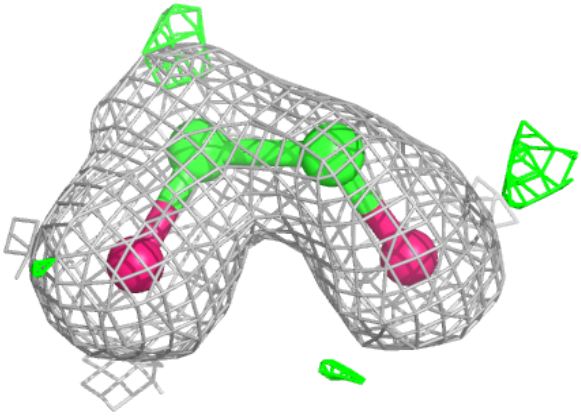


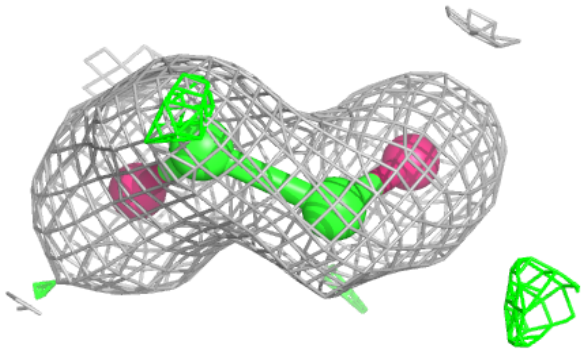


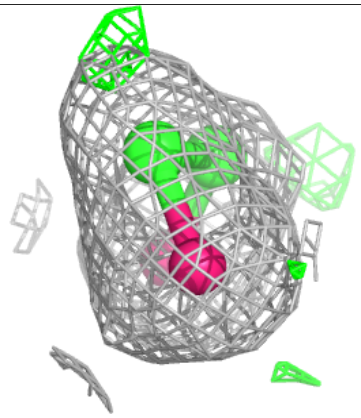


Electron density around EDO A 306:

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

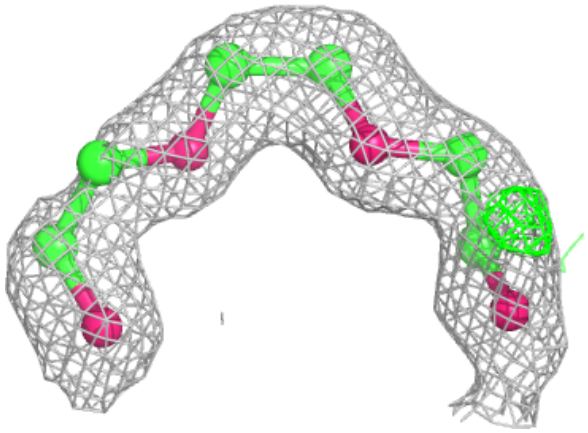


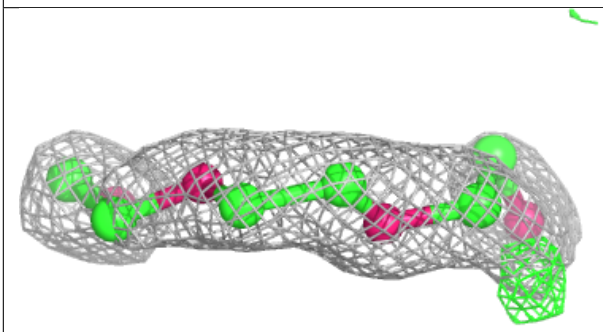


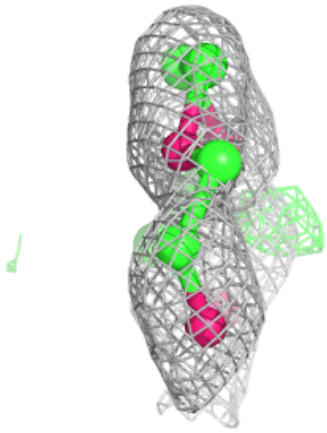


Electron density around PGE C 312:

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

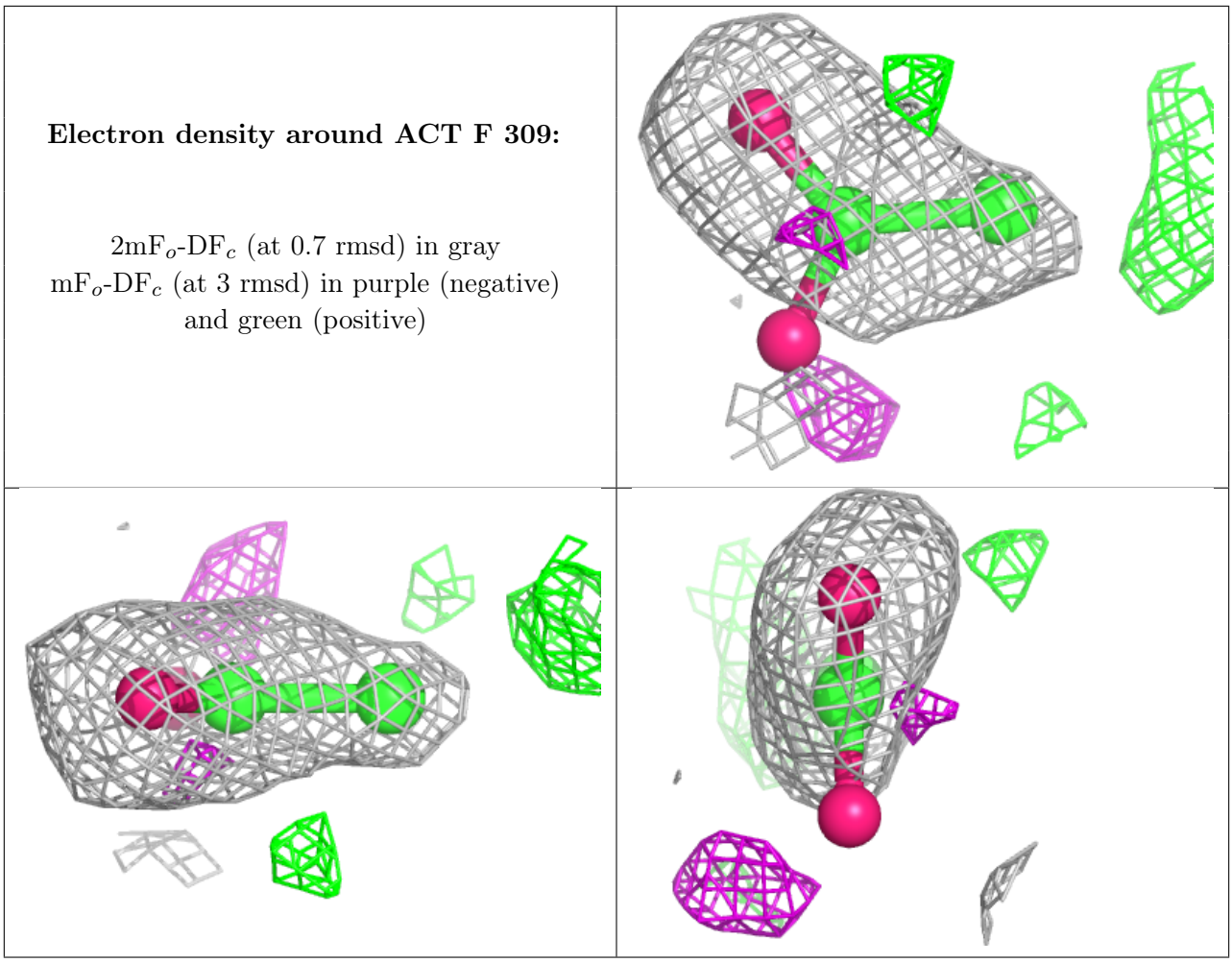






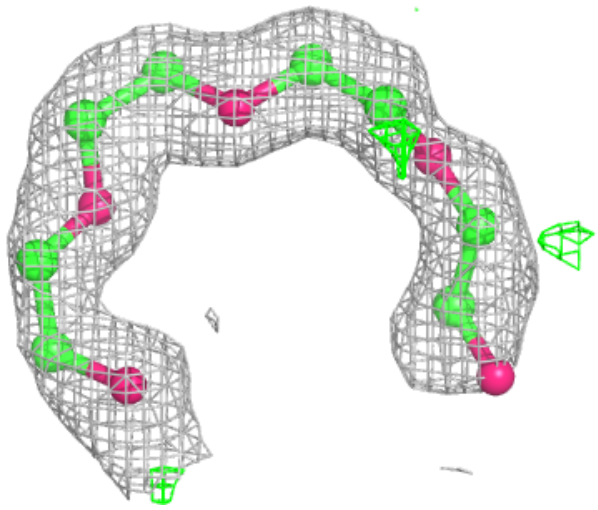
Electron density around ACT F 309:

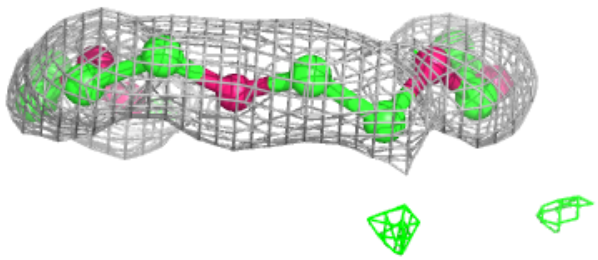
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

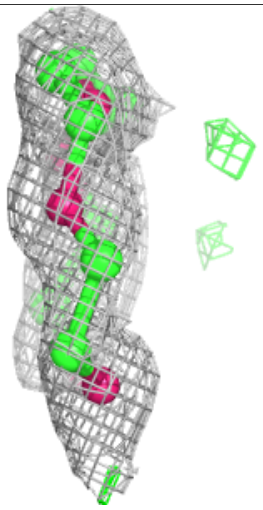


Electron density around PG4 A 303:

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

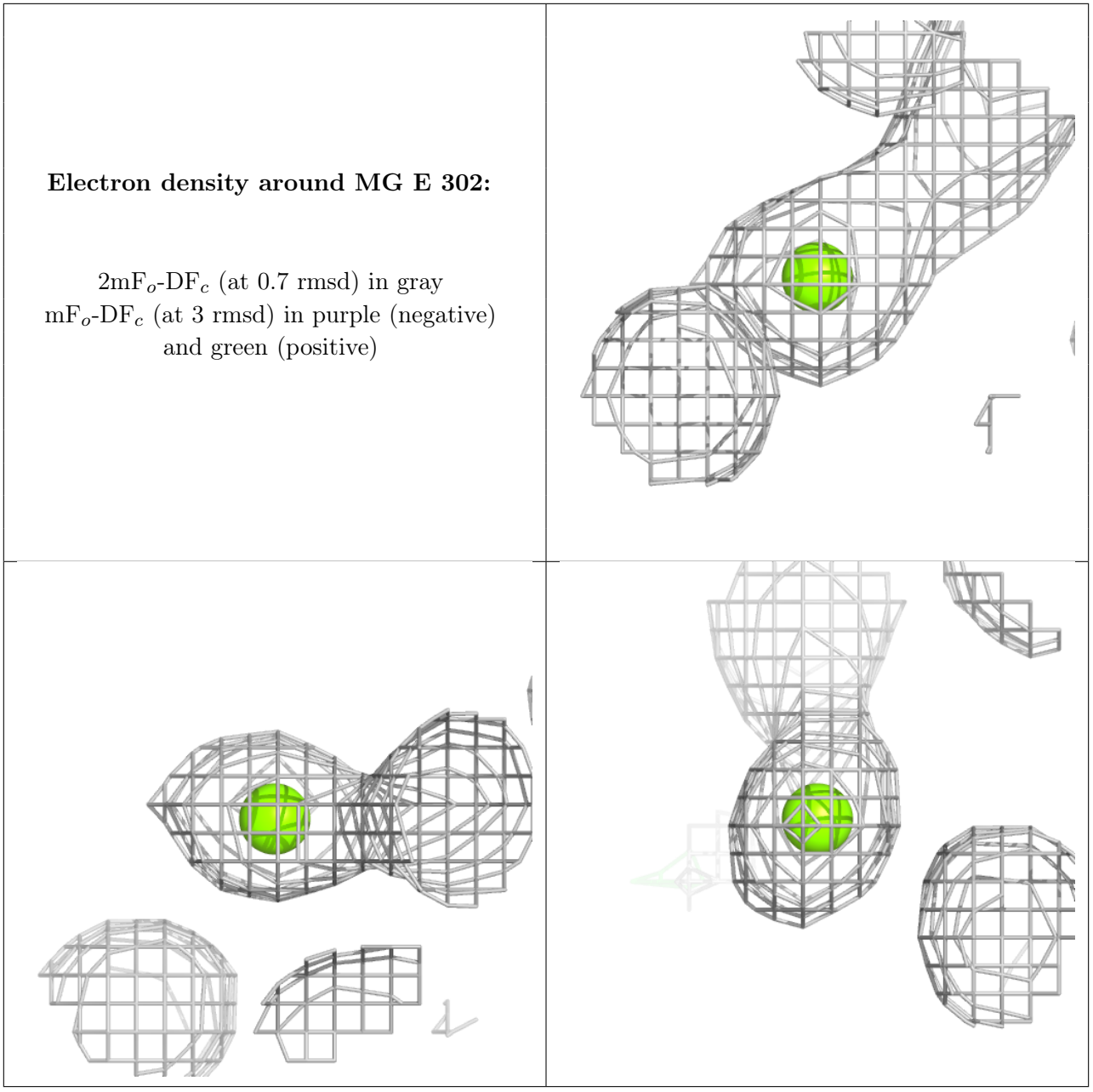






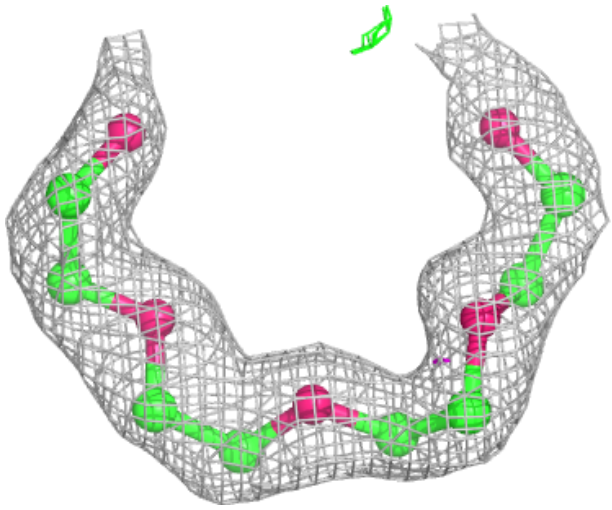
Electron density around MG E 302:

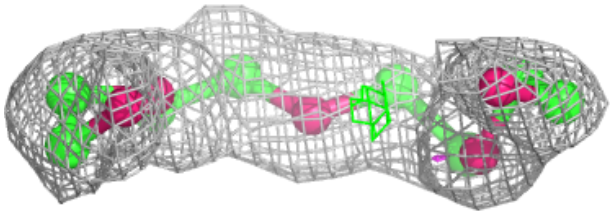
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

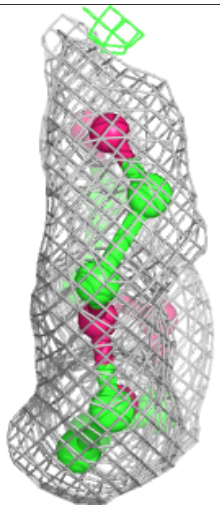


Electron density around PG4 B 305:

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

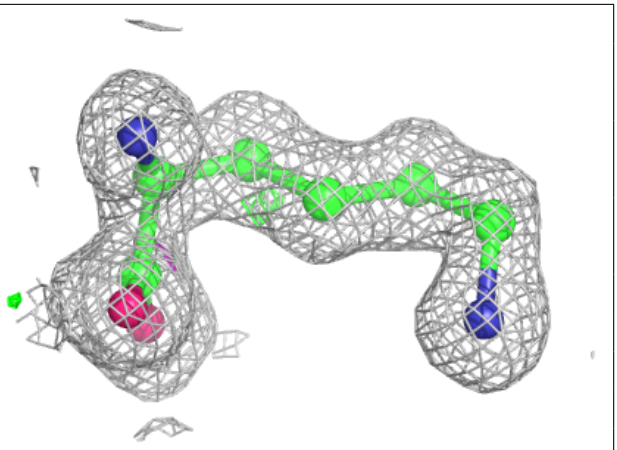


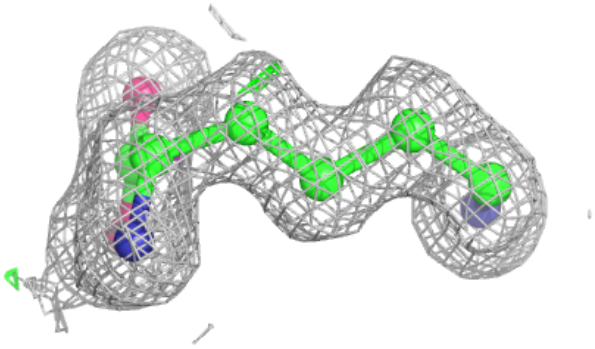


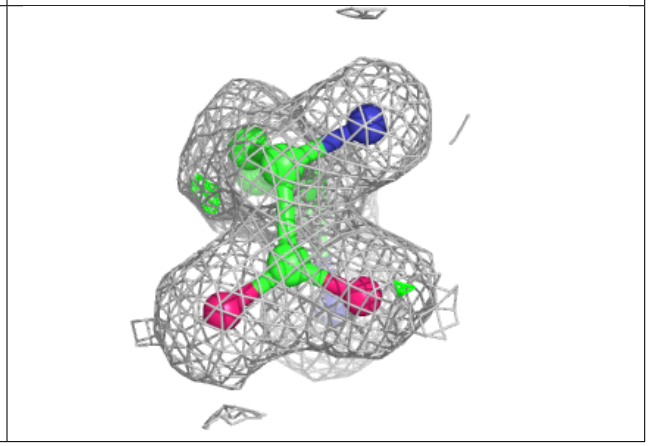


Electron density around LYS B 307:

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

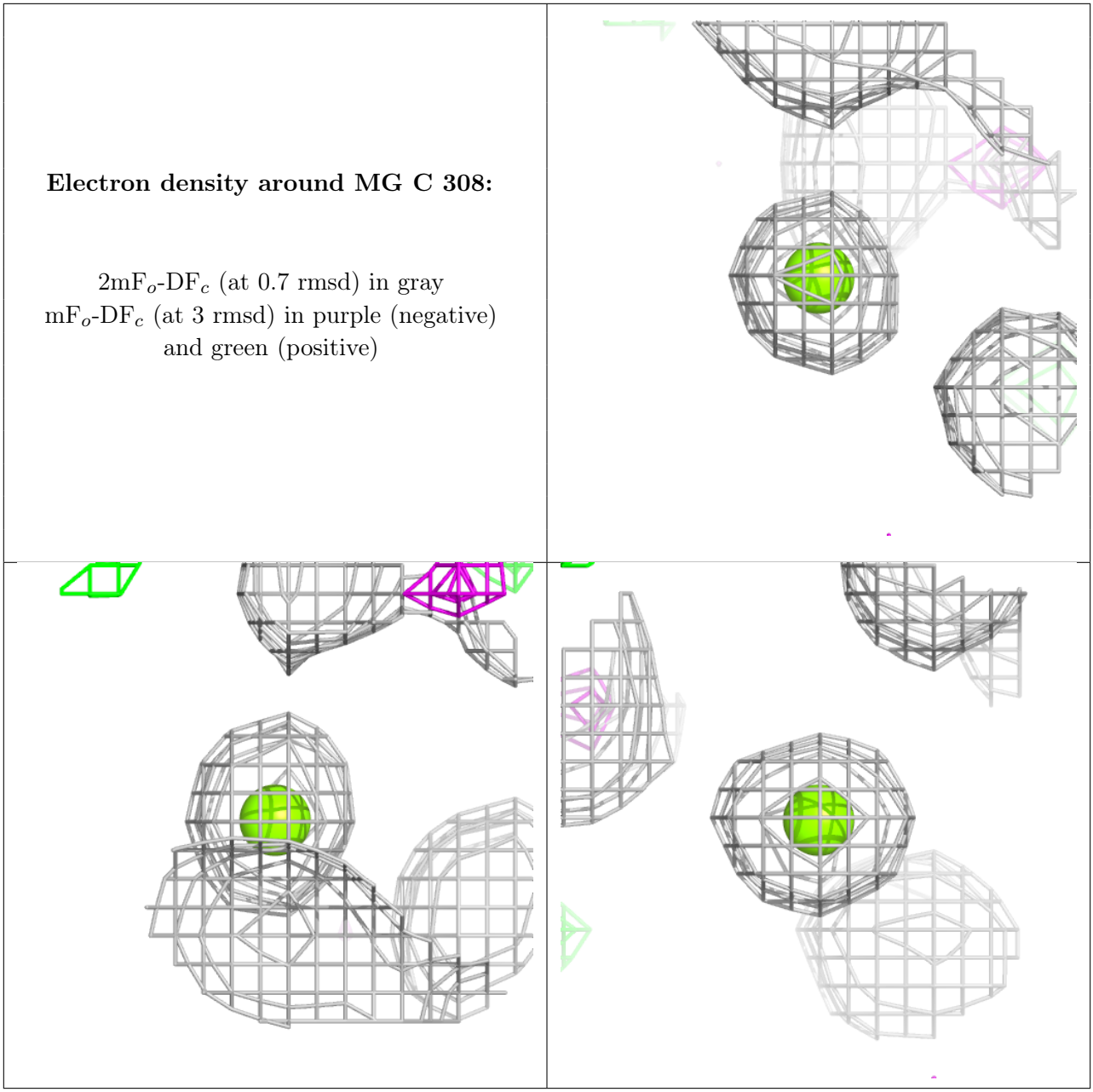






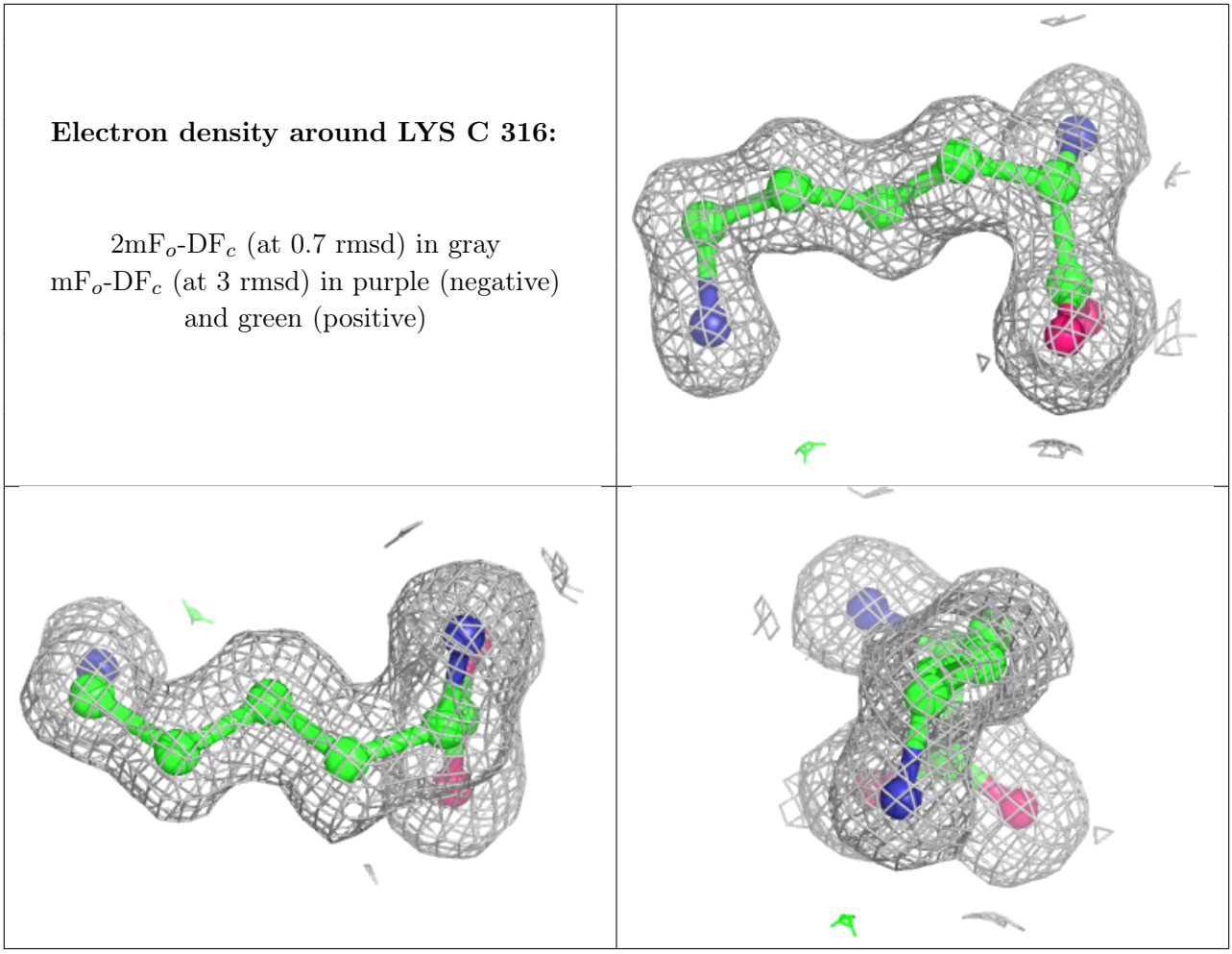
Electron density around MG C 308:

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



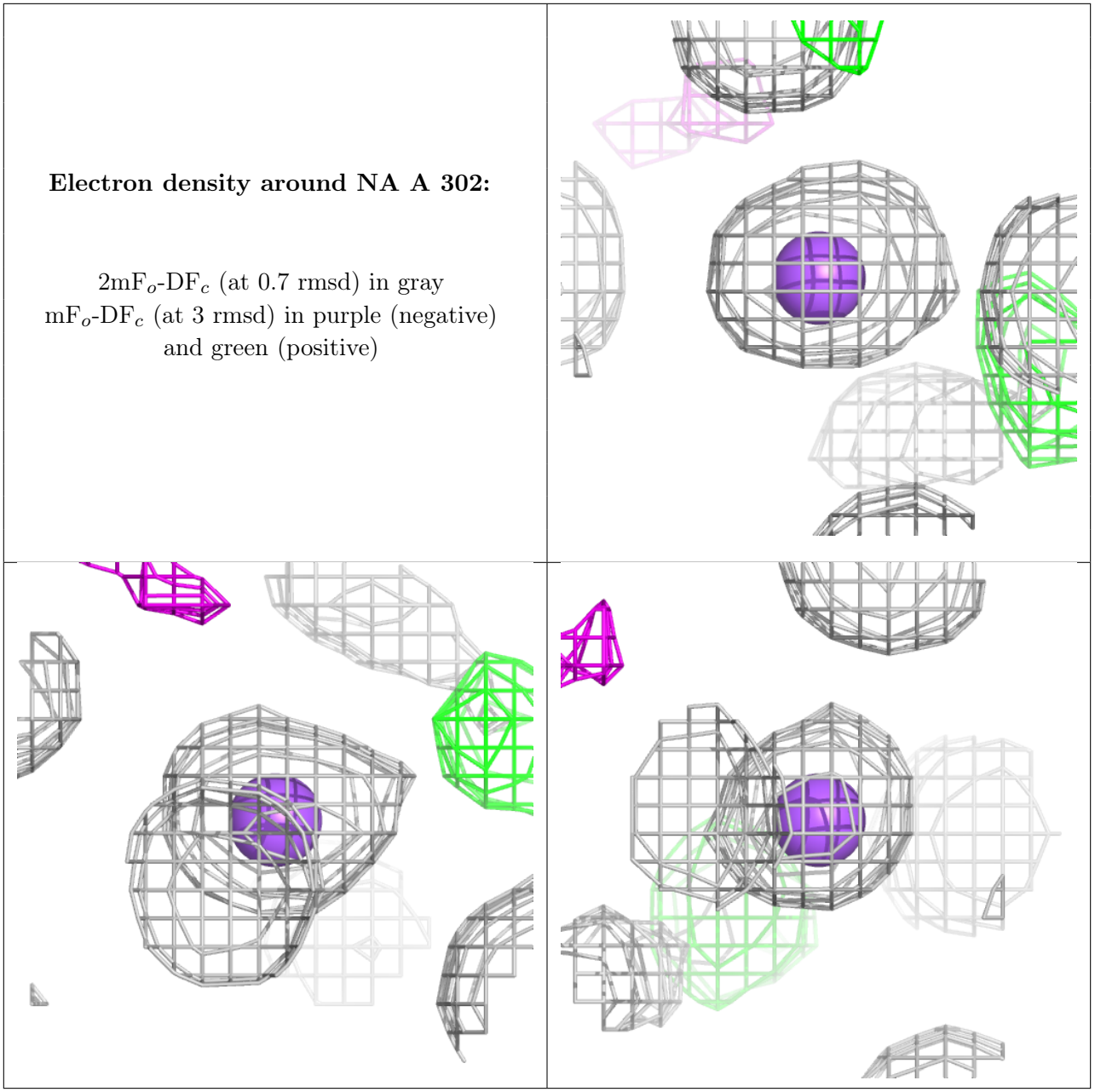
Electron density around LYS C 316:

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



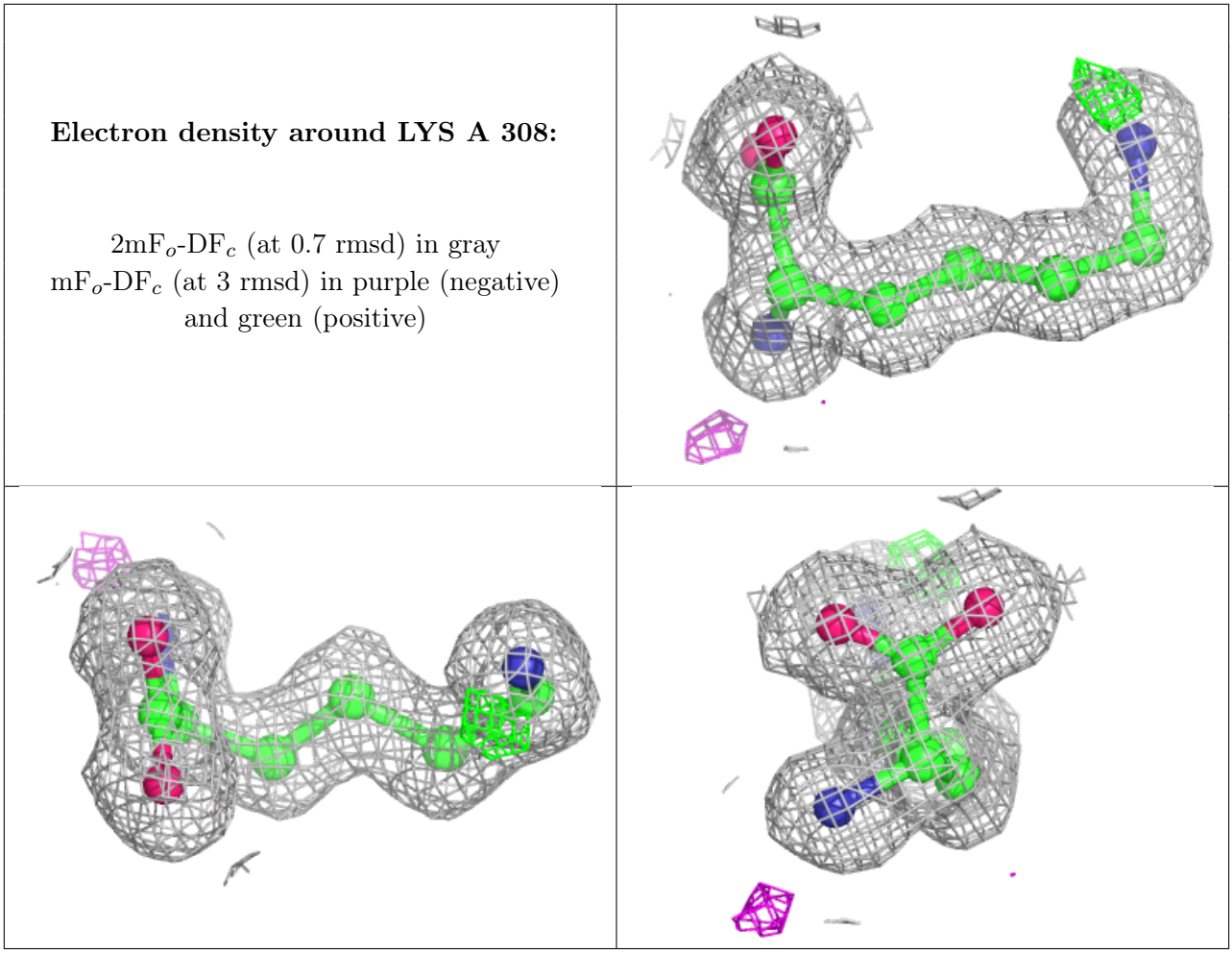
Electron density around NA A 302:

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



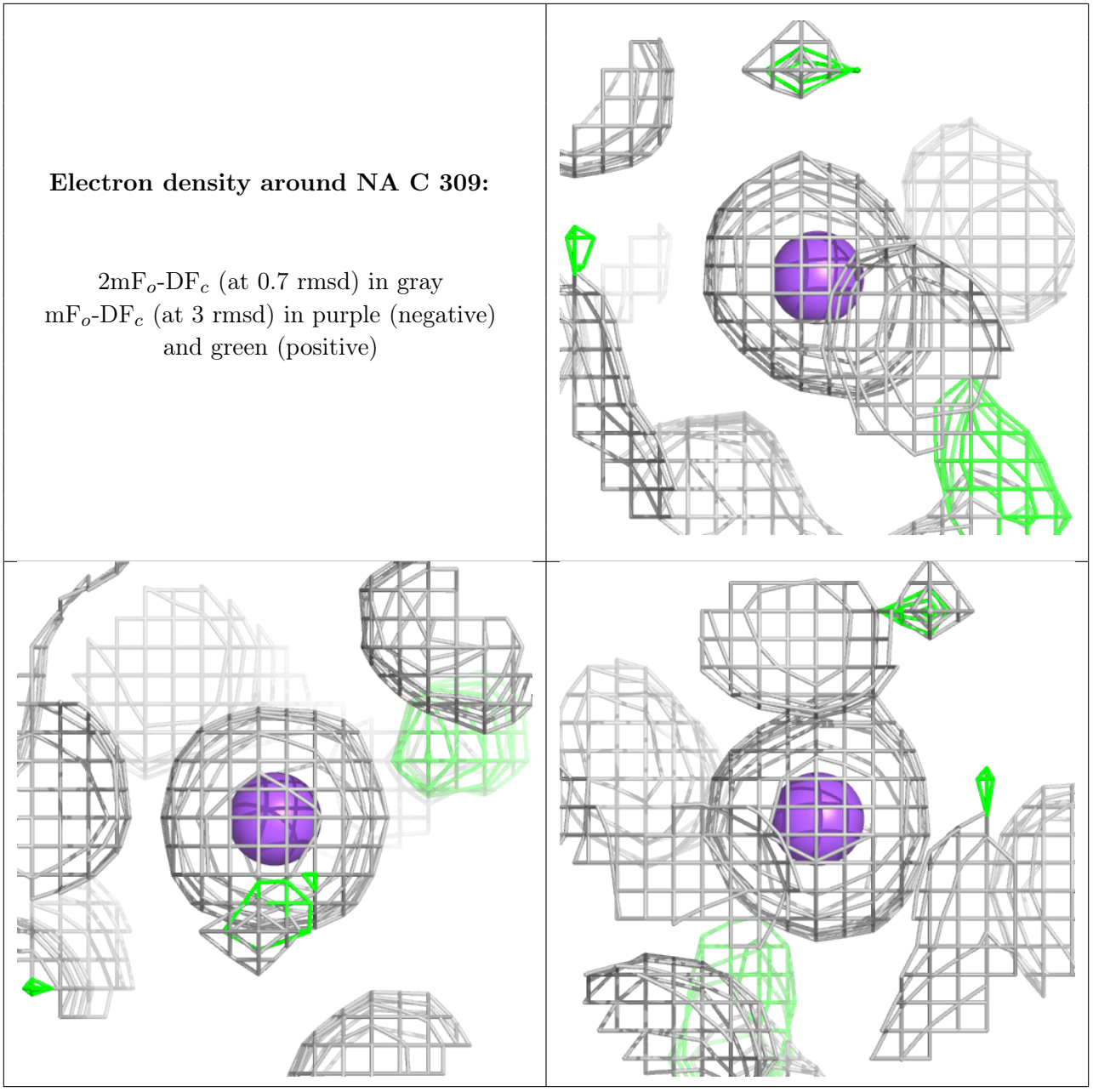
Electron density around LYS A 308:

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



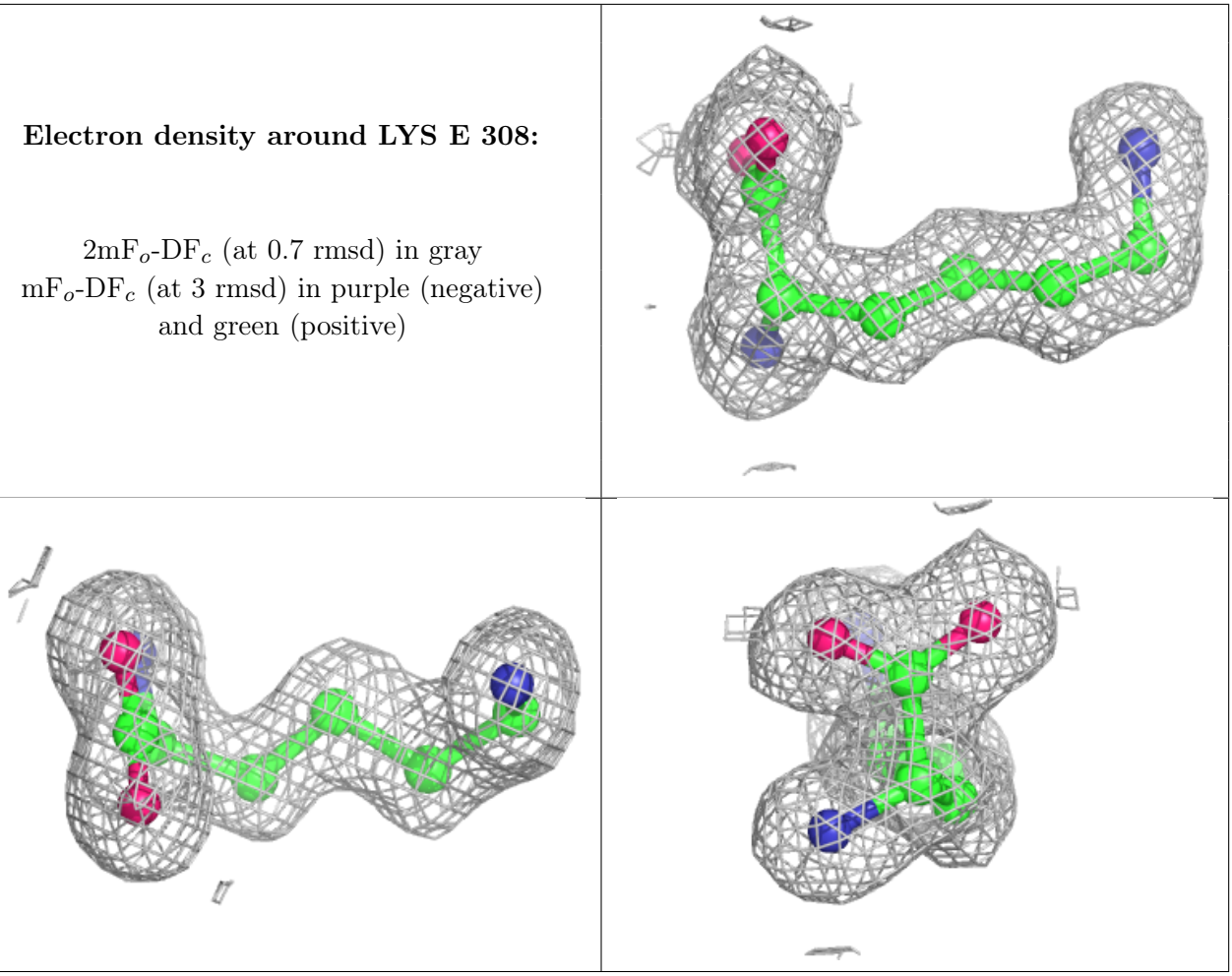
Electron density around NA C 309:

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



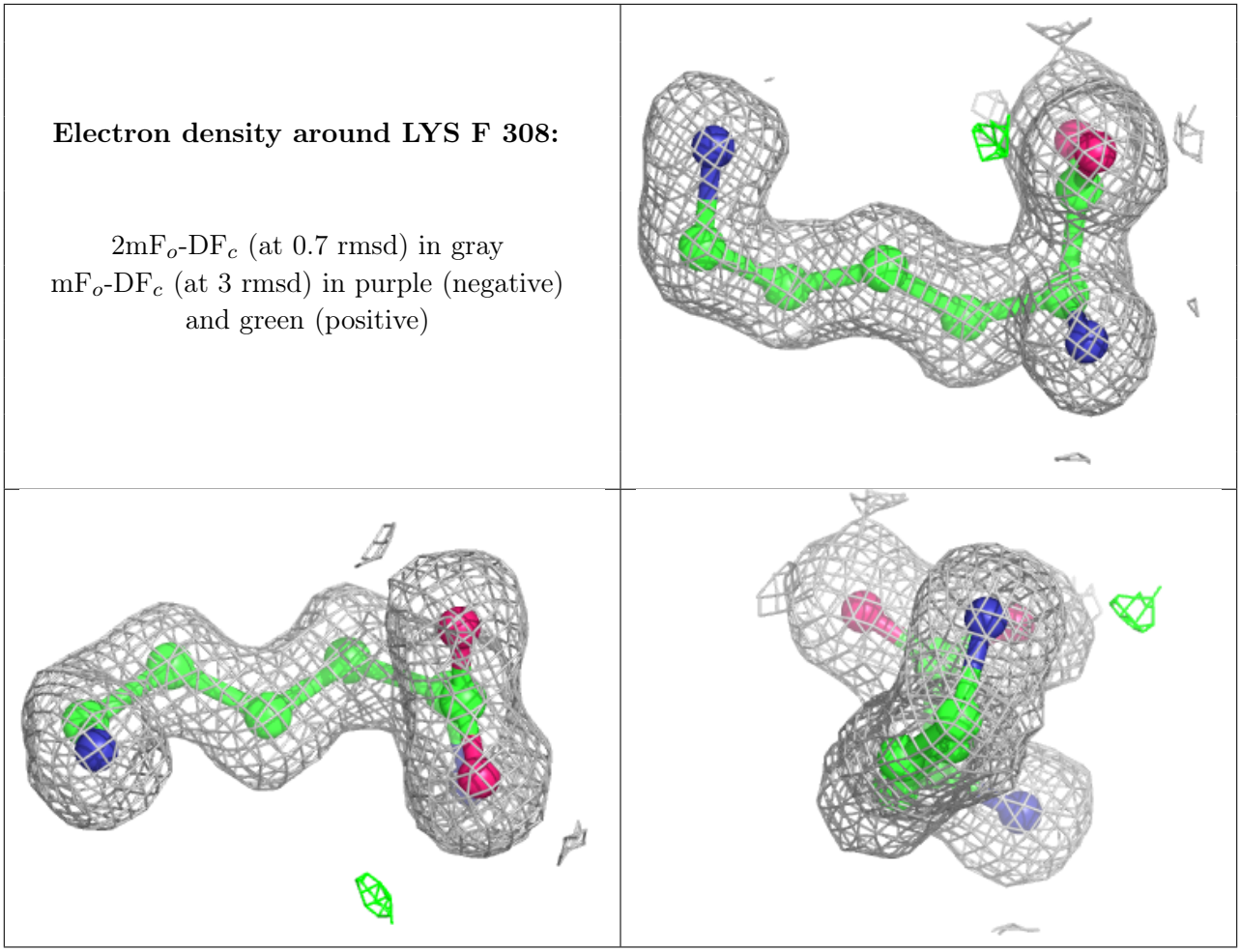
Electron density around LYS E 308:

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



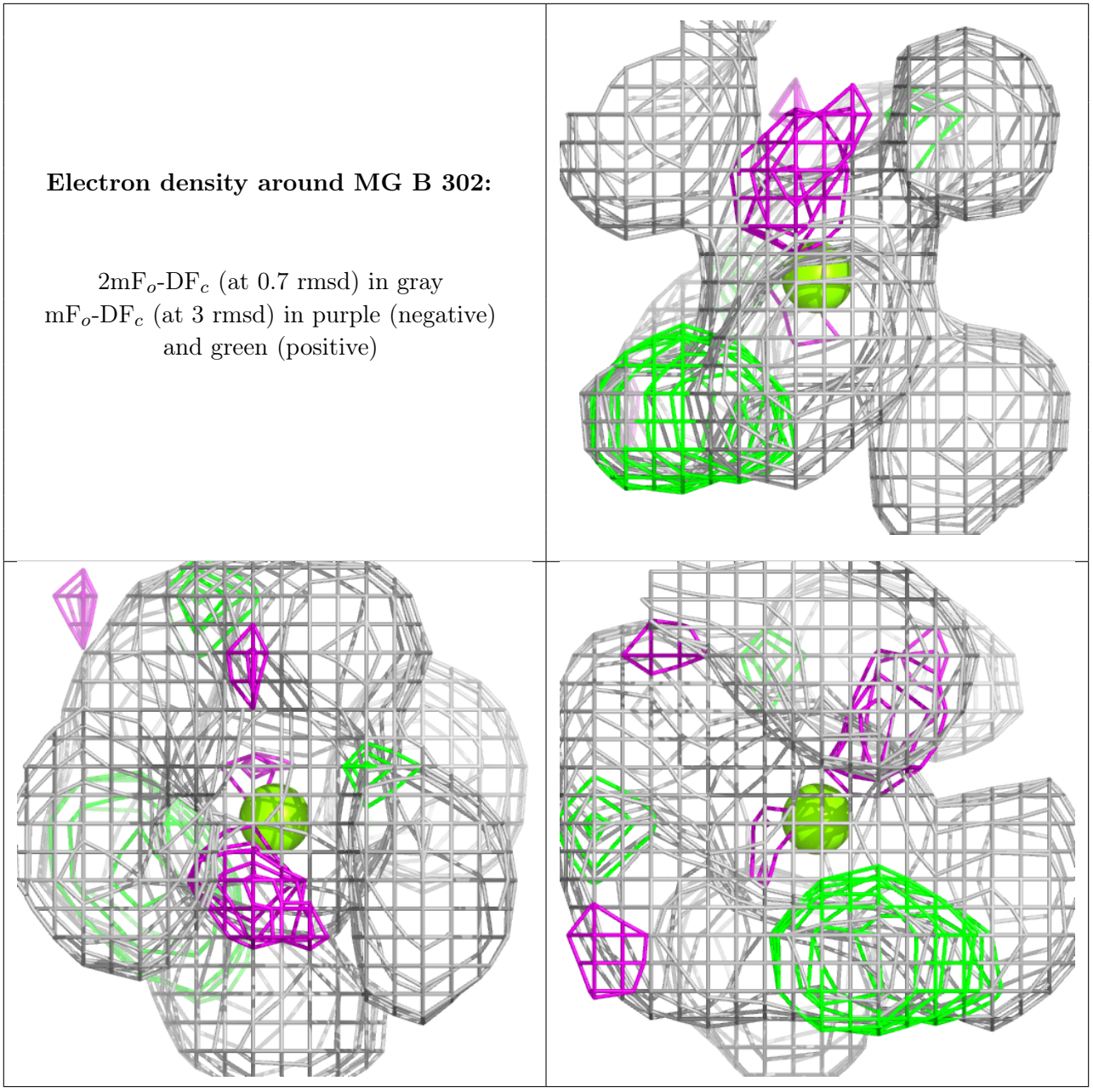
Electron density around LYS F 308:

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



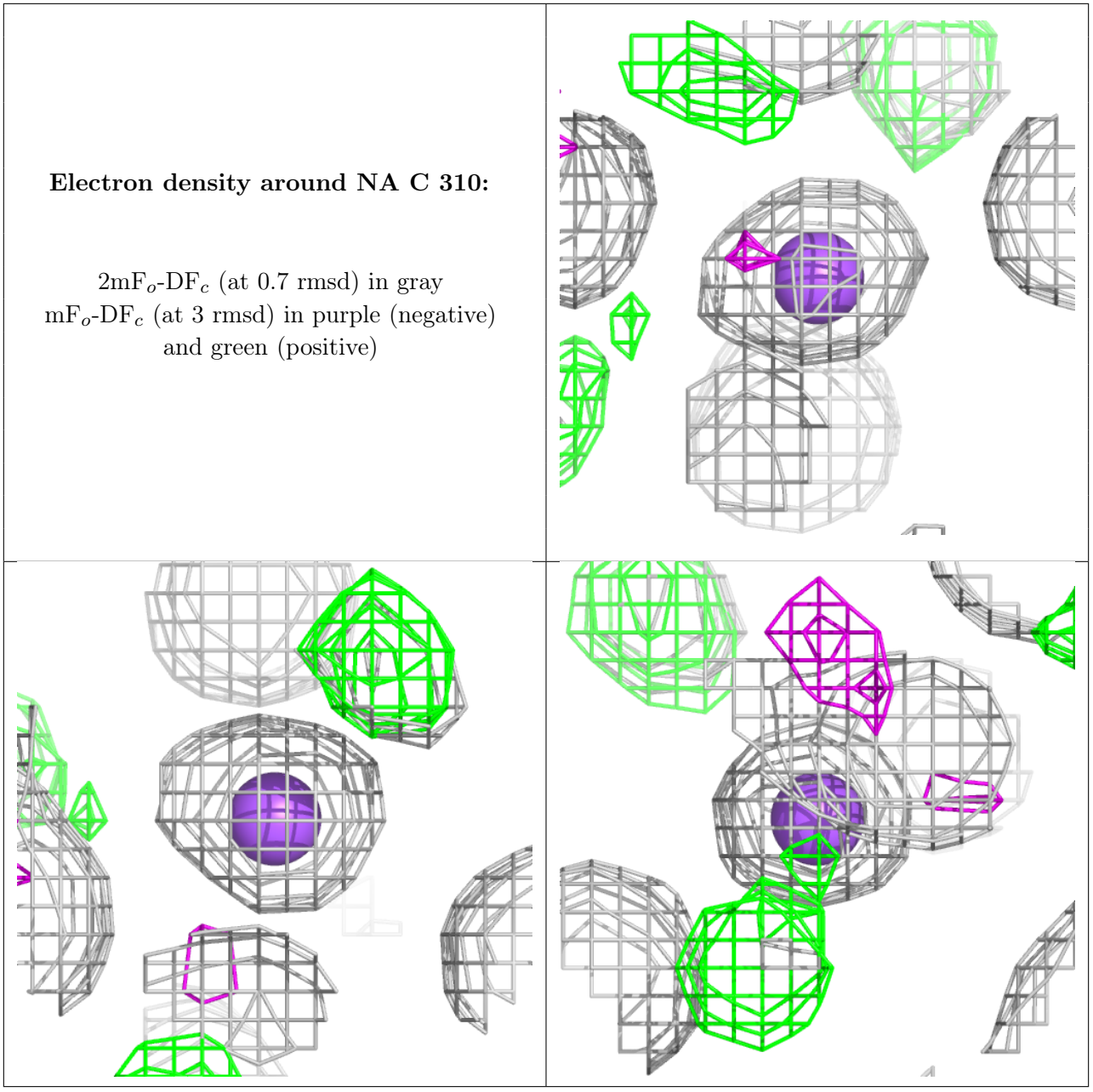
Electron density around MG B 302:

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



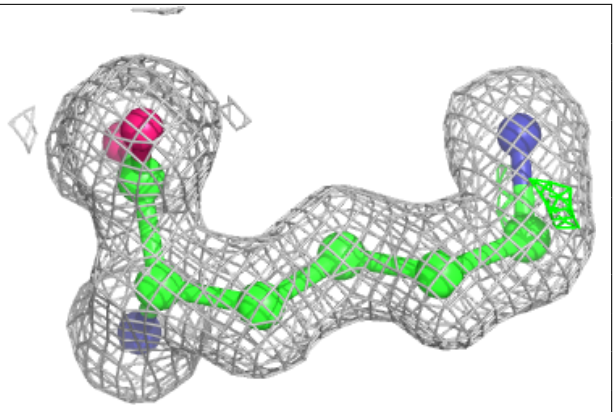
Electron density around NA C 310:

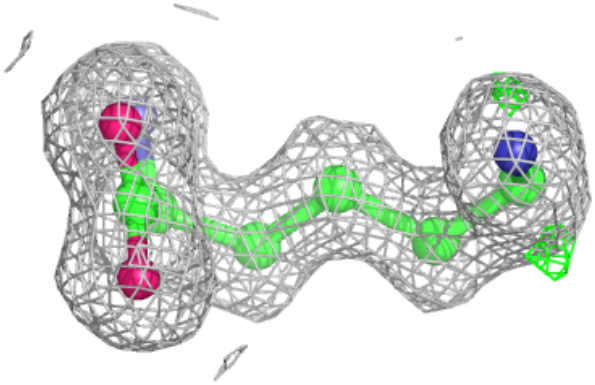
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

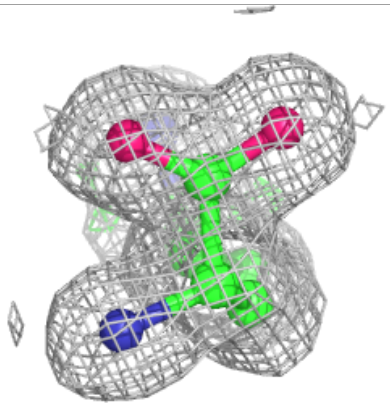


Electron density around LYS D 306:

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

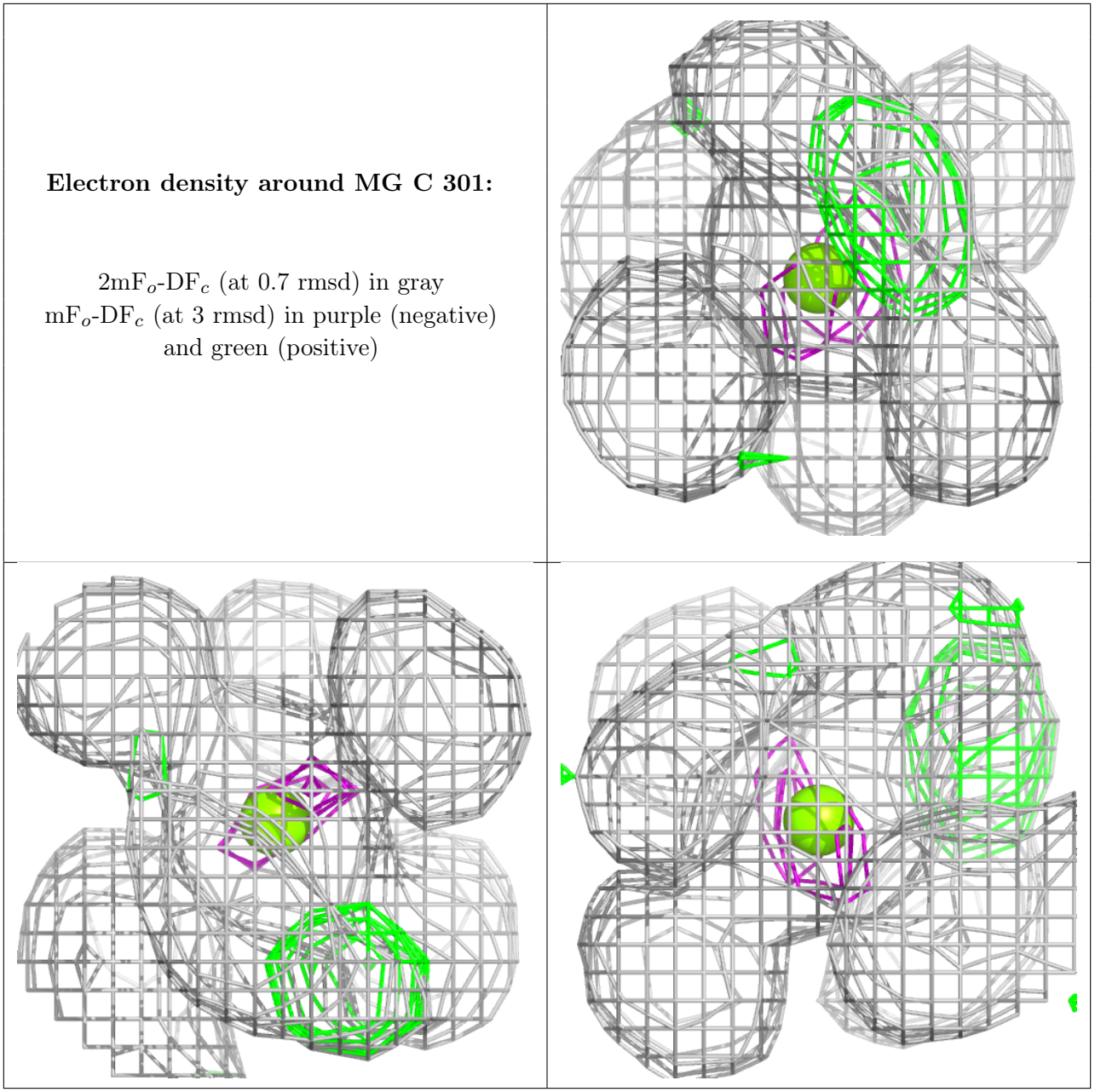






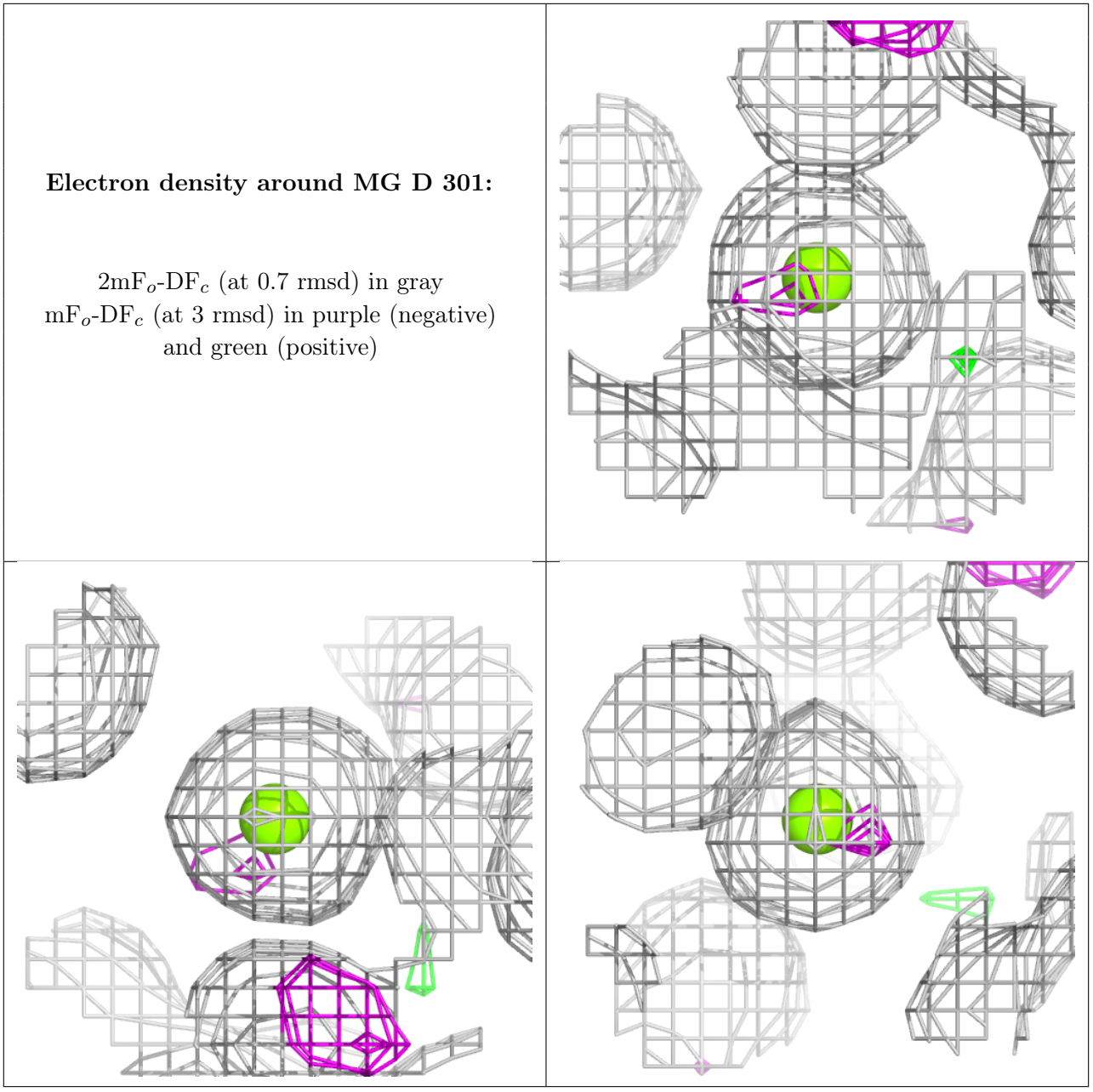
Electron density around MG C 301:

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



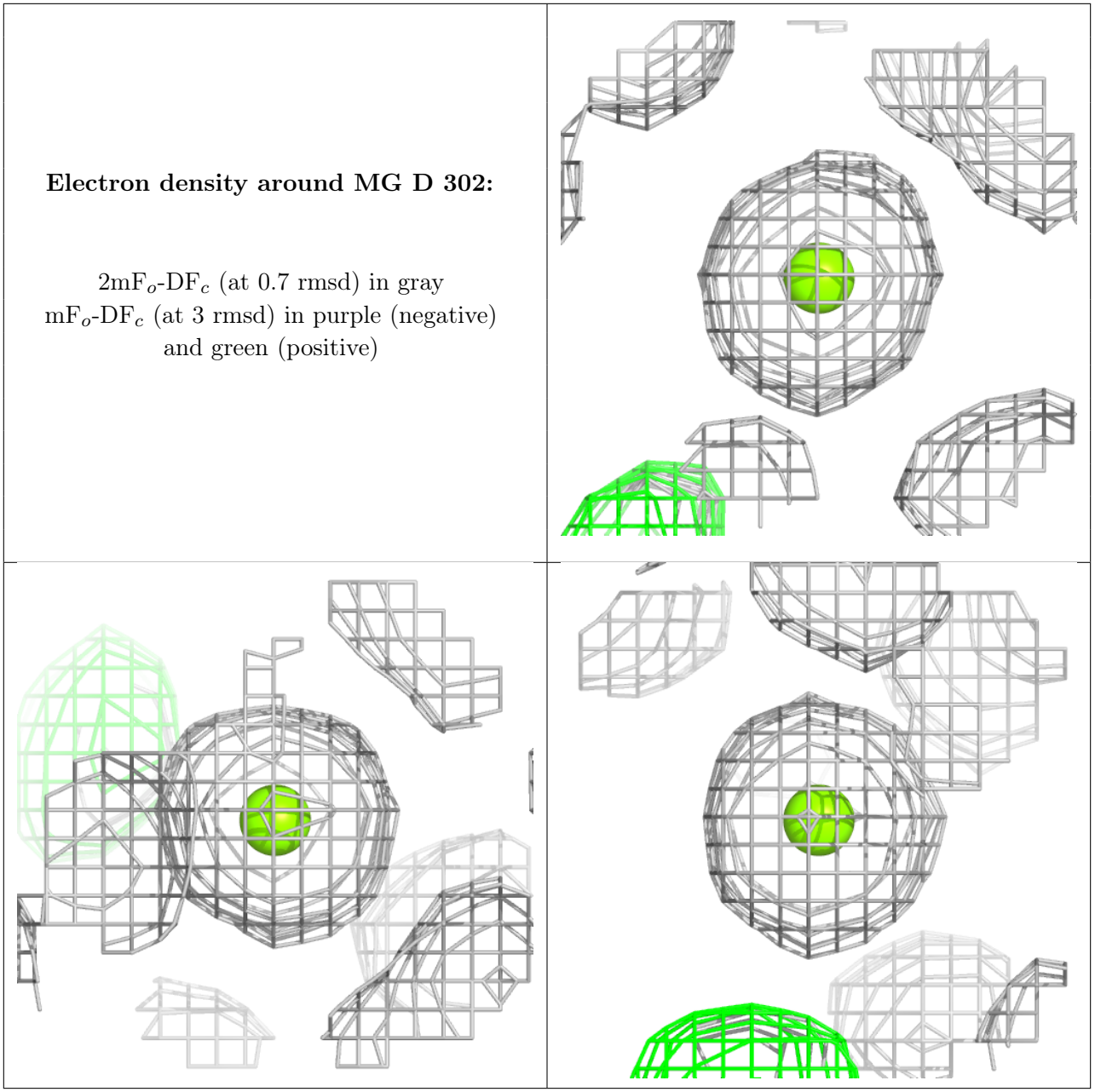
Electron density around MG D 301:

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



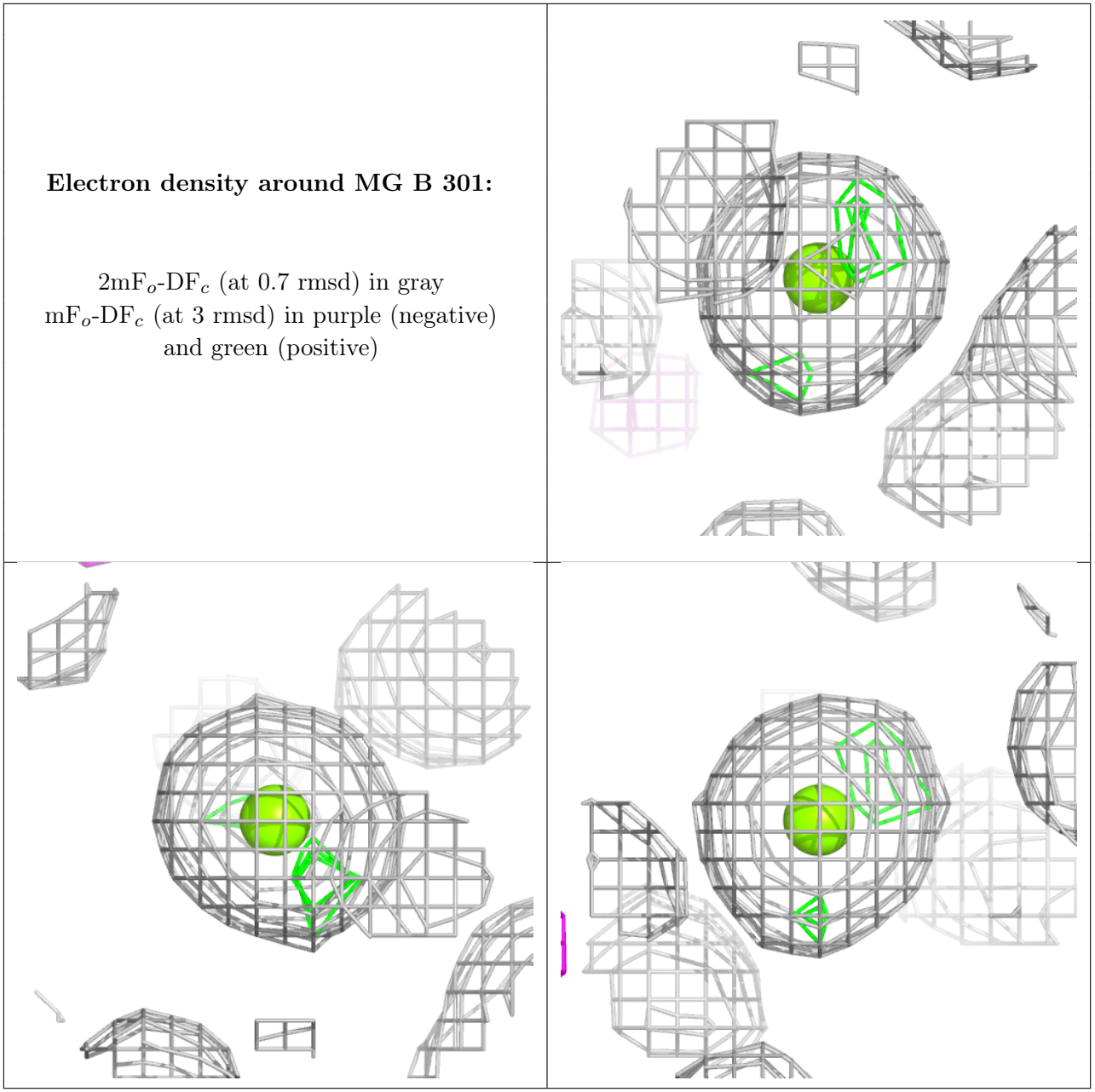
Electron density around MG D 302:

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



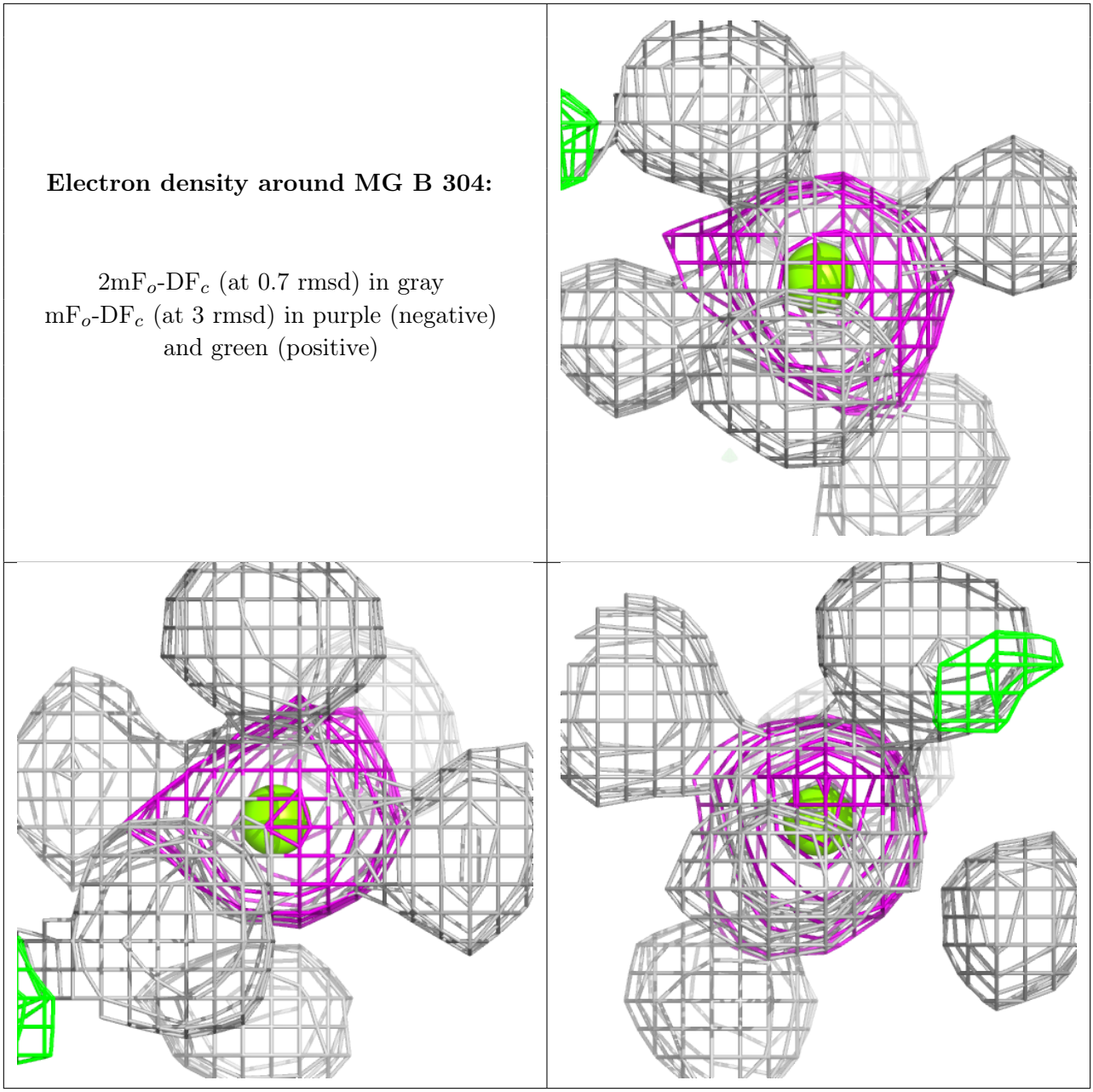
Electron density around MG B 301:

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



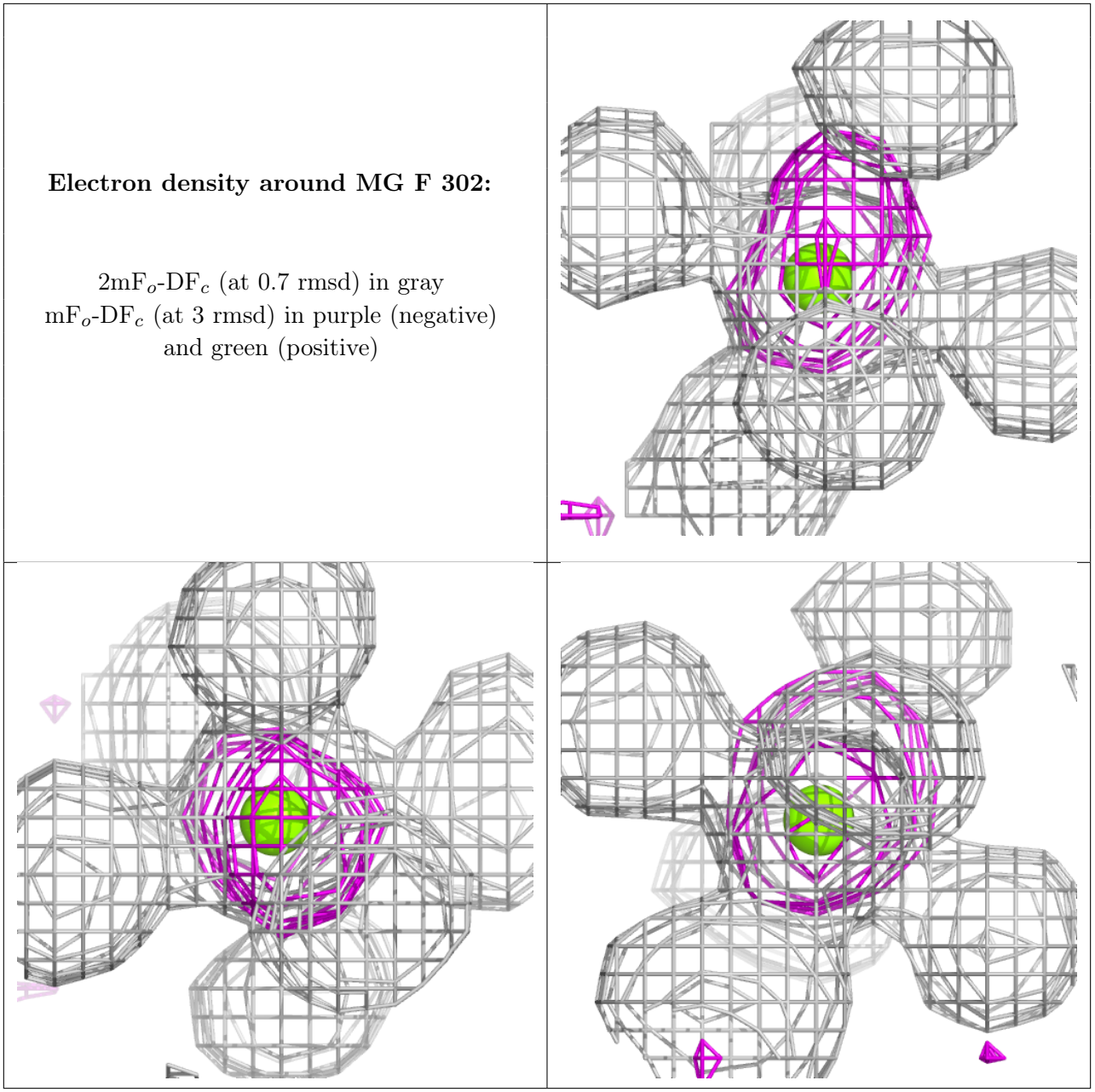
Electron density around MG B 304:

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



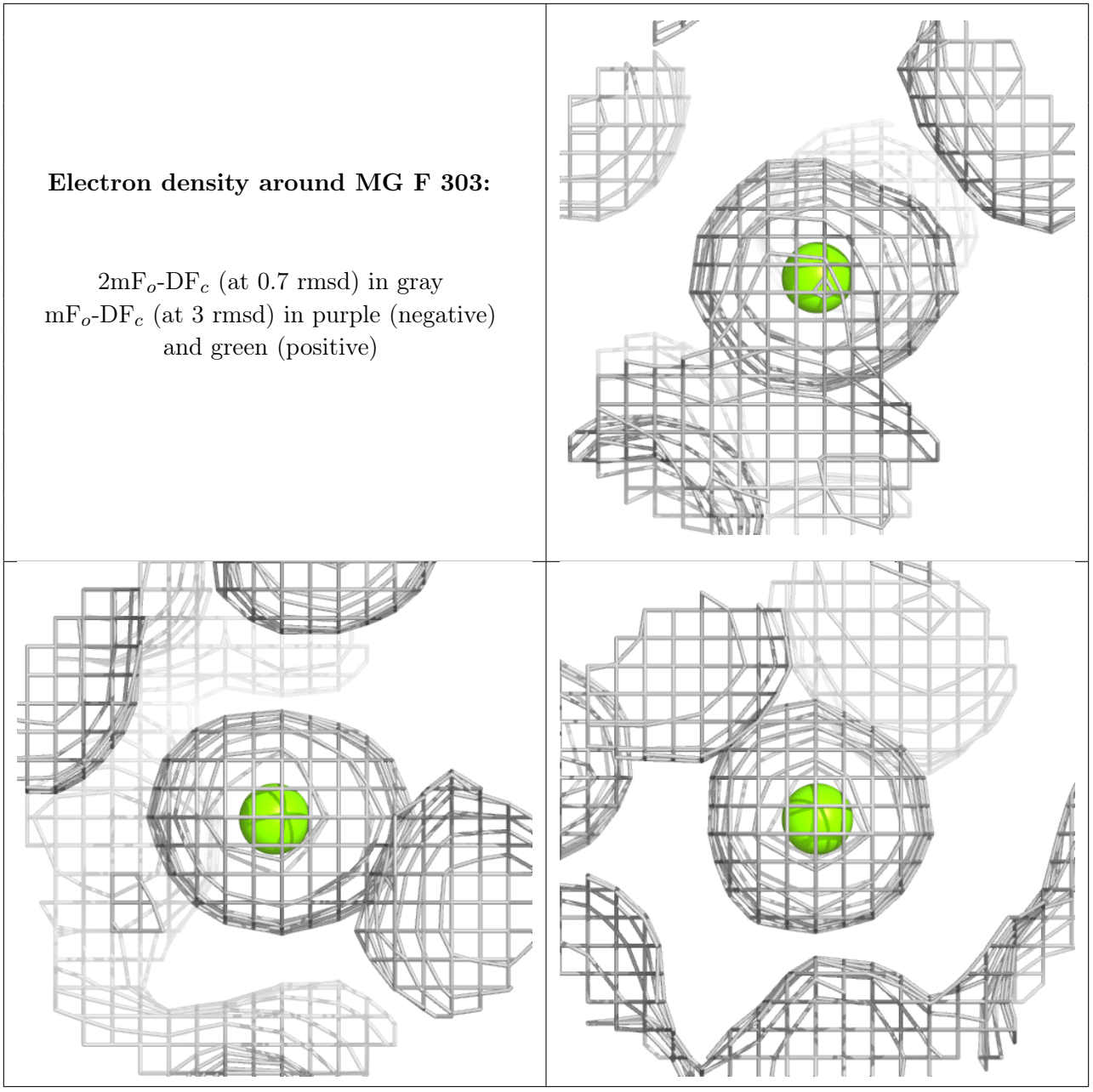
Electron density around MG F 302:

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



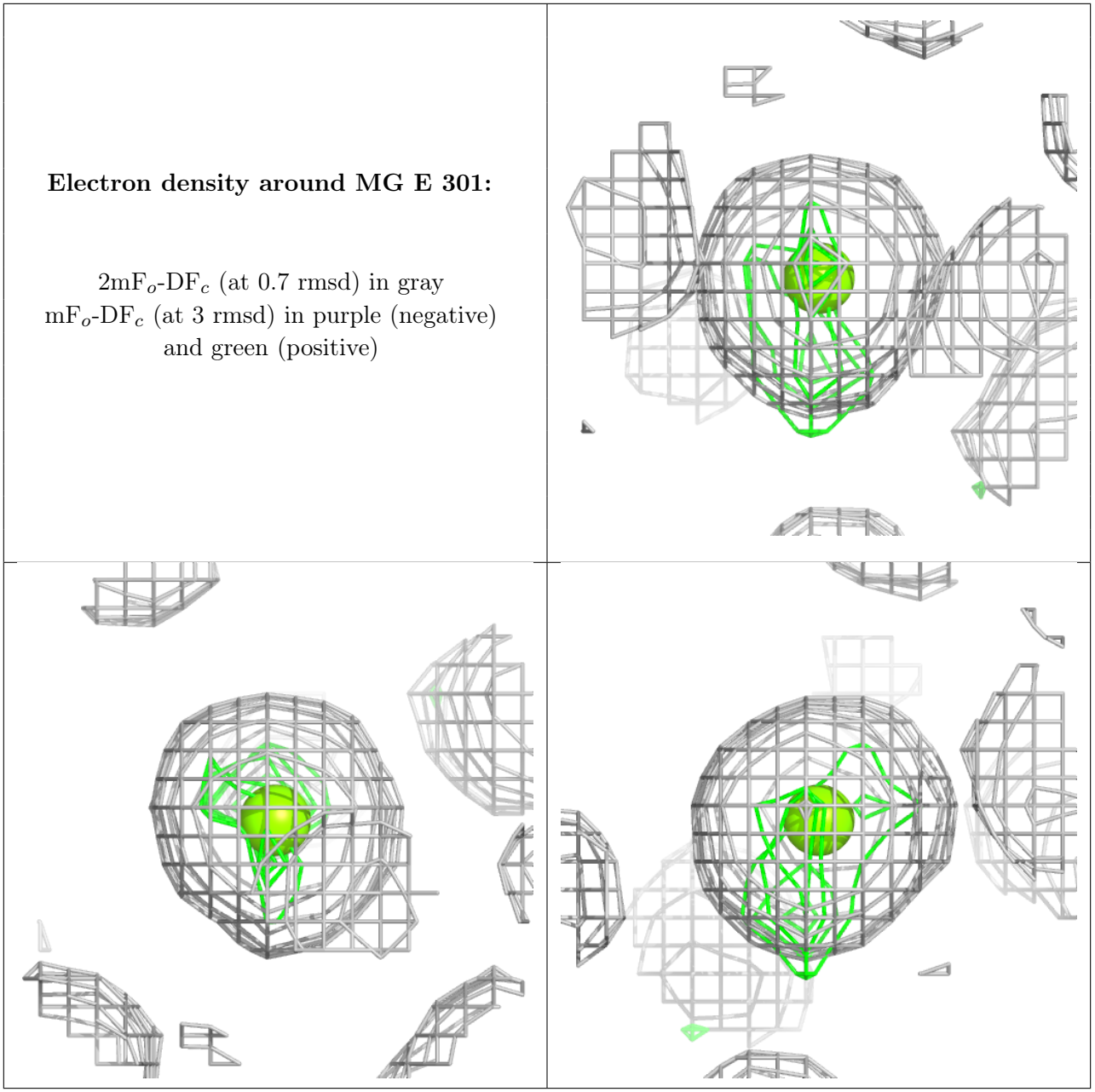
Electron density around MG F 303:

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



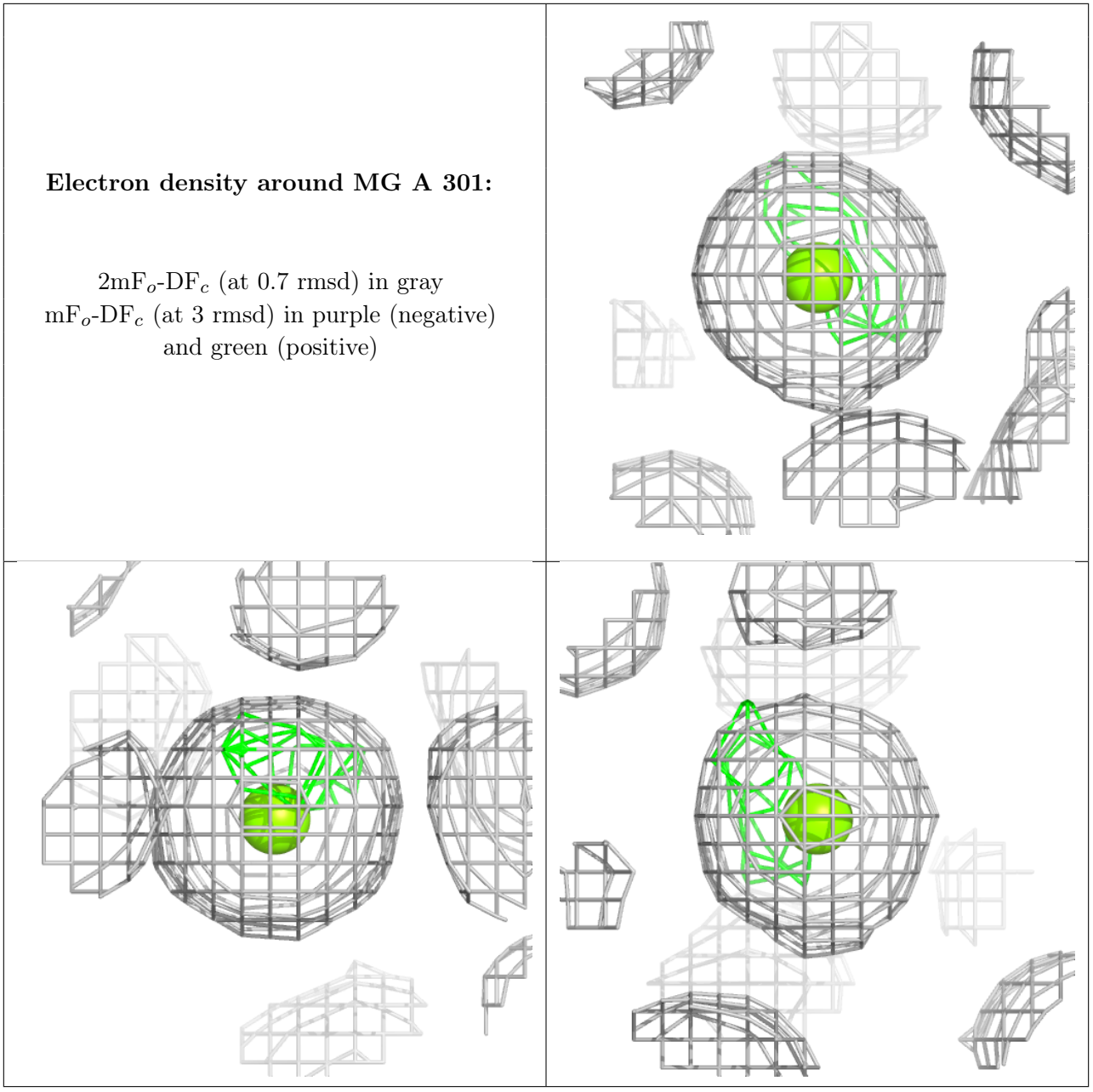
Electron density around MG E 301:

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



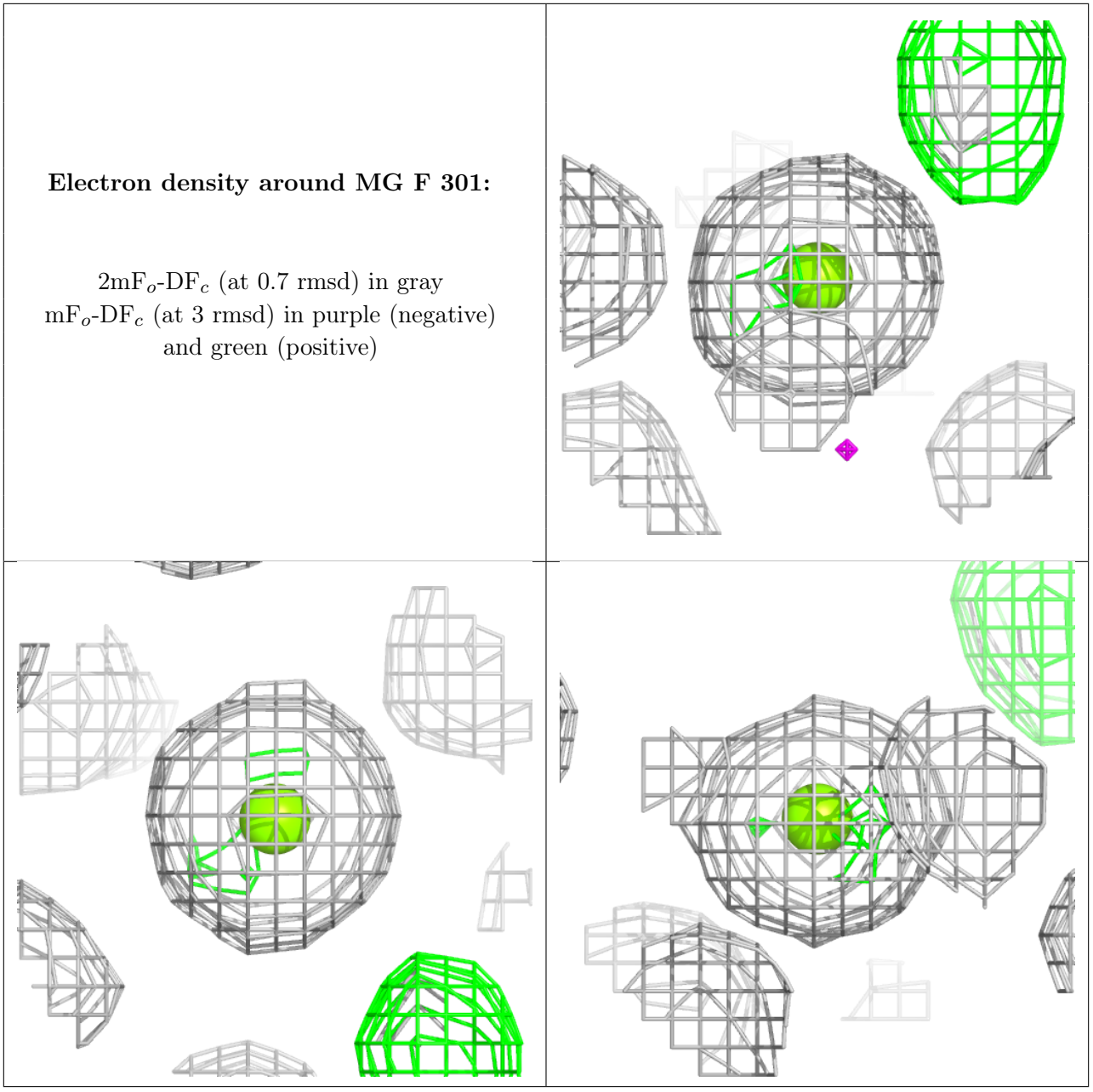
Electron density around MG A 301:

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



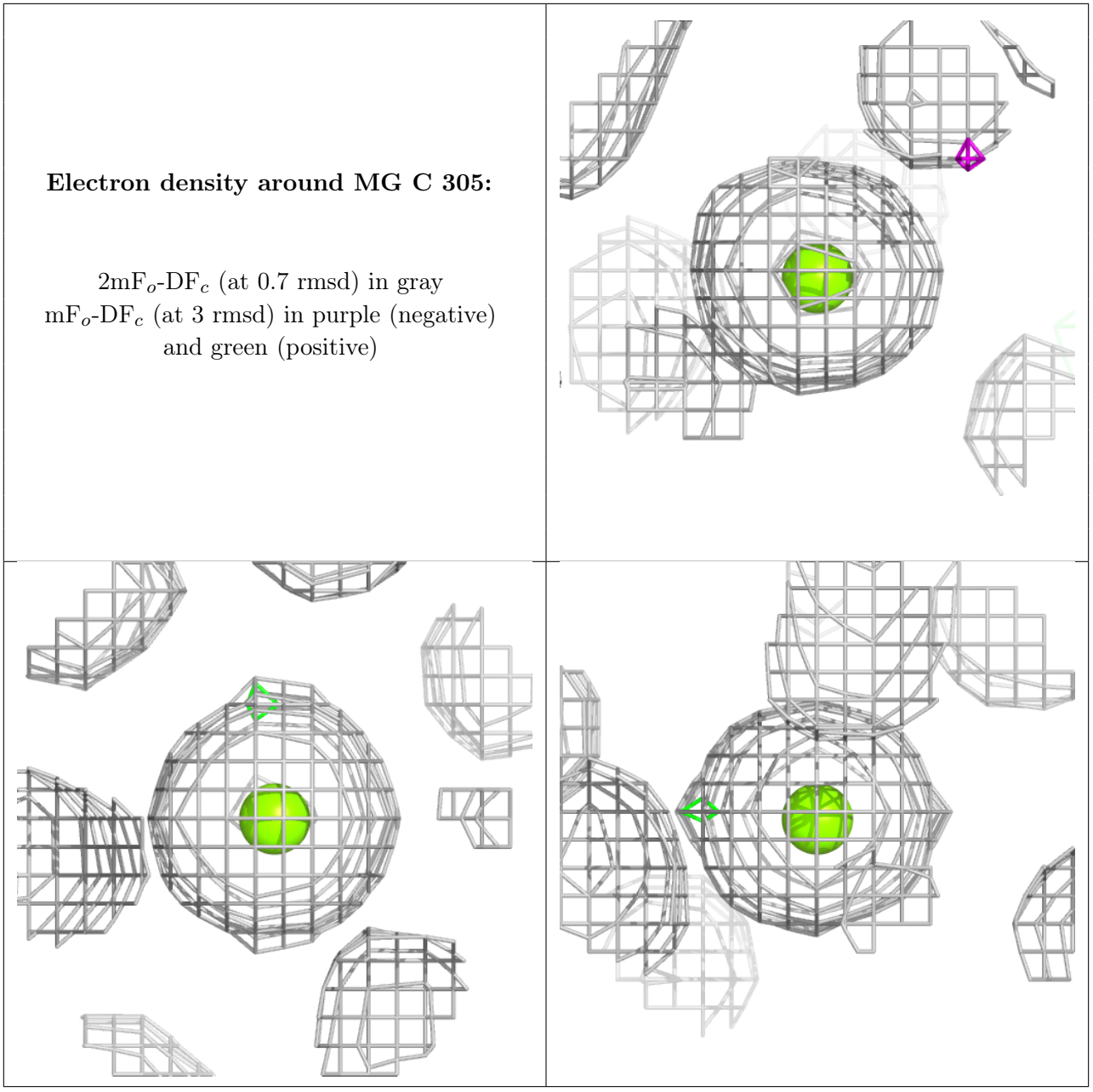
Electron density around MG F 301:

$2mF_o$-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 305:

$2mF_o$-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.